IRREVERSIBILITY AND NONPOTENTIALITY IN STATISTICAL MECHANICS

A reprint collection
edited by

ANTON SCHOBER
Division of Physics
The Institute For Basic Research
96 Prescott Street
Cambridge, MA 02138, U.S.A.

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TABLE OF CONTENTS:

FOREWORD

The compatibility between the idea of microscopic reversibility on one hand, and the irreversibility observed on the macroscopic scale on the other hand, remains one of the fundamental problems of contemporary Physics. Let us recall how I. Prigogine presents this problem in his recent work "From Being to Becoming. Time and Complexity in the Physical Sciences", W. H. Freeman, San Francisco 1980:[*]

"In classical and quantum dynamics, the fundamental laws of physics are taken to be symmetrical in time. Thermodynamic irreversibility corresponds to some kind of approximation added to dynamics. An often quoted example was given by Josiah Gibbs (1902): if we put a drop of black ink into water and stir it, the medium will look gray. This process would seem to be irreversible. But if we could follow each molecule we would recognize that in the microscopic realm the system has remained heterogeneous. Irreversibility would be an illusion caused by the observer's imperfect sense organs. It is true that the system has remained heterogeneous, but the scale of heterogeneity, initially macroscopic, has become microscopic. **The view that irreversibility is an illusion has been very influential and many scientists have tried to tie this illusion to mathematical procedures,**[†] *such as coarse graining, that would lead to irreversible processes. Others with similar aims have tried to work out the conditions of macroscopic observation. None of these attempts has led to conclusive results.*

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[*] Page 12

[†] The emphasis is ours.

It is difficult to believe that the observed irreversible processes, such as viscosity, decay of unstable particles, and so forth, are simply illusions caused by lack of knowledge or by incomplete observation. Because we know the initial conditions even in simple dynamical motion only approximately, future states of motion become more difficult to predict as time increases. Still, it does not seem meaningful to apply the second law of thermodynamics to such systems. Properties like specific heat and compressibility, which are closely associated with the second law, are meaningful for a gas formed by many interacting particles but are meaningless when applied to such simple dynamical systems as the planetary system. Therefore, irreversibility must have some basic connection with the dynamical nature of the system.

The opposite notion has also been considered: perhaps dynamics is incomplete; perhaps it should be expanded to include irreversibile processes.† *This attitude is also difficult to maintain, because for simple types of dynamical systems the predictions, both of classical and quantum mechanics, have been remarkably well verified. It is enough to mention the success of space travel, which requires very accurate computation of the dynamical trajectories.″*

It is true that it scarcely seems reasonable to try to break reversibility at the level of particle dynamics, since the current Hamiltonian formalism, which is symmetrical in time, is perfectly adapted to the dynamical description of all systems in which current long—range interactions are involved. However, it is not certain that this usual approach, which comes from consideration of particles as material points, is sufficient to describe the evolution of a system in the presence of short—range interactions. Indeed, any short—range interaction results from a state of contact i.e., for microscopic bodies, from a state of partial overlap between the interacting bodies. Thus there necessarily appear non—local effects which generally do not enter into the Hamiltonian framework. To us this constitutes sufficient justification for the theoretical study of non—Hamiltonian dynamics.

The papers gathered together below give an insight into the attempts made since the 1960's to associate non–Hamiltonian dynamics with irreversible statistical descriptions. These papers have been chosen because they show, even if their authors do not all know each other, a remarkable homogeneity of thought. Our compilation is evidently not exhaustive, and it is clear that our concern for homogeneity and conciseness has led us to leave out the many works concerning the hereditary and stochastic aspects of Evolution.

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The Institute For Basic Research
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LIST OF REPRINTED ARTICLES

NOTE

Sur la Théorie de la Variation des constantes arbitraires ;

PAR J. LIOUVILLE.

Soient n un nombre entier positif, x une fonction de t dont nous désignerons par x', x'',.... $x^{(n)}$ les dérivées successives, prises par rapport à t, et P une fonction quelconque de t, x, x',... $x^{(n-1)}$. Si l'on sait intégrer l'équation différentielle de l'ordre n,

$$(1) \qquad x^{(n)} = \mathrm{P},$$

il sera facile d'intégrer ensuite par approximation l'équation nouvelle

$$(2) \qquad x^{(n)} = \mathrm{P} + \mathrm{Q},$$

dans laquelle on suppose que le terme Q reste toujours très petit. Et même si Q désigne une fonction donnée quelconque de t, et que l'équation (1) soit linéaire, on parvient à intégrer complétement l'équation (2). La méthode que les géomètres suivent ordinairement pour atteindre ce but consiste à faire varier les constantes arbitraires contenues dans l'intégrale complète $x = f(t, a, b, \ldots c)$ de l'équation (1), de telle sorte que l'équation (2) soit satisfaite aussi par $x = f(t, a, b, \ldots c)$. Cela revient au fond à remplacer l'inconnue x par n inconnues $a, b, \ldots c$, entre lesquelles on pourra d'ailleurs établir à volonté $(n-1)$ relations. Les relations dont nous parlons deviennent très simples quand on assujétit les valeurs de $dx, d^2x, \ldots d^{n-1}x$ à conserver la même forme dans le cas de l'équation (2) et dans le cas de l'équation (1).

Reprinted from Journal Math. pures et appli., 3, 342 (1838)

Pour déterminer $a, b, \ldots c$ en fonction de t, on obtient dans cette hypothèse les équations suivantes :

$$\begin{array}{l}
\frac{dx}{da}\cdot\frac{da}{dt} + \frac{dx}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx}{dc}\cdot\frac{dc}{dt} = 0,\\
\frac{dx'}{da}\cdot\frac{da}{dt} + \frac{dx'}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx'}{dc}\cdot\frac{dc}{dt} = 0,\\
\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
\frac{dx^{(n-2)}}{da}\cdot\frac{da}{dt} + \frac{dx^{(n-2)}}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx^{(n-2)}}{dc}\cdot\frac{dc}{dt} = 0,\\
\frac{dx^{(n-1)}}{da}\cdot\frac{da}{dt} + \frac{dx^{(n-1)}}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx^{(n-1)}}{dc}\cdot\frac{dc}{dt} = Q.
\end{array}$$

Il s'agit d'en tirer les valeurs de $\frac{da}{dt}, \frac{db}{dt}, \ldots \frac{dc}{dt}$, et c'est ce qu'on peut toujours faire à l'aide de la règle donnée par Laplace pour résoudre les équations du premier degré, quel que soit le nombre des inconnues.

D'après cette règle on formera d'abord le dénominateur commun des inconnues $\frac{da}{dt}, \frac{db}{dt}, \ldots \frac{dc}{dt}$, à l'aide des coefficients $\frac{dx}{da}, \frac{dx}{db}$, etc., de ces inconnues. On aura ensuite le numérateur de la fraction qui exprime $\frac{da}{}$, par exemple, en remplaçant dans le dénominateur commun $\frac{dx^{(n-1)}}{da}$ par Q, et $\frac{dx^{(n-2)}}{da}, \ldots \frac{dx'}{da}, \frac{dx}{da}$ par zéro.

On peut simplifier le calcul toutes les fois que la fonction P est indépendante de $x^{(n-1)}$, c'est-à-dire toutes les fois que $\frac{dP}{dx^{(n-1)}} = 0$. Je me propose dans cette Note de prouver qu'alors le dénominateur commun des quantités $\frac{da}{dt}, \frac{db}{dt}, \ldots \frac{dc}{dt}$, ne contient pas t explicitement et n'est fonction que de $a, b, \ldots c$; on verra même qu'il se réduit à l'unité lorsque $a, b, \ldots c$ représentent les valeurs de x, $x', \ldots x^{(n-1)}$, relatives à une valeur particulière de t, telle que $t = 0$.

Pour donner de ce théorème une démonstration générale, je représente par u le dénominateur commun et je cherche sa dérivée $\frac{du}{dt}$ prise par rapport à t, en tant que cette lettre entre explicitement dans u, sans que l'on fasse varier les constantes $a, b, \ldots c$. La valeur de u se compose d'une série de termes, les uns positifs, les autres négatifs : le premier de ces termes est par exemple

$$\frac{dx}{da}\cdot\frac{dx'}{db}\;\ldots\;\frac{dx^{(n-1)}}{dc}.$$

D'après un théorème connu, la valeur de u doit devenir nulle si l'on rend égaux entre eux les coefficients de $\frac{da}{dt}$, ceux de $\frac{db}{dt}$,... ceux de $\frac{dc}{dt}$, dans deux des équations du problème. Si donc on remplace partout dans l'expression de u une des dérivées $x^{(i)}$ par une autre dérivée ayant un indice différent de i et compris dans la série 0, 1, 2,... $(n-1)$, il faudra que u se réduise à zéro après ce changement effectué.

Cela posé j'observe que, pour trouver $\frac{du}{dt}$, on peut différencier dans u successivement x, x',... $x^{(n-2)}$, $x^{(n-1)}$, et ajouter les résultats partiels ainsi obtenus. Or, différencier x, c'est remplacer x par x', et par ce changement u devient zéro; de même différencier x'... ou $x^{(n-2)}$, c'est remplacer x'... ou $x^{(n-2)}$ par x''... ou $x^{(n-1)}$, ce qui donne encore zéro pour résultat. Quant à la différenciation qui porte sur $x^{(n-1)}$, on l'effectuera en remplaçant $x^{(n-1)}$ par $x^{(n)}$ ou par P. Donc finalement la valeur de $\frac{du}{dt}$ se composera de termes de la forme

$$\frac{dx}{da}\cdot\frac{dx'}{db}\;\ldots\;\frac{dP}{dc}.$$

Mais P étant fonction de t, x, x',... $x^{(n-2)}$, on a

$$\frac{dP}{dc}=\frac{dP}{dx}\cdot\frac{dx}{dc}+\frac{dP}{dx'}\cdot\frac{dx'}{dc}+\ldots+\frac{dP}{dx^{(n-2)}}\cdot\frac{dx^{(n-2)}}{dc}.$$

On trouve des valeurs semblables pour les dérivées $\frac{dP}{da}$, $\frac{dP}{db}$,... En les substituant dans l'expression de $\frac{du}{dt}$, celle-ci se décompose en plusieurs parties qui ont pour facteurs respectifs $\frac{dP}{dx}$, $\frac{dP}{dx'}$,... $\frac{dP}{dx^{(n-2)}}$ et qui sont nulles d'elles-mêmes, comme il est aisé de le voir d'après ce que l'on a expliqué plus haut.

Donc enfin l'on a $\frac{du}{dt} = 0$, en sorte que le dénominateur u ne contient pas t explicitement, et se réduit à une simple fonction de $a, b, \ldots c$. Ainsi la valeur de u ne changera pas si l'on pose $t = 0$. Mais quand $a, b, \ldots c$ représentent les valeurs initiales de $x, x', \ldots x^{(n-1)}$, le premier terme de u, savoir $\frac{dx}{da} \cdot \frac{dx'}{db} \cdots \frac{dx^{(n-1)}}{dc}$, se réduit à l'unité pour $t = 0$, et les autres deviennent nuls dans la même hypothèse : on a par suite alors $u = 1$, ce qu'il fallait démontrer.

L'analyse précédente exige que P ne contienne pas la dérivée $x^{(n-1)}$, mais seulement les dérivées d'ordre inférieur à $(n-1)$. Si P contenait $x^{(n-1)}$, on trouverait de la même manière

$$\frac{du}{dt} = u \frac{dP}{dx^{(n-1)}}.$$

Ces considérations générales deviennent beaucoup plus claires lorsqu'on les applique au cas particulier où $n = 3$.

On a alors

$$\begin{aligned} u = {} & \frac{dx}{da} \cdot \frac{dx'}{db} \cdot \frac{dx''}{dc} - \frac{dx}{da} \cdot \frac{dx'}{dc} \cdot \frac{dx''}{db} \\ & + \frac{dx}{dc} \cdot \frac{dx'}{da} \cdot \frac{dx''}{db} - \frac{dx}{db} \cdot \frac{dx'}{da} \cdot \frac{dx''}{dc} \\ & + \frac{dx}{db} \cdot \frac{dx'}{dc} \cdot \frac{dx''}{da} - \frac{dx}{dc} \cdot \frac{dx'}{db} \cdot \frac{dx''}{da}; \end{aligned}$$

et par le calcul direct, on trouve, en omettant les termes qui se détruisent, et en remplaçant x''' par P,

$$\begin{aligned} \frac{du}{dt} = {} & \frac{dx}{da} \cdot \frac{dx'}{db} \cdot \frac{dP}{dc} - \frac{dx}{da} \cdot \frac{dx'}{dc} \cdot \frac{dP}{db} \\ & + \frac{dx}{dc} \cdot \frac{dx'}{da} \cdot \frac{dP}{db} - \frac{dx}{db} \cdot \frac{dx'}{da} \cdot \frac{dP}{dc} \\ & + \frac{dx}{db} \cdot \frac{dx'}{dc} \cdot \frac{dP}{da} - \frac{dx}{dc} \cdot \frac{dx'}{db} \cdot \frac{dP}{da}, \end{aligned}$$

expression qui devient nulle en effet, lorsqu'on met au lieu de $\frac{dP}{da}, \frac{dP}{db}, \frac{dP}{dc}$ leurs valeurs respectives

$$\frac{dP}{dx}\cdot\frac{dx}{da}+\frac{dP}{dx'}\cdot\frac{dx'}{da},$$
$$\frac{dP}{dx}\cdot\frac{dx}{db}+\frac{dP}{dx'}\cdot\frac{dx'}{db},$$
$$\frac{dP}{dx}\cdot\frac{dx}{dc}+\frac{dP}{dx'}\cdot\frac{dx'}{dc},$$

qui sont exactes dès que P est une fonction de t, x, x' indépendante de x''. Mais ces valeurs devraient être augmentées des termes suivants $\frac{dP}{dx''}\cdot\frac{dx''}{da}$, $\frac{dP}{dx''}\cdot\frac{dx''}{db}$, $\frac{dP}{dx''}\cdot\frac{dx''}{dc}$, si P contenait x''. Aussi dans ce cas $\frac{du}{dt}$ est $= u\frac{dP}{dx''}$ et non plus $= 0$.

En supposant P indépendant de $x^{(n-1)}$, et admettant que a, b, etc., soient les valeurs initiales de x, x', etc., on a

$$\frac{da}{dt} = -Q\frac{dx}{db},$$
$$\frac{db}{dt} = Q\frac{dx}{da},$$

pour $n = 2$; puis

$$\frac{da}{dt} = \left(\frac{dx}{db}\cdot\frac{dx'}{dc} - \frac{dx}{dc}\cdot\frac{dx'}{db}\right)Q,$$
$$\frac{db}{dt} = \left(\frac{dx}{dc}\cdot\frac{dx'}{da} - \frac{dx}{da}\cdot\frac{dx'}{dc}\right)Q,$$
$$\frac{dc}{dt} = \left(\frac{dx}{da}\cdot\frac{dx'}{db} - \frac{dx}{db}\cdot\frac{dx'}{da}\right)Q,$$

pour $n = 3$; et ainsi de suite.

Lorsque $n = 2$, si Q est de la forme $-\frac{dR}{dx}$, R étant une fonction de t et x seulement, il vient

$$\frac{da}{dt} = \frac{dR}{dx}\cdot\frac{dx}{db} = \frac{dR}{db},$$
$$\frac{db}{dt} = -\frac{dR}{dx}\cdot\frac{dx}{da} = -\frac{dR}{da},$$

ce qui s'accorde avec les formules connues.

Les résultats que nous venons d'obtenir s'étendent de la manière suivante à un nombre quelconque d'équations différentielles simultanées. On peut toujours supposer que ces équations sont du premier ordre; car si elles contiennent des différentielles d'ordre supérieur, il suffira de représenter les intégrales de ces différentielles par des lettres particulières, que l'on traitera comme de nouvelles variables, pour rabaisser au premier ordre les équations proposées : par exemple l'équation

$$\frac{d^3x_1}{dt^3} = x_1^2 + t^2$$

peut être remplacée par ces trois équations du premier ordre

$$\frac{dx_1}{dt} = x_2, \quad \frac{dx_2}{dt} = x_3,$$
$$\frac{dx_3}{dt} = x_1^2 + t^2.$$

Soient donc en général $x_1, x_2, \ldots x_n$, n fonctions de t liées entre elles par n équations différentielles de la forme

$$\frac{dx_1}{dt} = \mathrm{P}_1, \quad \frac{dx_2}{dt} = \mathrm{P}_2, \ldots \quad \frac{dx_n}{dt} = \mathrm{P}_n,$$

où $\mathrm{P}_1, \mathrm{P}_2, \ldots \mathrm{P}_n$ désignent des fonctions de $t, x_1, x_2, \ldots x_n$. Désignons par $a, b, \ldots c$ les constantes arbitraires qui entreront dans les expressions de $x_1, x_2, \ldots x_n$, fournies par l'intégration des équations différentielles proposées. Enfin considérons les n équations

$$\begin{aligned}
&\frac{dx_1}{da}\cdot\frac{da}{dt} + \frac{dx_1}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx_n}{dc}\cdot\frac{dc}{dt} = \mathrm{Q}_1, \\
&\frac{dx_2}{da}\cdot\frac{da}{dt} + \frac{dx_2}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx_n}{dc}\cdot\frac{dc}{dt} = \mathrm{Q}_2, \\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
&\frac{dx_n}{da}\cdot\frac{da}{dt} + \frac{dx_n}{db}\cdot\frac{db}{dt} + \ldots + \frac{dx_n}{}\cdot\frac{dc}{dt} = \mathrm{Q}_n,
\end{aligned}$$

où nous prenons pour inconnues $\frac{da}{dt}, \frac{db}{dt}, \ldots \frac{dc}{dt}$. Je dis qu'il est toujours facile de calculer *à priori* le dénominateur commun des fractions qui expriment ces inconnues. En effet, soit u ce dénominateur. D'après la règle de Laplace, il est formé d'une série de termes de la forme $\frac{dx_1}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}$, pris avec des signes convenables. C'est pourquoi nous écrirons

$$u = \Sigma\left(\pm \frac{dx_1}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right).$$

Cherchons maintenant $\frac{du}{dt}$. Il faudra pour cela différencier successivement $x_1, x_2, \ldots x_n$, par rapport à t : or la différenciation relative à x revient à remplacer x_1 par P_1, d'où résulte la quantité

$$\Sigma\left(\pm \frac{dP_1}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right),$$

qui, développée, devient

$$\begin{aligned} &\frac{dP_1}{dx_1} \Sigma\left(\pm \frac{dx_1}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right) \\ &+ \frac{dP_1}{dx_2} \Sigma\left(\pm \frac{dx_2}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right) \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &+ \frac{dP_1}{dx_n} \Sigma\left(\pm \frac{dx_n}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right), \end{aligned}$$

et se réduit simplement à

$$u \frac{dP_1}{dx_1},$$

parce que les sommes

$$\Sigma\left(\pm \frac{dx_2}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right), \ldots \quad \Sigma\left(\pm \frac{dx_n}{da} \cdot \frac{dx_2}{db} \ldots \frac{dx_n}{dc}\right)$$

sont nulles en vertu d'une propriété bien connue. La valeur complète de $\frac{du}{dt}$ est donc

$$\frac{du}{dt} = u\left(\frac{dP_1}{dx_1} + \frac{dP_2}{dx_2} + \ldots + \frac{dP_n}{dx_n}\right).$$

Toutes les fois que la somme

$$\frac{dP_1}{dx_1}+\frac{dP_2}{dx_2}+\ldots+\frac{dP_n}{dx_n}$$

se réduit à zéro, on a

$$\frac{du}{dt}=0,$$

en sorte que le dénominateur u est alors indépendant de t. Si donc on suppose que $a, b, \ldots c$ représentent les valeurs de $x_1, x_2, \ldots x_n$ pour $t=0$, et si l'on prend positivement le terme $\frac{dx_1}{da}\cdot\frac{dx_2}{db}\ldots\frac{dx_n}{dc}$ de l'expression de u, on aura toujours $u=1$. Mais quand, en adoptant cette dernière hypothèse, on regarde la somme

$$\frac{dP_1}{dx_1}+\frac{dP_2}{dx_2}+\ldots+\frac{dP_n}{dx_n}$$

comme ayant une certaine valeur φ différente de zéro, alors il vient

$$u=e^{\int_0^t \varphi dt}.$$

Pseudo-Hamiltonian Mechanics

R. J. DUFFIN

Communicated by W. NOLL

1. Introduction

This paper is concerned with the system of $2n$ ordinary differential equations

$$\frac{dq_j}{dt}=\frac{\partial H}{\partial p_j}, \qquad \varepsilon\frac{dp_j}{dt}=\frac{\partial H}{\partial q_j}. \tag{1}$$

Here $j=1, 2, \ldots, n$, and ε is a constant. The independent variable is t, and the dependent variables are $p_1, \ldots, p_n$ and $q_1, \ldots, q_n$. Also H denotes a given function of the p_j and the q_j and t; $H=H(p, q, t)$. In this paper equations (1) are termed the pseudo-Hamiltonian equations.

If $\varepsilon=-1$, then equations (1) are HAMILTON'S canonical equations. In this case it was shown by HAMILTON that equations (1) can be used to describe the motion of a mechanical system having n degrees of freedom. The q_j are interpreted as generalized coordinates of the system, and the p_j are intepreted as generalized momenta. HAMILTON'S equations have proved to offer a very fruitful mathematical technique for studying conservative mechanical systems. A system is said to be *conservative* if the total energy is constant. Moreover in such systems the Hamiltonian function H can be interpreted as the total energy, so H is said to be a constant of the motion.

This method of HAMILTON is not applicable to systems which dissipate energy. By contrast it is to be shown here the pseudo-Hamiltonian equations can describe the motion of common dissipative systems. For example, if $\varepsilon=1$ and if the Hamiltonian function H is a quadratic function of the p_j and the q_j, it results that relations (1) become a system of linear differential equations. This system can be used to describe the small motions of a dissipative mechanical system about a position of static equilibrium. Moreover this same system of pseudo-Hamiltonian equations can also be used to describe the flow of the charges q_j in an electrical network with lumped inductance, resistance and capacitance.

There is substantial theory relating to the true Hamiltonian equations [*1*]. Some of this theory can be extended to the case $\varepsilon\neq-1$. For example, it proves possible to extend LIOUVILLE'S theorem concerning a statistical ensemble of systems in phase space.

This paper may be regarded as a study of relations between conservative and dissipative systems. Previous work in this general direction appeared in references [*2*] and [*3*]. In particular, a special transformation was given in [*3*] which put conservative systems into correspondence with a class of dissipative systems. This motivated the present more general study.

Reprinted from Arch. Rational Mech. Anal., 9, 309 (1962)

It is well known that HAMILTON'S canonical equations can be regarded as the EULER equations of a variational principle [4]. Moreover H. BATEMAN [5] indicated a possible way of treating dissipative systems by a variational method. However no attempt is made here to relate the pseudo-Hamiltonian equations with the calculus of variations.

RAYLEIGH [6] made several contributions to dissipative mechanics. In particular, he introduced a new function R termed the *dissipation function.* Then RAYLEIGH could write LAGRANGE'S equations for a dissipative system as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial q'_k}\right) = \frac{\partial L}{\partial q_k} = \frac{\partial R}{\partial q'_k}. \tag{2}$$

Here L is LAGRANGE'S function, and q'_k denotes dq_k/dt. This method of RAYLEIGH has proved to be a suggestive mathematical technique for treating dissipative systems. However it is not in the spirit of the method of HAMILTON because two potentials L and R are required. In HAMILTON'S method the system is characterized by a single potential H.

In what follows all quantities are taken to be real unless the contrary is indicated. The continuity and differentiability conditions needed on the functions introduced are clear from the context and so are not explicitly stated.

2. The Hamiltonian equations

Let q_j for $j=1, \ldots, n$ be generalized coordinates of a system with n degrees of freedom. The velocity components are $q'_j = dq_j/dt$ where t is the time. Let f_j denote the external force components. Thus $\sum_1^n f_k q'_k$ is the power input to the system.

Suppose that there is a scalar function $L(q, q', t)$ such that for some constant $\varepsilon \neq 0$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial q'_j}\right) + \varepsilon^{-1}\frac{\partial L}{\partial q_j} = f_j. \tag{3}$$

Then L is termed a Lagrangian function. If $\varepsilon = -1$, then equations (3) are the classical equations of LAGRANGE.

The momentum components are defined to be

$$p_j = \frac{\partial L}{\partial q'_j}. \tag{4}$$

The Hamiltonian is then defined to be

$$H = \sum_1^n p_k - q'_k L. \tag{5}$$

Thus $-H$ is the Legendre transform of L and consequently can be considered to be a function of p_j, q_j and t, say $H(p, q, t)$. Differentiating (5) gives

$$dH = \sum_1^n q'_k\, dp_k - \sum_1^n \frac{\partial L}{\partial q_k} dq_k - \frac{\partial L}{\partial t} dt.$$

Then making use of (3) and (4) gives

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j}, \qquad \varepsilon \frac{\partial p_j}{\partial t} = \frac{\partial H}{\partial q_j} + \varepsilon f_j. \tag{6}$$

These are the (pseudo) Hamiltonian equations. In what follows the main concern will be the case of free motion. Then there are no external forces, so $f_j = 0$.

It is convenient to regard $q_1, q_2, \ldots, q_n$ as the components of a vector q in an n-dimensional Euclidean space E_n. Likewise $p_1, p_2, \ldots, p_n$ are regarded as components of a vector p. The scalar product of these two vectors is denoted by (p, q). Thus in terms of compound matrices equations (6) may be written as

$$\begin{vmatrix} 0 & I \\ \varepsilon I & 0 \end{vmatrix} \cdot \begin{vmatrix} p' \\ q' \end{vmatrix} = \begin{vmatrix} \dfrac{\partial H}{\partial p} \\ \dfrac{\partial H}{\partial q} \end{vmatrix}. \tag{7}$$

Here I is the n by n identity matrix.

Equation (7) may be written in a still more compact notation by introducing a $2n$-dimensional Euclidean space E_{2n} termed *phase space*. Let r be a vector of E_{2n} whose first n components are $p_1, p_2, \ldots, p_n$ and whose last n components are $q_1, q_2, \ldots, q_n$. Then equation (7) becomes

$$\Gamma r' = \frac{\partial H}{\partial r} \tag{8}$$

where Γ denotes the $2n$ by $2n$ matrix on the left side of equation (7). Clearly

$$\Gamma^2 = \varepsilon I. \tag{9}$$

By use of the pseudo-Hamiltonian equations in the form (8), it is seen how to develop the analogy. For example if u and v are two scalar variables, the Lagrange bracket $\{u, v\}$ is defined as

$$\left(\left(\Gamma \frac{\partial r}{\partial u}, \frac{\partial r}{\partial v}\right)\right) = \sum_1^n \left(\frac{\partial q_k}{\partial u}\frac{\partial p_k}{\partial v} + \varepsilon \frac{\partial p_k}{\partial u}\frac{\partial q_k}{\partial v}\right). \tag{10}$$

Here $((r, s))$ denotes the scalar product of two vectors in E_{2n}. If u and v are two scalar functions, the Poisson bracket $[u, v]$ is defined as

$$\left(\left(\Gamma \frac{\partial u}{\partial r}, \frac{\partial v}{\partial r}\right)\right) = \sum_1^n \left(\frac{\partial u}{\partial q_k}\frac{\partial v}{\partial p_k} + \varepsilon \frac{\partial v}{\partial q_k}\frac{\partial u}{\partial p_k}\right). \tag{11}$$

If v is any function of p_j and q_j, then the following relation holds:

$$[H, v] = \varepsilon \frac{dv}{dt}. \tag{12}$$

To prove this, use is made of (8) and (9). Thus

$$\begin{aligned} [H, v] &= ((\Gamma\, \partial H/\partial r, \partial v/\partial r)) = ((\Gamma^2 r', \partial v/\partial r)) \\ &= \varepsilon \sum_1^{2n} \frac{\partial v}{\partial r_k} r_k' = \varepsilon \frac{dv}{dt}. \end{aligned}$$

This formulation of Hamiltonian mechanics is patterned after the new treatment given by SYNGE [7]. The older approach does not use matrix methods, and it results that certain basic concepts are obscured.

3. Definition of canonical transformations

Transformations of phase space which leave Hamilton's equations invariant in form are termed *canonical transformations*. Attention will be restricted to the case when the Hamiltonian function is not an explicit function of the time t.

Consider then a transformation of phase space taking each vector r into a transformed vector R, say $R=f(r)$. Thus

$$dR=J\,dr \quad\text{and}\quad R'=J\,r', \tag{13}$$

where J is the Jacobian matrix. Also

$$\frac{\partial H}{\partial r}=J^T\frac{\partial H}{\partial R} \tag{14}$$

where J^T denotes the transpose of J. Substitution of these two relations in (8) gives

$$\Gamma J^{-1}R'=J^T\frac{\partial H}{\partial R}.$$

These equations can be written in the canonical form $\Gamma R'=\partial H/\partial R$ provided

$$\Gamma=J^T\Gamma J. \tag{15}$$

These are the necessary and sufficient conditions that $R=F(r)$ is a canonical transformation.

Theorem 1. *The Lagrange and Poisson brackets are invariant under a canonical transformation.*

Proof. By relations (13) and (15)

$$\left(\left(\Gamma\frac{\partial R}{\partial u},\frac{\partial R}{\partial v}\right)\right)=\left(\left(\Gamma J\frac{\partial r}{\partial u},J\frac{\partial r}{\partial v}\right)\right)=\left(\left(J^T\Gamma J\frac{\partial r}{\partial u},\frac{\partial r}{\partial v}\right)\right)=\left(\left(\Gamma\frac{\partial r}{\partial u},\frac{\partial r}{\partial v}\right)\right).$$

This shows that the Lagrange brackets are invariant.

To treat the second part the following identity is needed:

$$\Gamma=J\Gamma J^T. \tag{16}$$

To prove this, the inverse of (15) is taken giving $\Gamma^{-1}=J^{-1}\Gamma^{-1}(J^T)^{-1}$. Then $J\Gamma^{-1}J^T=\Gamma^{-1}$, but by (9) it is seen that $\Gamma^{-1}=\Gamma/\varepsilon$, and this gives (16).

The Poisson bracket is

$$\left(\left(\Gamma\frac{\partial u}{\partial r},\frac{\partial v}{\partial r}\right)\right)=\left(\left(\Gamma J^T\frac{\partial u}{\partial R},J^T\frac{\partial v}{\partial R}\right)\right)=\left(\left(J\Gamma J^T\frac{\partial u}{\partial R},\frac{\partial v}{\partial R}\right)\right)=\left(\left(\Gamma\frac{\partial u}{\partial R},\frac{\partial v}{\partial R}\right)\right).$$

This completes the proof of Theorem 1.

It is well known that true canonical transformations do not have to be linear. Because of this fact the following theorem reveals a major difference between pseudo-Hamiltonian and true Hamiltonian equations.

Theorem 2. *A canonical transformation is a linear transformation if* $\varepsilon\neq-1$.

Proof. Let the relation $\Gamma=J^T\Gamma J$ be differentiated with respect to the coordinate r_c, and denote the derivative of J as J_c, so

$$J_c^T\Gamma J+J^T\Gamma J_c=0.$$

Let X denote $J^T\Gamma$, and let Y denote $(\Gamma J)^{-1}$, so

$$J_c^T=-XJ_cY. \tag{17}$$

Let J_{ab} denote the matrix elements of J, and let J_{abc} denote the matrix elements of J_c. Thus (17) becomes

$$J_{bac} = -X_{ad} J_{dec} Y_{eb}. \tag{18}$$

Here the summation convention has been employed. By the definition of the Jacobian matrix it follows directly that $J_{dec} = J_{dce}$. Then the transformation (18) is applied twice to give

$$J_{bac} = X_{ad} X_{cf} J_{fge} Y_{gd} Y_{eb}.$$

Changing J_{fge} to J_{feg} and again using (18) gives

$$-J_{bac} = X_{ad} J_{bcg} Y_{gd} = J_{bgc} Y_{gd} X_{ad}.$$

In the notation of equation (17) this relation may be written as

$$-J_c = J_c Y X^T = J_c J^{-1} \Gamma^{-1} \Gamma^T J.$$

Thus $J_c J^{-1}(I + \Gamma^{-1}\Gamma^T) J = 0$. But

$$\Gamma^{-1}\Gamma^T = \begin{vmatrix} 0 & \varepsilon^{-1} \\ I & 0 \end{vmatrix} \begin{vmatrix} 0 & \varepsilon \\ I & 0 \end{vmatrix} = \begin{vmatrix} \varepsilon^{-1} & 0 \\ 0 & \varepsilon \end{vmatrix}.$$

Clearly $I + \Gamma^{-1}\Gamma^T$ is singular if and only if $\varepsilon = -1$. Hence $J_c = 0$, and the proof is complete.

4. Representations of canonical transformations

As is well known, if S is an antisymmetric matrix, then e^S is an orthogonal transformation. The aim of this section is to give representations of this type for linear canonical transformations.

Theorem 3. *Let $f(z)$ be a function which is analytic at $z=0$ and satisfies the identity*

$$f(z)\, f(-z) = 1. \tag{19}$$

Then if $\varepsilon = 1$ or $\varepsilon = -1$, a canonical transformation is defined by $R = Jr$ where J is a constant matrix defined as

$$J = f(\Gamma S). \tag{20}$$

Here S is an arbitrary symmetric matrix if $\varepsilon = -1$ and S is an arbitrary antisymmetric matrix if $\varepsilon = 1$. (The precise meaning of (20) is given below.)

Proof. If $f(z)$ has the power series expansion

$$f(z) = a_0 + a_1 z + a_2 z^2 + \cdots, \tag{21}$$

then define

$$f(z\Gamma S) = a_0 I + a_1 z \Gamma S + a_2 z^2 (\Gamma S)^2 + \cdots. \tag{22}$$

This series converges if the parameter z has small absolute value. The expression (20) is defined as the continuation of (22) for $z=1$. A continuation is assumed to exist along some path in the complex z-plane which is symmetrical with respect to the origin. The path is to extend from $z=-1$ to $z=1$. Thus if

$f(z\Gamma S)$ is defined, so also is $f(-z\Gamma S)$. Clearly (19) implies that

$$f(z\Gamma S)\,f(-z\Gamma S)=I, \tag{23}$$

and this holds if $z=1$.

To prove that J is a canonical matrix it is sufficient to show that

$$\Gamma^{-1}J^T\Gamma=J^{-1}. \tag{24}$$

Consider that $(S\Gamma)^T=\Gamma^T S^T=\varepsilon\Gamma S^T=-\Gamma S$. The last step follows from the hypothesis on S. It is seen that $\{(S\Gamma)^n\}^T=(-\Gamma S)^n$. Thus

$$\Gamma^{-1}\{(S\Gamma)^n\}^T\Gamma=(-S\Gamma)^n. \tag{25}$$

Using this in (22) gives

$$\Gamma^{-1}[f(z\Gamma S)]^T\Gamma=f(-z\Gamma S). \tag{26}$$

Then the continuation of identities (23) and (26) yield (24), and the proof is complete.

Let $u(z)$ be an odd function analytic at the origin. Then it is clear that

$$f(z)=u(z)\pm\left(1+u^2(z)\right)^{\frac{1}{2}} \tag{27}$$

satisfies (19). Moreover it is easy to show that this gives the general solution of (19). Special cases are:

$$f(z)=\sinh z+\cosh z=e^z, \tag{28}$$

$$f(z)=z+(1+z^2)^{\frac{1}{2}}, \tag{29}$$

$$f(z)=(1-z)/(1+z). \tag{30}$$

The function (30) was introduced by CAYLEY to represent orthogonal transformations. It is clear that orthogonal transformations in Euclidean space are obtained by replacing Γ by the identity matrix. The function (29) was proposed by SYNGE to represent Lorentz transformations. The case of Lorentz transformations may be obtained by choosing Γ to be a diagonal matrix with

$$\Gamma_{11}=\Gamma_{22}=\Gamma_{33}=1 \quad\text{and}\quad \Gamma_{44}=-1. \tag{31}$$

The group of canonical transformations corresponding to $\varepsilon=-1$ have been termed the symplectic group by H. WEYL [*8*]. The symplectic geometry and the orthogonal geometry as studied by ARTIN [*9*] correspond to $\varepsilon=-1$ and $\varepsilon=1$ respectively.

5. Quadratic Lagrangians

Consider a Lagrangian which is a general quadratic form in q and q'. Thus

$$2L=(Aq',q')+2(Bq,q')+(Cq,q) \tag{32}$$

where A, B, and C are constant matrices. It may be assumed without loss of generality that A and C are symmetric matrices. Then

$$\frac{\partial L}{\partial q'}=Aq'+Bq, \tag{33}$$

$$\frac{\partial L}{\partial q}=B^Tq'+Cq. \tag{34}$$

Substituting these expressions in LAGRANGE's equations (3) gives

$$A q'' + B_1 q' + C_1 q = f \tag{35}$$

where

$$B_1 = B + \varepsilon^{-1} B^T \quad \text{and} \quad C_1 = \varepsilon^{-1} C. \tag{36}$$

To obtain the Hamiltonian function the first step is to take the product of relation (33) with q'. Thus

$$(p, q') = (A q', q') + (B q, q'). \tag{37}$$

Substitution of equation (37) in equation (5) then gives

$$2H = (A q', q') - (C q, q). \tag{38}$$

To obtain HAMILTON's equations it is now necessary to eliminate q' from the right side of equation (38).

Let E be a symmetric matrix such that

$$A = A E A. \tag{39}$$

If A has an inverse, then it is clear that $E = A^{-1}$. In any case relation (39) can always be satisfied. (This is seen by transforming A to diagonal form.) Then

$$A q' = p - B q, \tag{40}$$

$$E A q' = E p - E B q. \tag{41}$$

Forming the scalar product of equations (40) and (41) and then using equations (38) and (39) gives

$$2H = (E p, p) + 2(F q, p) + (G q, q), \tag{42}$$

where

$$F = -E B, \quad G = -C + B^T E B. \tag{43}$$

Then HAMILTON's equations for free motion are

$$\Gamma r' = K r \tag{44}$$

where K is the $2n$ by $2n$ matrix

$$K = \begin{vmatrix} E & F \\ F^T & G \end{vmatrix}.$$

It is seen that K is a symmetric matrix because E and G are symmetric.

Of especial interest are *normal modes of motion.* These are solutions of equation (44) of the form

$$r = e^{zt} w. \tag{45}$$

Here w is a constant vector termed an *eigenvector,* and z is a constant termed an *eigenvalue.* Both w and z may be complex. Substituting (45) in (44) gives

$$z \Gamma w = K w. \tag{46}$$

If $\varepsilon=1$, then Γ, as well as K, is a symmetric matrix. Let w_1 and w_2 be eigenvectors corresponding to different eigenvalues, z_1 and z_2. Then the following orthogonality relations hold:

$$0=((\Gamma w_1, w_2))=((K w_1, w_2)). \tag{47}$$

If $\varepsilon=-1$, then Γ is antisymmetric, and it is seen that the eigenvalues are pure imaginary. Thus if z is an eigenvalue corresponding to the eigenvector w, then $-z$ is an eigenvalue corresponding to w^*. (The asterisk denotes the complex conjugate.) The following orthogonality relationship holds:

$$0=((\Gamma w_1, w_2^*))=((K w_1, w_2^*)). \tag{48}$$

Here w_1 and w_2 are eigenvectors with different eigenvalues.

6. Typical linear systems and networks

It has just been seen that a quadratic Lagrangian function results in the set of linear differential equations (35). These equations may be regarded as relating the coordinates q_j of a system with the applied forces f_j. Equations (35) are sufficiently general to treat linear mechanical systems or linear electrical systems.

Greatest generality is attained in equations (35) when $\varepsilon^2 \neq 1$. In that case equation (36) can be solved for B. Thus

$$B=(B_1-\varepsilon^{-1} B_1^T)/(1-\varepsilon^{-2}). \tag{49}$$

Consequently the matrix B_1 is arbitrary.

The matrices A and C_1 can be arbitrary as long as they are symmetric. This is not an essential restriction since all electrical and mechanical theories lead to such symmetry.

If $\varepsilon=1$, then it follows from equation (36) that the matrix B_1 is symmetric. Then all the matrices in the LAGRANGE equations (35) are symmetric. Also the matrices Γ and K in HAMILTON'S equations (44) are symmetric. It is seen that the case $\varepsilon=1$ may be used to treat small damped vibration of a mechanical system about a position of equilibrium.

The case $\varepsilon=1$ also corresponds to an electrical network with lumped parameters. The matrices A, B_1 and C_1 correspond to inductance, resistance and capacitance respectively. The quadratic form $2R=(B_1 q', q')$ is the energy dissipated in heat. R is RAYLEIGH'S dissipation function.

The case $\varepsilon=-1$ is the classical case. It is seen from equation (36) that B_1 is necessarily antisymmetric. Thus $(B_1 q', q')=0$, so no energy can be dissipated. Equations (35) can be interpreted as the equations which determine the small vibrations of a conservative mechanical system about a position of *steady motion*. Then Bq' is interpreted as gyroscopic force.

HOWITT [*10*] proposed a method of finding equivalent networks by making a transformation $Q=f(q)$ in coordinate space E_n. A simple example of this method is given in reference [*11*]. A coordinate transformation is a special canonical transformation, so this suggests the following generalization of HOWITT'S method. Instead of a coordinate transformation make a canonical transformation $R=f(r)$ in phase space E_{2n}. This may lead to a more general class of equivalent networks.

7. Liouville's theorem for dissipative systems

Consider an ensemble of identical conservative systems in phase space. Then, according to LIOUVILLE's well known theorem, the ensemble density is constant along a trajectory [*12*]. Of concern here is the extension of this theorem to certain systems with dissipative forces.

The type of dissipative force to be permitted is a resistance proportional to the velocity. It is convenient to define this precisely in terms of the Hamiltonian function of the system as follows. A system is said to have *linear velocity forces* if $\partial^2 H/\partial p_j \partial q_k$ is a constant for $j, k=1, 2, \ldots, n$. The following theorem will be based on this hypothesis. It is worth noting that the theorem will follow under the weaker hypothesis that

$$\sum_1^n \frac{\partial^2 H}{\partial p_k\, \partial q_k} = \text{constant}. \tag{50}$$

Theorem 4. *Let S be a system with linear velocity forces. Let $\varrho(r, t)$ be the density in phase space of an ensemble of systems identical to S. Then along a free trajectory*

$$\varrho = \varrho_0\, e^{bt} \tag{51}$$

where b is an absolute constant.

Proof. The equation of continuity is $\partial\varrho/\partial t + \operatorname{div} \varrho r' = 0$, so

$$0 = \frac{\partial \varrho}{\partial t} + \sum_1^{2n} r'_k \frac{\partial \varrho}{\partial r_k} + \varrho \sum_1^{2n} \frac{\partial r'_k}{\partial r_k}. \tag{52}$$

Also if $D\varrho/Dt$ denotes the rate of growth of ϱ along a free trajectory, it is clear that

$$\frac{D\varrho}{Dt} = \frac{\partial \varrho}{\partial t} + \sum_1^{2n} \frac{\partial \varrho}{\partial r_k} r'_k. \tag{53}$$

Subtracting equation (52) from equation (53) gives

$$\frac{D\varrho}{Dt} = -\varrho \sum_1^{2n} \frac{\partial r'_k}{\partial r_k} = -\varrho \sum_1^{n} \left(\frac{\partial p'_k}{\partial p_k} + \frac{\partial q'_k}{\partial q_k} \right).$$

Substituting HAMILTON's equations on the right gives

$$\frac{1}{\varrho} \frac{D\varrho}{Dt} = -(1+\varepsilon) \sum_1^n \frac{\partial^2 H}{\partial p_k\, \partial q_k}. \tag{54}$$

Integrating this equation gives

$$\log \varrho = bt + c$$

where b and c are constants, and the proof is complete.

Conceivably Theorem 4 could aid in the study of non-equilibrium statistical mechanics.

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Carnegie Institute of Technology
Pittsburgh, Pennsylvania

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MATEMATICĂ

EVOLUȚIA DENSITĂȚII DE PROBABILITATE ÎN SPAȚIUL FAZELOR, PENTRU SISTEMELE MECANICE NECONSERVATIVE

DE

SILVIU GUIAȘU

Comunicare prezentată de C. IACOB, membru corespondent al Academiei R.P.R., în ședința din 7 iulie 1962

1. Să consideram un sistem mecanic neconservativ, cu n grade de libertate. Mișcarea sistemului este dată de sistemul de ecuații cvasi-canonic :

$$\dot{q}^k = \frac{\partial \mathcal{H}}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q^k} + Q_k, \qquad (k = 1, \ldots, n), \tag{1}$$

unde q^k, p_k $(k = 1, \ldots, n)$ sînt respectiv coordonatele generalizate și impulsurile generalizate, Q_k componentele forței generalizate, iar hamiltonianul

$$\mathcal{H} = \sum_{k=1}^{n} p_k \dot{q}^k - T, \tag{2}$$

T fiind energia cinetică. Mișcarea sistemului cu n grade de libertate revine la mișcarea unui punct reprezentativ în spațiul fazelor E_{2n} care este un spațiu euclidian cu $2n$ dimensiuni. Poziția punctului reprezentativ la momentul t, indică starea sistemului mecanic la acel moment.

2. **Evoluția în timp a volumului în spațiul fazelor.** Fie un domeniu $D \subset E_{2n}$. Fie un punct care la momentul inițial se găsește în D și are coordonatele $p_1, \ldots, p_n, q^1, \ldots, q^n$. După intervalul de timp dt, el va avea coordonatele

$$p'_i = p_i + \dot{p}_i \, dt, \quad q'^i = q^i + \dot{q}^i \, dt, \qquad (i = 1, \ldots, n), \tag{3}$$

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în care derivatele sînt date de ecuaţiile cvasicanonice (1). Volumul domeniului D ocupat de puncte la momentul iniţial este

$$V = \int_{D} \cdots \int dp_1 \ldots dp_n \, dq^1 \ldots dq^n , \tag{4}$$

iar volumul ocupat de puncte după dt

$$V' = \int_{D'} \cdots \int dp'_1 \ldots dp'_n \, dq'^1 \ldots dq'^n .$$

Relaţiile (3) reprezintă o schimbare de variabile, de determinant funcţional

$$\Delta = 1 + \sum_{k=1}^{n} \left(\frac{\partial \dot{p}_k}{\partial p_k} + \frac{\partial \dot{q}^k}{\partial q^k} \right). \tag{5}$$

Ţinînd cont de sistemul cvasicanonic, avem

$$\Delta = 1 + \sum_{k=1}^{n} \frac{\partial Q_k}{\partial p_k} dt. \tag{6}$$

Deci

$$V' = V + \int_{D} \cdots \int \sum_{k=1}^{n} \frac{\partial Q_k}{\partial p_k} dp_1 \ldots dp_n \, dq^1 \ldots dq^n \, dt.$$

Cum $V' - V = dV$, cunoscînd volumul V_0 al lui D la momentul t_0, volumul V la momentul t va fi

$$V = V_0 + \int_{t_0}^{t} \int_{D} \cdots \int \sum_{k=1}^{n} \frac{\partial Q_k}{\partial p_k} dp_1 \ldots dp_n \, dq^1 \ldots dq^n \, dt \tag{7}$$

şi deci:

Teoremă. *Dacă se consideră fiecare punct al domeniului D_0 de volum V_0 ca stare iniţială a sistemului la un moment iniţial t_0 şi se urmăreşte deplasarea în timp de-a lungul traiectoriei sale pînă la un anumit moment final t, atunci totalitatea acestor puncte finale formează un domeniu D, al cărui volum V este dat de relaţia* (7).

Remarcă. În cazul forţelor conservative $Q_k = \dfrac{\partial U}{\partial q^k}$, unde $U = U(q, t)$ şi deci $\dfrac{\partial Q_k}{\partial p_k} = 0$, în care caz avem teorema lui Liouville de conservare a volumului în spaţiul fazelor.

3. Evoluţia în timp a densităţii de probabilitate. Să presupunem că avem o densitate de probabilitate în spaţiul fazelor $\mathfrak{P}(p, q, t)$. Să considerăm un domeniu d infinit mic, situat în jurul punctului de coordonate (p, q), avînd deci volumul $v = dp_1 \ldots dp_n \, dq^1 \ldots dq^n$. Probabilitatea ca la momentul t un punct să aparţină domeniului d este

$$\mathfrak{P}(p, q, t) \, dp_1 \ldots dp_n \, dq^1 \ldots dq^n . \tag{8}$$

După intervalul de timp dt, aceeaşi probabilitate, ca punctul să aparţină domeniului infinit mic d', obţinut din d, este

$$\mathfrak{P}(p', q', t + dt)\, dp_1' \dots dq'^n = \mathfrak{P}(p, q, t)\, dp_1 \dots dq^n ,$$

şi cum

$$v' = dp_1' \dots dp_n' dq'^1 \dots dq'^n = \Delta\, dp_1 \dots dp_n dq^1 \dots dq^n = \Delta \cdot v,$$

avem :

$$\Delta \cdot \mathfrak{P}(p', q', t + dt) = \mathfrak{P}(p, q, t).$$

Cum însă

$$\mathfrak{P}(p', q', t + dt) - \mathfrak{P}(p, q, t) = d\mathfrak{P}(p, q, t),$$

rezultă :

$$\frac{d\mathfrak{P}(p, q, t)}{\mathfrak{P}(p, q, t)} = -\sum_{k=1}^{n} \frac{\partial Q_k}{\partial p_k}\, dt, \tag{9}$$

de unde obţinem :

$$\mathfrak{P}(p(t), q(t), t) = \mathfrak{P}(p(t_0), q(t_0), t_0)\, e^{-\sum\limits_{k=1}^{n}\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt} . \tag{10}$$

$\mathfrak{P}(p(t_0), q(t_0), t_0)$ se obţine din condiţia de normare a densităţii de probabilitate :

$$\mathfrak{P}(p(t_0), q(t_0), t_0) = \frac{1}{\underset{E_{2n}}{\int \dots \int} e^{-\sum\limits_{k=1}^{n}\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt}\, dp_1 \dots dp_n dq^1 \dots dq^n} . \tag{11}$$

Pentru ca $\mathfrak{P}(p, q, t)$ dată de relaţia (10) să fie o densitate de probabilitate, mai rămîne să arătăm că condiţia de normare este independentă de timp, adică, probabilitatea ca punctul (p, q) să se găsească în spaţiul fazelor la orice moment t, este egală cu 1. Într-adevăr, se vede că

$$dv' = v' - v, \quad \text{adică} \quad \frac{dv}{v} = \sum_{k=1}^{n} \frac{\partial Q_k}{\partial p_k}\, dt,$$

de unde rezultă

$$v = v_0\, e^{\sum\limits_{k=1}^{n}\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt} . \tag{12}$$

Deci, produsul factorilor care depind de t, din condiţia de normare,

$$e^{-\sum\limits_{k=1}^{n}\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt} \cdot v = e^{-\sum\limits_{k=1}^{n}\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt} \cdot e^{\sum\limits_{k=1}^{n}\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt} \cdot v_0 = dp_1(t_0) \dots dq^n(t_0)$$

şi deci nu depind de t. Prin urmare am demonstrat :

Teoremă. *Cunoscînd valoarea densităţii de probabilitate la un moment iniţial, într-un anumit punct iniţial, valoarea acestei densităţi de* *probabilitate; la un moment final t oarecare, în punctul obținut prin deplasarea punctului inițial de-a lungul traiectoriei sale din spațiul fazelor, este dată de relația* (10).

Remarcă. În cazul în care forțele care acționează asupra sistemului sînt conservative, se vede din (10) că densitatea de probabilitate în spațiul fazelor rămîne constantă.

ЭВОЛЮЦИЯ ПЛОТНОСТИ РАСПРЕДЕЛЕНИЯ ВЕРОЯТНОСТЕЙ В ФАЗОВОЙ ПЛОСКОСТИ ДЛЯ НЕКОНСЕРВАТИВНЫХ МЕХАНИЧЕСКИХ СИСТЕМ

РЕЗЮМЕ

Пусть дана неконсервативная механическая система с n степенями свонбоды, E_{2n} — фазовое пространство, Q_k — компоненты обобщенной силы. Если известно значение плотности распределения вероятностей в начальном моменте, в некоторой начальной точке, то значение этой плотности распределения вероятностей в некотором конечном моменте t в той точке, которая получается при перемещении начальной точки вдоль трасктории в фазовом пространстве, дается соотношением

$$\mathfrak{X}(p(t), q(t), t) = \mathfrak{X}(p(t_0), q(t_0), t_0) \cdot e^{-\sum\limits_{k=1}^{n} \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} dt}$$

Если каждая точка области $D_0 \subset E_{2n}$ объема V_0 рассматривается как начальное состояние системы в начальном моменте и затем следуют за перемещением вдоль трасктории до некоторого конечного момента t, то совокупность этих конечных точек образует область D, объем V которой дается соотношением

$$V = V_0 + \int_{t_0}^{t} \underbrace{\int \ldots \int}_{D} \sum_{k=1}^{n} \frac{\partial Q_k}{\partial p_k} dp_1 \ldots dp_n \, dq^1 \ldots dq^n \, dt.$$

В случае консервативных сил $Q_k = \dfrac{\partial U}{\partial q^k}$, где $U = U(q, t)$ и, следовательно, $\dfrac{\partial Q_k}{\partial p_k} = 0$; получаем в этом случае теорему Лиувилля о сохранении объема и плотности распределения вероятностей в фазовом пространстве.

ÉVOLUTION DE LA DENSITÉ DE PROBABILITÉ DANS L'ESPACE DES PHASES, DANS LE CAS DES SYSTÈMES MÉCANIQUES NON CONSERVATIFS

RÉSUMÉ

Soit un système mécanique non conservatif à n degrés de liberté; E_{2n} l'espace des phases, Q_k les composantes de la force généralisée. Si l'on connaît la valeur de la densité de probabilité à un moment initial, dans un point initial déterminé, la valeur de cette densité de probabilité à un moment final t quelconque, au point obtenu par le déplacement du point initial le long de sa trajectoire dans l'espace des phases, sera fournie par la relation

$$\mathfrak{L}(p(t), q(t), t) = \mathfrak{L}(p(t_0), q(t_0), t_0)\; e^{-\sum\limits_{k=1}^{n}\int_{t_0}^{t}\frac{\partial Q_k}{\partial p_k}\,dt}.$$

Si l'on considère chaque point du domaine $D_0 \subset E_{2n}$ de volume V_0 comme état initial du système à un moment initial t_0 et que l'on suive le déplacement dans le temps le long de sa trajectoire jusqu'à un certain moment final t, la totalité de ces points finals forment un domaine D, dont le volume V est donné par la relation

$$V = V_0 + \int_{t_0}^{t}\underbrace{\int\ldots\int}_{D}\sum_{k=1}^{n}\frac{\partial Q_k}{\partial p_k}\,dp_1\ldots dp_n\,dq^1\ldots dq^n\,dt.$$

Dans le cas des forces conservatives, $Q_k = \dfrac{\partial U}{\partial q^k}$, où $U = U(q, t)$ et par conséquent $\dfrac{\partial Q_k}{\partial p_k} = 0$; or, en ce cas on a le théorème de Liouville, de la conservation du volume et de la densité de probabilité dans l'espace des phases.

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C. R. Acad. Sc. Paris, t. 260 p. 3873-3876 (5 avril 1965). Groupe 4.

PHYSIQUE THÉORIQUE. — *Incompatibilité de la dynamique hamiltonienne et des théorèmes d'irréversibilité en Mécanique statistique classique.* Note (*) de M. **Francis Fer**, présentée par M. Louis de Broglie.

1. Définitions et notations. — Soit un système isolé S de la Mécanique statistique classique, défini par ses coordonnées généralisées et son hamiltonien $\mathcal{H}$; X désignera un point quelconque de l'extension en phase Γ. Soit Σ l'hypersurface de Γ définie par $\mathcal{H}(X) = E$, constante donnée. Nous prenons pour mesure sur Σ (notation $d\Omega$ pour la plage $d\Sigma$) la mesure définie par Khinchine (¹); elle est invariante dans le mouvement.

Nous supposons que nous avons, pour représenter un état macroscopique de S, une règle qui fait correspondre à cet état un ensemble C de points de Σ de mesure positive. Nous appellerons C une constellation; Σ est la réunion de constellations C_i ($i = 1$ à s). Pour un système à N particules (que nous supposerons identiques pour simplifier) un moyen particulier et bien connu pour définir un état macroscopique et la constellation correspondante consiste à diviser l'espace des phases μ de la particule en cubes identiques D_ρ ($\rho = 1, 2, \ldots$) de grandeur finie et à caractériser cet état par une distribution $\{n_\rho\}$, n_ρ étant le nombre des particules attribuées à D_ρ. Bien entendu, en sus de la condition $\sum_\rho n_\rho = N$, la distribution et la position des particules dans μ doivent respecter la condition d'énergie donnée. A $\{n_\rho\}$ correspond dans l'espace Γ un certain nombre de cubes Δ, produits cartésiens de cubes de l'espace μ, et permutant entre eux par les permutations des particules entre elles; la constellation C est la portion de Σ découpée par cet ensemble de cubes [on définit généralement la constellation comme cet ensemble lui-même (²), mais ici nous faisons expressément intervenir la condition d'énergie donnée]. Quand nous prendrons en considération plusieurs constellations nous désignerons par $\{n_\rho^i\}$ la distribution de particules relative à la constellation C_i.

Revenant à notre définition générale nous désignerons par $\Omega_i = \int_{C_i} d\Omega$ la mesure de C_i; nous appellerons fonction de constellation toute fonction Φ du point X sur Σ astreinte à garder une valeur constante Φ_i sur chaque constellation C_i (la discontinuité sur les frontières n'ont pas d'importance, l'ensemble de ces frontières étant de mesure nulle).

2. Théorème de compensation. — Un état macroscopique C_i (définition générale) étant donné à l'instant initial, on attribue à la plage $d\Sigma$ de C_i la probabilité $d\Omega/\Omega_i$ pour que le point représentatif de S s'y trouve (équiprobabilité). Soit X un point de C_i; en un temps Δt donné quelconque, le mouvement le fait passer dans une constellation C_j, qui dépend de X, et la fonction de constellation passe pour X de Φ_i à Φ_j. L'espérance mathé-

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matique de la variation de Φ pendant Δt à partir de l'état initial C_i est par définition

$$\overline{(\Delta\Phi)_i} = \left(\frac{1}{\Omega_i}\right)\int_{C_i}[\Phi_j(X) - \Phi_i]\,d\Omega.$$

Nous allons montrer que *pour tout mouvement à mesure invariante on a* $\sum_i \Omega_i \overline{(\Delta\Phi)_i} = 0$ ($i = 1$ à s); *en conséquence il est impossible que* $\overline{(\Delta\Phi)_i}$ *ait un signe défini sur* Σ (il est clair que $\overline{(\Delta\Phi)_i}$ a « aussi souvent » le signe + que le signe —).

Soit T la transformation dynamique pendant le temps Δt, et posons $\omega_{ij} = \text{mes}(TC_i \cap C_j)$ (ω_{ij} est positif ou nul suivant que TC_i coupe C_j ou non). On a les deux égalités $\sum_j \omega_{ij} = \Omega_i$ (invariance de la mesure dans le mouvement) et $\sum_k \omega_{ki} = \Omega_i$ (invariance de Σ, C_i étant complètement recouverte par un certain nombre de transformées TC_k). D'autre part, la définition de $\overline{(\Delta\Phi)_i}$ nous donne

$$\overline{(\Delta\Phi)_i} = \left(\frac{1}{\Omega_i}\right)\sum_j (\Phi_j - \Phi_i)\,\omega_{ij}.$$

D'où

$$\sum_i \Omega_i \overline{(\Delta\Phi)_i} = \sum_{ij} \omega_{ij}(\Phi_j - \Phi_i) = \sum_j \Phi_j \sum_i \omega_{ij} - \sum_i \Phi_i \sum_j \omega_{ij}$$
$$= \sum_j \Phi_j \Omega_j - \sum_i \Phi_i \Omega_i = 0.$$

C.Q.F.D.

On voit que, *si un mouvement admet une intégrale première d'énergie et une mesure invariante, il est impossible de trouver une fonction de constellation ayant une variation moyenne de signe défini qui puisse servir à caractériser une irréversibilité.*

Corollaire. — La fonction H de Boltzmann est une fonction de constellation (je me réfère ici à la définition particulière obtenue par le découpage de l'espace μ) puisque, pour un état macroscopique donné C_i, elle a pour valeur $\sum_\rho n_\rho^i \log n_\rho^i$ et que n_ρ^i est constant sur C_i. Le théorème H énonce que $\overline{(dH/dt)_i} \leq 0$, $\overline{(dH/dt)_i}$ désignant la moyenne de dH/dt prise pour toutes les évolutions possibles à partir *d'un* état C_i donné, quel que soit d'ailleurs cet état. $\overline{(dH/dt)_i}$ est donc un cas particulier des moyennes $\overline{(\Delta\Phi)_i}$, et l'on voit par conséquent que le théorème H et le théorème ci-dessus sont contradictoires (sauf évidemment pour l'équilibre $\overline{(dH/dt)_i} = 0, \forall i$).

3. L'incompatibilité des conclusions découle à n'en pas douter de l'incompatibilité des hypothèses sur lesquelles elles s'appuient, et il est par suite indiqué de rechercher en quoi les hypothèses du théorème H sont inconciliables avec un modèle purement hamiltonien. Prenons par exemple la démonstration du théorème H pour un gaz homogène à molécules sphériques sans champ de forces externe. On peut reconnaître qu'il

y est fait appel au postulat suivant : la probabilité pour qu'une molécule donnée I_0 de vitesse donnée quelconque se trouve dans un volume dV de l'espace physique est dV/V, V volume total du gaz. On admet toujours que ce postulat découle de celui de l'équiprobabilité du point représentatif X sur la constellation considérée de Σ.

Il n'en est rien. Si l'hamiltonien $\mathcal{H}$ est de classe C_1, on peut montrer que l'équiprobabilité de X sur C_i de Σ n'entraîne l'équiprobabilité de la position de I_0 dans l'espace physique que si I_0 est sans interaction avec le reste S^* du système S, auquel cas le modèle perd tout sens physique. *Si, au contraire, il y a interaction entre* S^* *et* I_0, *le premier postulat n'entraîne plus, en général, le second.* Dans les exposés classiques cette difficulté est masquée parce qu'on néglige la condition d'énergie constante : on prend pour constellation un ensemble de cubes Δ (voir § 1), et l'on raisonne comme si le point X pouvait se transformer en n'importe quel point d'un autre ensemble de cubes d'énergie « à peu près » égale. Mais ceci est illégitime car, même en admettant une imprécision d'énergie au départ, X doit se déplacer entre deux hypersurfaces Σ et Σ' déterminées par la constellation initiale, et ne faire ensuite qu'écorner les autres. On retombe alors sur la difficulté signalée.

Le paradoxe de Loschmidt est donc techniquement réfutable : comme tous les paradoxes il tire son origine dans la croyance que sont équivalentes des hypothèses qui ne le sont pas en réalité.

4. Théorème $\overline{\mathrm{H}}$ généralisé. — Il introduit, comme on sait, une densité de probabilité semi-fine P_i sur C_i à partir d'une densité fine de probabilité ρ définie sur Σ au moyen de la relation $\Omega_i P_i = \int_{C_i} \rho \, d\Omega$. L'examen du formalisme de sa démonstration fait voir qu'il ne démontre strictement que ceci : *si* à l'instant o on a $\rho = P_i$ sur chaque C_i, et *si* à l'instant t on a $\rho \neq P_i$ sur quelque C_i, alors $\overline{H}(o) > \overline{H}(t)$. Mais on ne peut démontrer que, pour $t > t'$, on a $H(t) > H(t')$ puisqu'en t la première hypothèse n'est plus vérifiée. On peut d'ailleurs démontrer que, pour un hamiltonien $\mathcal{H}$ et surface Σ donnés, *on peut trouver une infinité de distributions* ρ *(donc aussi* P_i*) sur* Σ *telles que* $d\overline{H}/dt$ *soit positif et même ait telle valeur qu'on veut.*

Mais, fut-il vrai, le théorème $\overline{H}$ généralisé tombe sous le coup d'une critique très grave, qui remet totalement en question sa signification physique. Le premier théorème de Birkhoff permet à lui seul de définir une probabilité de présence sur Σ : si σ est une plage de Σ, ∂ sa fonction caractéristique d'ensemble, et X_0 un point donné de Σ à l'instant zéro,

$$\partial (X_0) = \lim_{\theta \to \infty} \left(\frac{1}{\theta} \right) \int_0^{\theta} \partial (T_\theta X_0) \, d\theta$$

(T_θ, transformation dynamique de o à θ) existe; c'est le temps relatif moyen passé par $T_\theta X_0$ dans σ, et il permet de définir avec un sens physique parfaitement clair ce que nous appellerons la « probabilité d'observation » de $T_0 X_0$ dans σ. Généralisons à un état initial C_0, doté de l'équiprobabilité; la probabilité d'observation du système sur σ est $(1/\Omega_0)\int_{C_0}\hat{\partial}(X_0)\,d\Omega$, et l'on montre facilement que cette valeur est égale à $\lim\limits_{\theta\to\infty}(1/\theta)\int_0^\theta m(\theta)\,d\theta$, $m(\theta)$ étant la masse provenant de C_0 qui se trouve à l'instant θ dans σ. La moyenne temporelle $\hat{m}(\theta)$ de $m(\theta)$ existe donc et nous définit une probabilité d'observation *sans qu'il soit nullement besoin que $m(\theta)$ soit constant*, jusques et y compris dans le cas où il y a ergodisme, c'est-à-dire où $\hat{m}(\theta)$ est proportionnel à la mesure de σ. Or le théorème $\overline{\text{H}}$ exigerait, au moins pour l'ergodisme, que $m(\theta)$ soit constant [$m_i(\theta)$ sur C_i n'est autre que $\Omega_i P_i$]. *On se trouve donc en face de deux définitions de la probabilité de présence irréductibles l'une à l'autre.*

La raison de cette dualité est évidente. La probabilité d'observation puise sa source dans *les lois* du mouvement, la probabilité semi-fine P_i dans *notre* ignorance des conditions initiales exactes du système. Le théorème $\overline{\text{H}}$ se rattache donc plutôt à la théorie de l'information [$\text{H} = \sum\limits_i \Omega_i P_i \log P_i$ est une quantité analogue à la neg-entropie d'information, qui serait $-\sum\limits_i \Omega_i P_i \log(\Omega_i P_i)$], et n'a pas de véritable signification physique. Il est d'ailleurs heureux qu'il en soit ainsi : il est difficile d'admettre que l'irréversibilité, fait physique, tienne au défaut d'information de l'observateur.

5. Il me semble résulter de ce qui précède que la distinction entre état macroscopique (constellation) et état microscopique est impuissante à concilier l'irréversibilité des phénomènes naturels et la réversibilité de la Mécanique hamiltonienne, et que l'opinion reçue suivant laquelle cette distinction esquive la contradiction n'a pas de fondement : *on ne peut en définitive tirer une irréversibilité de la réversibilité.* Comme la première s'impose physiquement, et que le contenu physique du théorème $\overline{\text{H}}$ est trop clair pour l'abandonner, il est préférable de renoncer à la Mécanique hamiltonienne et de rechercher une dynamique qui, *tout en étant déterministe, renferme pour l'observateur un élément d'imprévision* qui explique la probabilité, *y compris pour un système unique.* L'irréversibilité prendrait alors son origine dans le processus élémentaire, et non dans notre vision macroscopique.

(*) Séance du 29 mars 1965.

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(*Institut du Radium, boul. Clemenceau, Orsay*
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Meccanica statistica. — *Sur la Mécanique statistique pour les systèmes non-conservatifs.* Nota di SILVIU GUIAŞU, presentata (*) dal Socio B. FINZI.

Hommage à M. le Professeur MAURO PICONE à l'occasion
de son 80ᵉ anniversaire.

1. Les systèmes à double structure ont été élucidés par O. Onicescu [1], [2].

Soit maintenant $\mathcal{S}$ un système mécanique non-conservatifs, avec liaisons holonomes. Le mouvement est donné par les équations [3], [4],

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_k}\right) - \frac{\partial T}{\partial q_k} = Q_k \qquad (k = 1, 2, \cdots, s) \tag{1}$$

où $q_1, q_2, \cdots, q_s$ sont les coordonnées généralisées, T l'énergie cinétique, et $Q_1, Q_2, \cdots, Q_s$ les composantes généralisées de la force dans l'espace des configurations. Soient maintenant

$$p_k = \frac{\partial T}{\partial \dot{q}_k} \qquad (k = 1, 2, \cdots, s) \tag{2}$$

et la fonction

$$\mathcal{H} = \sum_{k=1}^{s} p_k \dot{q}_k - T$$

En calculant les dérivées partielles de la fonction $\mathcal{H}$ par rapport à p_k, respectivement à q_k, et en tenant compte de (1) et (2) nous obtenons le système des équations quasi-canoniques

$$\dot{q}_k = \frac{\partial \mathcal{H}}{\partial p_k} \quad ; \quad \dot{p}_k = -\frac{\partial \mathcal{H}}{\partial q_k} + Q_k \qquad (k = 1, 2, \cdots, s) \tag{3}$$

2. Le courant attaché au système des équations (3) jouit les propriétés suivantes:

THÉORÈME: *Si dans l'espace des phases* Γ, *l'on considere chaque point du domaine* $D_0 \subset \Gamma$, *de volume* V_0, *comme l'état initial du système au moment* t_0 *et si l'on suit le déplacement de ces points dans le temps, le long de leurs trajectoires jusqu'à un certain moment final* t, *alors la totalité des positions réalisées à ce moment forment un domaine* D_t *dont le volume* V_t *est donné par la relation*

$$V_t = \int_{D_0} e^{\sum_{k=1}^{s} \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} du} \, dq_0 \, dp_0 . \tag{4}$$

(*) Nella seduta dell'11 dicembre 1965.

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Roma, 39, 447 (1965)

Démonstration: Soit

$$q = q(q_0, p_0, t_0, t) \quad , \quad p = p(q_0, p_0, t_0, t)$$

la solution du système (3) et soit Δ le détermination fonctionnel de cette transformation au moment t. Alors

$$\frac{d\Delta}{dt} = \Delta \sum_{k=1}^{s} \frac{\partial Q_k}{\partial p_k} .$$

Pour $t = t_0$ la transformation est identique, donc $\Delta_0 = 1$, et donc nous avons pour le volume V_t la formule (4).

3. Comme conséquence du théorème précédant nous avons une relation bien déterminée entre la densité de probabilité dans le point (q_0, p_0) au moment t_0 et la densité de probabilité dans le point $(q = q(q_0, p_0, t_0, t)$, $p = p(q_0, p_0, t_0, t))$ au moment t:

$$\rho_t(q(q_0, p_0, t_0, t), p(q_0, p_0, t_0, t)) = \rho_{t_0}(q_0, p_0)\, e^{-\sum_{k=1}^{s} \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} du} \tag{5}$$

Cette relation résulte de la conservation de la probabilité

$$\int_{D_t} \rho_t(q, p)\, dq\, dp = \int_{D_0} \rho_{t_0}(q_0, p_0)\, dq_0\, dp_0 \tag{6}$$

parce que grâce au courant, tous les points du domaine D_0 au moment t_0, vont au domaine D_t au moment t et donc la probabilité que le point representatif du système se trouve au moment t_0 dans le domaine D_0 est egale à la probabilité que le point representatif du système se trouve au moment t dans le domaine D_t. Mais puisque

$$\int_{D_t} \rho_t(q, p)\, dq\, dp = \int_{D_0} \rho_t(q(q_0, p_0, t_0, t), p(q_0, p_0, t_0, t))\, \Delta\, dq_0\, dp_0 \tag{7}$$

il resulte de (6), (7) et (4) la formule (5).

4. La formule (5) nous donne la loi d'évolution de la densité de probabilité à condition de connaître la densité de probabilité au moment initial t_0. Pour la déterminer, nous ferons l'application du principe de l'entropie maximale de E.T. Jaynes [5]. Si nous connaissons les valeurs moyennes $\langle f_i \rangle_{t_0}$ $(i = 1, 2, \cdots, n)$ de n fonctions de phase f_i $(i = 1, 2, \cdots, n)$ au moment t_0, alors, par l'application de ce principe nous obtenons pour la densité de probabilité au moment t_0 l'expression

$$\rho_{t_0}(q_0, p_0) = e^{-\beta - \sum_{i=1}^{n} \alpha_i f_i(q_0, p_0, t_0)} \tag{8}$$

où les constantes $\beta, \alpha_1, \alpha_2, \cdots, \alpha_n$ seront déterminées par les égalités

$$\beta = \log \Phi_{t_0}(\alpha_1, \alpha_2, \cdots, \alpha_n)$$

$$\langle f_i \rangle_{t_0} = -\frac{\partial \log \Phi_{t_0}(\alpha_1, \alpha_2, \cdots, \alpha_n)}{\partial \alpha_i} \qquad (i = 1, 2, \cdots, n)$$

où nous avons posé

$$\Phi_{t_0}(\alpha_1, \alpha_2, \cdots, \alpha_n) = -\int_{\Gamma} e^{-\sum_{i=1}^{n} \alpha_i f_i(q_0, p_0, t_0)} \, dq_0 \, dp_0 .$$

L'expression (8) compléte la formule (5) pour la densité de probabilité au moment t.

5. Le processus correspondant au courant de l'espace des phases, tenant compte de considérations précédantes est encore un processus déterministe; aléatoires sont seulement les conditions initiales. La probabilité de passage du point (q_0, p_0) au moment t_0 au point (q, p) arbitraire, au moment $t\,(t > t_0)$ sera

$$\rho_{t_0,t}(q_0, p_0 ; q, p) = \begin{cases} 1 & \text{si } q = q(q_0, p_0, t_0, t) \quad , \quad p = p(q_0, p_0, t_0, t) \\ 0 & \text{si } q \neq q(q_0, p_0, t_0, t) \quad \text{ou} \quad p \neq p(q_0, p_0, t_0, t) \end{cases}$$

où $q(q_0, p_0, t_0, t)$, $p(q_0, p_0, t_0, t)$ est la solution du système des équations quasi-canoniques (3), avec les conditions initiales (q_0, p_0) au moment t_0.

6. La Thérmodynamique des processus irréversibles s'occupe des lois phénoménologiques qui gouvernent le comportement des systèmes macroscopiques en évolution et la Mécanique statistique des processus irréversibles essaye d'expliquer ces lois, comme une conséquence de la Mécanique microstructurale. Les grandeurs macroscopiques sont assimilées aux valeurs moyennes de certaines variables aléatoires, fonctions de phase attachées aux système. Si nous avons m variables macroscopiques

$$\langle f_r \rangle_t = \int_{\Gamma} f_r \, \rho_t \, dv \qquad (r = 1, 2, \cdots, m)$$

où nous avons noté, pour simplifier l'écriture, avec dv l'élément de volume dans Γ, leur variation en fonction de temps, grâce à la relation (5) sera donné par les équations

$$(9) \qquad \frac{d\langle f_r \rangle_t}{dt} = \left\langle \frac{df_r}{dt} - f_r \sum_{k=1}^{s} \frac{\partial Q_k}{\partial p_k} \right\rangle_t = \langle \xi_r(f_r) \rangle_t , \qquad (r = 1, 2, \cdots, m).$$

Considérons à présent v fonctions de ces m variables macroscopiques

$$F_l(t) = F_l(\langle f_1 \rangle_t, \langle f_2 \rangle_t, \cdots, \langle f_m \rangle_t), \qquad (l = 1, 2, \cdots, v)$$

Alors, nous avons pour les flux de ces grandeurs, en tenant compte de (9),

$$J_l = \frac{dF_l}{dt} = \sum_{r=1}^{m} L_{lr} X_r , \qquad (l = 1 , 2 , \cdots , v)$$

où nous avons noté avec

$$L_{lr} = \frac{\partial F_l}{\partial \langle f_r \rangle_t} , \quad X_r = \langle \xi_r (f_r) \rangle_t , \qquad (l = 1 , 2 , \cdots , v ; r = 1 , 2 , \cdots , m).$$

7. Il est facile de montrer que si pour chaque $q_0 = q(t_0)$, $p_0 = p(t_0)$ les intégrales

$$\int_{t_0}^{\infty} \frac{\partial Q_k}{\partial p_k} du < + \infty \qquad (k = 1 , 2 , \cdots , s)$$

sont convergentes et s'il existe une constante $M > 0$, telle que, pour chaque $t > t_0$ et $q_0 = q(t_0)$, $p_0 = p(t_0)$ l'on a

$$- \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} du < M$$

alors le système mécanique tend vers l'équilibre, c'est-à-dire, pour chaque $\varepsilon > 0$ et chaque $(q_0 , p_0) \in \Gamma$ tel que $0 < \rho_{t_0}(q_0 , p_0) < + \infty$ il existe le nombre réel $T = T(\varepsilon , q_0 , p_0)$ tel que, aussitot ayant $t' > T$, $t'' > T$ il en résulte

$$| \rho_{t'}(q(q_0 , p_0 , t_0 , t') , p(q_0 , p_0 , t_0 , t') - \rho_{t''}(q(q_0 , p_0 , t_0 , t'') , p(q_0 , p_0 , t_0 , t'')) | < \varepsilon .$$

8. Nous supposons que la solution du système des équations quasi-canoniques (3) est une application biunivoque de Γ sur Γ. Alors le théorème H de L. Boltzmann démontré dans [6] reste valable.

9. Si nous supposons maintenant qu'il existe une fonction de force $U = U(q , t)$ telle que

$$Q_k = \frac{\partial U}{\partial q_k} \qquad (k = 1 , 2 , \cdots , s)$$

alors, il résulte de (4) et (5) que le volume et la densité de probabilité dans l'espace des phases se conservent dans le temps, c'est-à-dire le théorème classique de Liouvile. Il résulte que les forces non-conservatives déterminent les lois d'évolution.

10. Les détails de ces problemes seront donnés dans [7].

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RIASSUNTO. — In questo lavoro, noi presentiamo la Meccanica statistica per un sistema meccanico non conservativo, rinunziando all'ipotesi restrittiva che le forze generalizzate nello spazio delle configurazioni derivino da un potenziale.

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L' ENTROPIE ET LA PHYSIQUE MODERNE

par

J. Fronteau

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RESUME

La thermodynamique et le théorème de Liouville sont apparus à la même époque sur la scène scientifique (à quinze ans d'intervalle[*]). La coïncidence aurait pu en faire des alliés. L'histoire en a fait des ennemis. En effet, c'est bien sur la base d'un cas particulier du théorème de Liouville[**] qu'on a construit la mécanique statistique qui n'avait d'autre but que de s'opposer à l'hégémonie d'une thermodynamique envahissante.[***] Nous avons hérité de cette lutte l'idée que l'entropie est un concept statistique.

L'auteur croit que l'histoire a eu tort. Une autre voie eût été possible, qu'il essaie de tracer aujourd'hui : définir à l'aide du théorème de liouville vrai[x] une entropie fine (valable au niveau du phénomène élémentaire) puis l'amener de la mécanique prérelativiste à la physique des particules élémentaires, la mécanique relativiste et la mécanique statistique n'étant que des étapes comme les autres. L'auteur suggère en conclusion que l'entropie serait peut-être plus fructueuse encore en théorie des hautes énergies que partout ailleurs.

ABSTRACT

Thermodynamics and Liouville's theorem made their appearance at about the same time on the scientific scene (at an interval of fifteen years[*]). Accordingly, they might well have become allies. History made them enemies. In fact, it was a special application of Liouville's theorem[**] which served as the basis for statistical mechanics, the sole aim of which was to rebut the hegemony of thermodynamics[***]. The legacy of this struggle was the present idea that entropy is a statistical concept.

In the author's opinion, history was wrong. There was another possible solution, which he is now trying to outline : this would be to use the original version[x] of Liouville's theorem for the definition of "fine" entropy (true for elementary phenomena) and then to take entropy from pre-relativistic mechanics to elementary particle physics, relativistic mechanics and statistical mechanics being mere stages on the way like the others. The author suggests in conclusion that entropy could perhaps be even more productive in high-energy theory than anywhere else.

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[*] Ref. 1 et 2

[**] Ref. 5 (p. 82)

[***] Ref. 5 (p. 2), Ref. 9 (p. 2-06-6)

[x] Ref. 2, Ref. 24

"If we place a vessel full of water over a fire, it is only probable, and not certain, that the water will boil instead of freezing".

J.H. Jeans (1925)[*]

"Die Wärme selbst kann meiner Ansicht nach nie vereinigend, sondern immer nur trennend wirken".

R. Clausius (1865)[**]

Qui a raison ?

Et maintenant, pourquoi cette opposition ? Voici peut-être la réponse :

"Die Annahmen über die Wechselwirkung der Moleküle während eines Zusammenstosses haben ganz den Charakter des provisorischen und werden sicher einmal durch andere ersetzt werden. Ich war sogar versucht, eine Gastheorie anzudeuten, wo an Stelle der während der Zusammenstösse wirkenden Kräfte blosse Bedingungsgleichungen im Sinne der posthumen Mechanik Hertz' treten sollten, die allgemeiner sind, als die des elastischen Stosses; ich unterliess es aber, da ich doch nur wieder neue willkürliche Annahmen hätte machen müssen".

L. Boltzmann (1895)[***]

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[*] Ref. 6 (p. 181)

[**] Ref. 3 (p. 269)

[***] Ref. 5 (p. 3)

CHAPITRE I

L'ENTROPIE EN MECANIQUE CLASSIQUE

1. LE BUT DE CE RAPPORT

De même qu'on définit analytiquement l'"énergie" et l'"impulsion" d'un point matériel mobile, l'auteur pense qu'il est possible de définir une "entropie" du point matériel.

Cette idée, quoique empruntée à Louis de Broglie [Ref. 18 (p. 40)], reste aujourd'hui contraire aux habitudes de pensée : l'entropie est un concept essentiellement collectif; l'entropie "fine" n'a pas de sens. Aussi eût-il été moins téméraire d'introduire cette grandeur sous un autre nom. Cependant, le fait qu'elle permette de retrouver très simplement le $dS = \frac{dQ}{T}$ de la thermodynamique (voir page 14) et la fonction H de Boltzmann (voir page 37) justifie la liberté que l'auteur a prise à l'encontre de la tradition.

Par ailleurs, au risque *certain* de paraître s'en tenir à des banalités, l'auteur introduira cette notion d'entropie fine dès la mécanique prérelativiste, ce qui lui permettra de rappeler cette évidence, trop souvent oubliée, que la mécanique hamiltonienne n'est qu'un cas très particulier de la mécanique classique. Il essaiera alors de montrer qu'on ne peut réellement comprendre la notion d'entropie qu'en s'écartant de ce cas particulier. C'est là qu'il fera appel au théorème de Liouville "vrai", c'est-à-dire pris dans toute la généralité que lui a reconnue son auteur [Ref. 2], et qu'on a si peu exploitée.

Le texte présenté aujourd'hui n'est guère qu'un essai, fort incomplet, qui mériterait d'être critiqué en détail sur la base de tout ce qui a été fait jusqu'à présent dans les divers domaines qu'il touche. Il y a là un travail énorme. L'auteur ne l'a pas fait; il n'aura peut-être jamais le loisir de le faire. Cependant, sans en saisir nettement la portée, l'auteur pense que les idées qu'il expose dans ce texte pourront un jour apporter quelques éclaircissements à divers problèmes de physique.

2. DEFINITION DE L'ENTROPIE LOCALE

La mécanique du point matériel est régie par le système différentiel

$$\boxed{\frac{d\vec{p}}{dt} = \vec{F}}$$

Dans le cas relativiste [Ref. 24 (p. 24)] de même que dans l'approximation prérelativiste, il est possible de remplacer ces équations par un système de la forme suivante :

$$\boxed{\frac{d\vec{X}}{dt} = \vec{f}(X,t)} \qquad \text{où} \quad \vec{X} = \begin{pmatrix} x \\ y \\ z \\ x' \\ y' \\ z' \end{pmatrix}$$

Soit maintenant Δ le jacobien de l'espace des conditions initiales [espace (x,y,z,x',y',z')]

$$\Delta = \frac{D[x,y,z,x',y',z']}{D[x_0,y_0,z_0,x'_0,y'_0,z'_0]} \;.$$

Nous définirons*) l'entropie locale S par la relation

$$\boxed{S = \text{Log}|\Delta|}$$

D'après Liouville [Ref. 2, Ref. 24 (p. 3)], il vient

$$\frac{dS}{dt} = \frac{d}{dt}\,\text{Log}\,|\Delta| = \text{Div}\,\vec{f} \quad ,$$

d'où

$$\boxed{\begin{array}{l} \text{Transfert d'énergie , } dE/dt = \vec{F}\cdot\vec{v} \\ \text{Transfert d'entropie, } dS/dt = \text{Div}\,\vec{f} \end{array}}$$

---

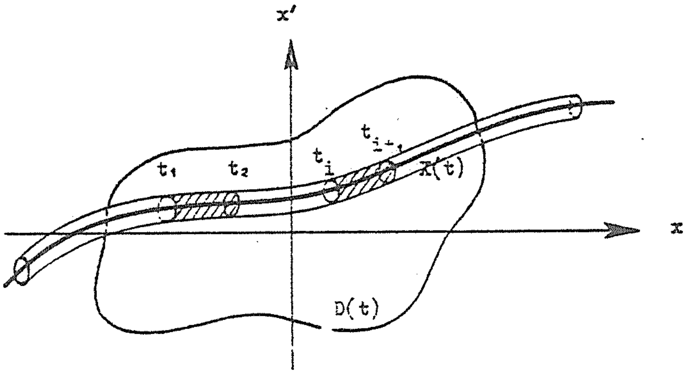
*) Il ne faut pas confondre l'entropie "locale" ainsi définie (qui, normalement, varie lorsque le temps s'écoule) avec l'entropie quantique "microscopique" de von Neumann (qui ne varie pas avec le temps, mais en raison seulement d'éventuels processus de mesure) [Ref. 10 (p. 399), Ref. 21 (p. 87)].

CHAPITRE V

UTILISATION STATISTIQUE DE L'ENTROPIE

1. DEFINITION DE LA DENSITE LOCALE

L'évolution de tout système de points matériels peut toujours être étudiée dans l'espace des conditions initiales $E_6(x,y,z,x',y',z')$. Soit $D(t)$ l'hypervolume limité par une hypersurface fermée de E_6; $D(t)$ se déplace et se déforme quand le temps s'écoule [sur la figure on s'est borné à représenter l'espace $E_2(x,x')$].



Soit, dans E_6, un certain tube de trajectoires, centré sur une trajectoire nominale $X(t)$. Supposons maintenant que ce tube soit très fin et que les trajectoires qu'il contient satisfassent toutes à un même système différentiel

$$\frac{d\vec{X}}{dt} = \vec{f}_{X,t}\,[X,t] \quad .$$

La notation qui vient d'être introduite est lourde; elle nous paraît cependant nécessaire. Voici comment nous la comprenons. Les lettres X,t qui figurent dans les crochets rappellent que la fonction $\vec{f}$ peut dépendre analytiquement de x,y,z,x',y',z' et de t. Les mêmes lettres X,t écrites en indices, signifient que la fonction $\vec{f}$ peut varier quand on passe d'un certain tube $X_1(t)$ à un autre tube $X_2(t)$ et que, pour un tube donné, elle peut être différente suivant le tronçon considéré (de t_1 à t_2, de t_2 à t_3 ...., de t_i à t_{i+1}) .

Au système différentiel $d\vec{X}/dt = \vec{f}_{X,t}$ correspond un jacobien qui dépend également du tube considéré, et même du tronçon de tube considéré

$$\Delta_{X,t} = \frac{D(X)}{D(X_0)} .$$

Ce jacobien commande l'évolution du volume élémentaire de E_6 qui accompagne le point $X(t)$ dans son mouvement

$$dX(t) = |\Delta_{X,t}|\ dX(t_0) .$$

On pourrait donc définir la densité locale comme l'inverse du volume élémentaire. En fait, si l'on veut introduire une densité qui ait un sens physique, il faut remplacer le volume élémentaire (c'est-à-dire un volume qui tend vers 0 au sens mathématique du terme) par un volume petit, mais fini, δX. On pourra ainsi parler, aux environs du point <u>mobile</u> $X(t)$, d'une densité locale de points qui ont le même comportement moyen

$$\rho[X(t)] = \frac{\rho[X(t_0)]}{|\Delta_{X,t}[X(t)]|}$$

$$\boxed{\rho = \frac{\rho_0}{|\Delta_{X,t}|}} .$$

2. CALCUL DE LA VALEUR MOYENNE D'UNE FONCTION

Supposons que les états $X(t)$ de tous les points du système considéré soient contenus dans le domaine $D(t)$.

Conformément aux habitudes de la mécanique statistique, toute fonction $\Phi_{X,t}$ aura pour valeur moyenne à l'instant t,

$$\bar{\Phi}(t) = \frac{\displaystyle\int_{D(t)} \Phi_{X,t}\, \rho \; dv}{\displaystyle\int_{D(t)} \rho \; dv} \quad .$$

Le dénominateur est égal au nombre de particules qui constituent le système. Nous supposerons qu'il reste constant

$$\boxed{N(t) = N(t_0) = N_0}$$

d'où

$$\bar{\Phi}(t) = \frac{1}{N_0} \int_{D(t)} \Phi_{X,t}\, \rho \; dv \quad .$$

Calculons maintenant la dérivée de cette valeur moyenne, $d\bar{\Phi}/dt$. En répétant le raisonnement des pages 4 et 5 du rapport CERN 65-38 [Ref. 24], il vient :

$$\frac{d}{dt}\, \bar{\Phi} = \frac{1}{N_0} \int_{D(t)} \left[\Phi_{X,t}\, \rho \; \mathrm{Div}\, \vec{f} + \frac{d}{dt}\, (\Phi\rho) \right] dv \quad .$$

Réintroduisons maintenant la relation de transfert d'entropie, $dS/dt = \mathrm{Div}\, \vec{f}$. Il vient, en résumé :

$$\boxed{\begin{gathered} \bar{\Phi}(t) = \frac{1}{N_0} \int_{D(t)} \Phi\, \rho \; dv \\[2em] \frac{d}{dt}\, \bar{\Phi} = \frac{1}{N_0} \int_{D(t)} \left[\Phi\rho(\mathrm{Div}\, \vec{f}) + \frac{d}{dt}\, (\Phi\rho) \right] dv = \frac{1}{N_0} \int_{D(t)} \left[\Phi\rho\, \frac{dS}{dt} + \frac{d}{dt}\, (\Phi\rho) \right] dv \end{gathered}}$$

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LA MÉCANIQUE STATISTIQUE NON CONSERVATIVE

PAR

SILVIU GUIAŞU

Dans ce travail, on présente une Mécanique statistique non conservative, en renonçant à l'hypothèse restrictive que les forces généralisées dérivent d'un pontentiel. Nous donnons ici la loi d'évolution de la densité de probabilité dans l'espace des phases, le problème de la détermination de la densité de probabilité au moment initial, les équations phénoménologiques des processus irréversibles, l'évolution des systèmes vers l'état d'équilibre, la variation de l'entropie du système mécanique et la loi de la variation dans le sens croissant de l'entropie macroscopique.

§ 1. INTRODUCTION

La Mécanique statistique étudie le comportement des ensembles constitués par un grand nombre de points matériels. Ces ensembles interviennent dans le microcosme (un système des particules élémentaires) ou dans le mégacosme (un système des étoiles dans une galaxie). Une longue période de temps, la Mécanique statistique a eu comme objet d'étude la justification microscopique des états macroscopiques d'équilibre et le comportement des processus réversibles. Ce problème a été élucidé grâce au théorème limite central de la théorie des probabilités [11], et puis, grâce à la théorie de l'information [12]. Mais, la majorité des processus dans la nature sont irréversibles et, en général, les états des divers systèmes matériels sont états de non-équilibre. L'interprétation microscopique des processus macroscopiques irréversibles forme l'objet de la Mécanique statistique actuelle.

En général, nous pouvons étudier une collection de plusieurs particules matérielles : a) d'une manière incomplète, par un petit nombre de variables macroscopiques, qui satisfont certaines équations phénoménologiques, c'est-à-dire équations différentielles de type déterministique; b) d'une manière complète, par la description du mouvement de chaque particule individuelle, ce qui nécessite un nombre très grand de variables

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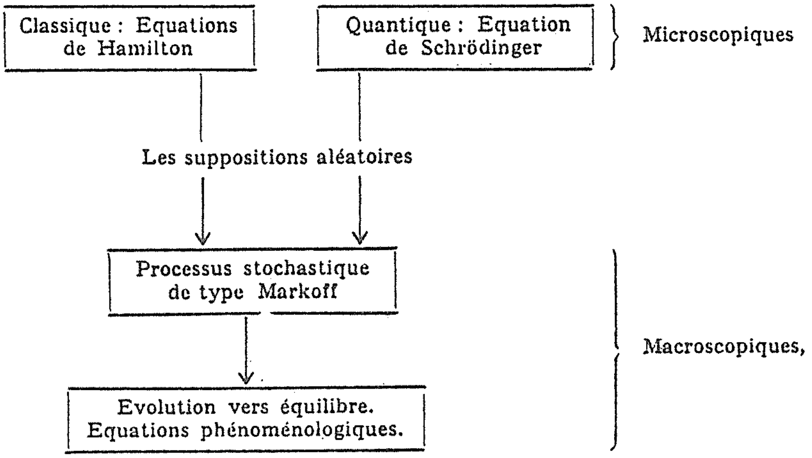
micro- ou mégascopiques. Ce mouvement des particules se fait conformément à la Mécanique classique (avec approximation) ou quantique dans le cas des systèmes microscopiques et conformément à la Mécanique classique dans le cas des systèmes mégascopiques. Nous supposerons, dans ce travail, que le mouvement des particules qui constituent le système mécanique donné se fait conformément aux équations de la Mécanique classique. Du reste, comme l'a remarqué G. E. Uhlenbeck [23], les problèmes fondamentaux de la Mécanique statistique fondée sur la Mécanique classique et ceux de la Mécanique statistique fondée sur la Mécanique quantique sont les mêmes.

Alors, nous étudions des systèmes microscopiques ou mégascopiques de points matériels, dont le mouvement se fait conformément à la Mécanique classique et à l'échelle macroscopique, nous faisons des observations et des mesurages sur ces systèmes.

En synthétisant les résultats des travaux consacrés à la Mécanique statistique des processus irréversibles, N. G. Van Kampen [17] donne le schéma général suivant :



Toutes les suppositions aléatoires supplémentaires comme « Stosszahlansatz », « molecular chaos hypothesis » ou « random phase approximation » cherchent à suppléer la pauvreté des résultats impliqués par le fait qu'à l'échelle microscopique le système de points matériels est supposé conservatif. Les équations canoniques de Hamilton, qui sont considérées habituellement comme point de départ, ne permettent pas d'obtenir les lois d'évolution à l'échelle macroscopique sans des suppositions supplémentaires.

Dans ce travail, nous donnons une Mécanique statistique des systèmes non conservatifs, en renonçant à l'hypothèse restrictive que les forces généralisées dérivent d'un potentiel. Nous donnons ici la loi d'évolution de la densité de probabilité dans l'espace des phases, le problème de la détermination de la densité de probabilité au moment initial, les équations phénoménologiques des processus irréversibles, l'évolution des systèmes vers l'état d'équilibre, la variation de l'entropie du système micro- ou mégascopique, et la loi de la variation dans le sens croissant de l'entropie macroscopique. En renonçant à la restriction que le système matériel soit conservatif, nous admettons tant la possibilité d'un échange d'énergie avec l'extérieur, que la transformation de l'énergie mécanique du système dans d'autres formes d'énergie, d'une qualité supérieure, dans le système lui-même. Nous poursuivrons, en général, deux problèmes : a) l'obtention de l'irréversibilité macroscopique : b) la cause microscopique (ou mégascopique) de l'irréversibilité macroscopique.

L'auteur profite de cette occasion pour remercier le Professeur Octav Onicescu, membre de l'Académie de la République Socialiste de Roumanie pour les nombreuses discussions et suggestions sur la Mécanique statistique. Dans [19], O. Onicescu a élucidé les systèmes à double structure et dans [20] il a étudié les processus irréversibles du point de vue des liaisons microscopiques aléatoires, en obtenant une justification pour l'interprétation des processus irréversibles comme processus stochastiques de type Markoff.

§ 2. LE SYSTÈME DES ÉQUATIONS QUASI-CANONIQUES

Soit un système mécanique holonome à s degrés de liberté. Le mouvement est donné par les équations de Lagrange

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_k}\right)-\frac{\partial T}{\partial q_k}=Q_k \qquad (k=1,2,\ldots,s) \tag{1}$$

où T est l'énergie cinétique $q_1, q_2, \ldots, q_s$ sont les coordonnées généralisées et $Q_1, Q_2, \ldots, Q_s$ sont les composantes généralisées de la force dans l'espace des configurations. Soient maintenant les variables

$$p_k=\frac{\partial T}{\partial \dot{q}_k} \qquad k=1,2,\ldots,s. \tag{2}$$

La résolution du système linéaire (2) par rapport à $\dot{q}_1, \dot{q}_2, \ldots, \dot{q}_s$ nous donne

$$\dot{q}=\dot{q}(q, p, t).$$

Soit maintenant la fonction

$$\mathcal{H}=\sum_{k=1}^{s} p_k\dot{q}_k-T.$$

En calculant les dérivées partielles de la fonction $\mathcal{H}$ par rapport à p_k, respectivement à q_k, et en tenant compte de (1) et (2), nous obtenons le système des équations quasi-canoniques

$$\begin{aligned} \dot{q}_k &= \frac{\partial \mathcal{H}}{\partial p_k} && (k=1,2,\ldots,s)\\ \dot{p}_k &= -\frac{\partial \mathcal{H}}{\partial q_k}+Q_k && (k=1,2,\ldots,s). \end{aligned} \tag{3}$$

Soit Γ l'espace des phases, c'est-à-dire l'espace euclidien à $2s$-dimensions, de coordonnées $q_1, q_2, \ldots, q_s, p_1, p_2, \ldots, p_s$. L'état du système mécanique à chaque moment est représenté par un point dans l'espace Γ. L'évolution en temps du système mécanique est représentée par une courbe dans l'espace Γ. Supposons que les fonctions

$$\mathcal{H} = \mathcal{H}(q, p, t), \qquad Q_k = Q_k(q, p, t) \qquad (k = 1, 2, \ldots, s)$$

soient suffisamment régulières parce que, dans l'espace des phases, le courant généré par les équations quasi-canoniques (3) est à chaque moment, une application biunivoque de Γ sur Γ et que la solution du système (3) soit unique déterminée dans tout l'espace Γ par les conditions initiales.

Dans le cas conservatif, il existe une fonction de force

$$U = U(q, t)$$

elle que

$$Q_k = \frac{\partial U}{\partial q_k} \qquad (k = 1, 2, \ldots, s)$$

et le système des équations quasi-canoniques (3) devient le système des équations canoniques de Hamilton

$$\begin{aligned} \dot{q}_k &= \frac{\partial H}{\partial p_k} \qquad (k = 1, 2, \ldots, s) \\ \dot{p}_k &= -\frac{\partial H}{\partial q_k} \qquad (k = 1, 2, \ldots, s) \end{aligned} \tag{4}$$

où la fonction hamiltonienne

$$H = \sum_{k=1}^{s} p_k \dot{q}_k - (T + U) = \mathcal{H} - U.$$

Nous pouvons remarquer encore qu'en général, le système des équations quasi-canoniques (3) n'est pas invariable si nous posons $-t$ au lieu de t.

§ 3. LE THÉORÈME DE LIOUVILLE GÉNÉRALISÉ

Le courant dans l'espace Γ, généré par le système des équations quasi-canoniques, a la propriété suivante :

THÉORÈME 1 : *Si l'on considère chaque point du domaine $D_0 \subset \Gamma$, de volume V_0, comme état initial du système au moment initial t_0 et que l'on suit le déplacement dans le temps le long de sa trajectoire jusqu'à un certain* *moment final t, la totalité de ces points finals forment un domaine D, dont le volume V_t est donné par la relation*

$$V_t = \int_{D_0} e^{\sum_{k=1}^{s} \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} du} \, dq_0 \, dp_0 . \tag{5}$$

Démonstration : Notons, pour simplifier l'écriture,

$$x_k = q_k, \qquad x_{s+k} = p_k \qquad (k = 1, 2, \ldots, s)$$

$$X_k = \frac{\partial \mathcal{H}}{\partial p_k}, \quad X_{s+k} = - \frac{\partial \mathcal{H}}{\partial q_k} + Q_k \qquad (k = 1, 2, \ldots, s).$$

Alors, le système des équations quasi-canoniques (3) devient

$$\frac{dx_i}{dt} = X_i \qquad i = 1, 2, \ldots, 2s. \tag{6}$$

Soit la transformation

$$x_i = f_i(x_1^0, x_2^0, \ldots, x_{2s}^0, t) \qquad (i = 1, 2, \ldots, 2s)$$

la solution du système (6) et soit Δ le déterminant fonctionnel de la transformation, au moment t,

$$\Delta = \frac{\partial(x_1, x_2, \ldots, x_{2s})}{\partial(x_1^0, x_2^0, \ldots, x_{2s}^0)} .$$

Alors

$$\frac{d\Delta}{dt} = \sum_{i=1}^{2s} \Delta_i \tag{7}$$

où Δ_i, est le déterminant qui s'obtient par Δ, si nous dérivons par rapport à t les éléments de la colonne i. En tenant compte de (6) nous avons

$$\frac{d}{dt}\left(\frac{\partial x_i}{\partial x_k^0}\right) = \frac{\partial}{\partial x_k^0} \frac{dx_i}{dt} = \frac{\partial X_i}{\partial x_k^0} = \sum_{l=1}^{2s} \frac{\partial X_i}{\partial x_l} \cdot \frac{\partial x_l}{\partial x_k^0}$$

et donc

$$\Delta_i = \sum_{l=1}^{2s} \frac{\partial X_i}{\partial x_l} \Delta_{il}$$

où Δ_{il} s'obtient par Δ en remplaçant la colonne i par la colonne l, d'où il résulte

$$\Delta_i = \Delta \frac{\partial X_i}{\partial x_i} .$$

Alors, la relation (7) nous donne

$$\frac{d\Delta}{dt} = \Delta \sum_{i=1}^{2s} \frac{\partial X_i}{\partial x_i}$$

c'est-à-dire

$$\Delta = \Delta_0 \, e^{\int_{t_0}^{t} \sum_{i=1}^{2s} \frac{\partial X_i}{\partial x_i} du} .$$

Pour $t = t_0$ la transformation est identique, donc $\Delta_0 = 1$. En tenant compte du système d'équations quasi-canoniques (3) nous avons

$$\sum_{i=1}^{2s} \frac{\partial X_i}{\partial x_i} = \sum_{k=1}^{s} \frac{\partial Q_k}{\partial p_k} .$$

Il résulte que le déterminant fonctionnel du courant généré par le système des équations quasi-canoniques, est

$$\Delta = e^{\sum_{k=1}^{s} \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} du}$$

donc, nous avons pour le volume V_t la formule (5), q.e.d.

Remarque 1° : Dans le cas conservatif

$$\frac{\partial Q_k}{\partial p_k} = \frac{\partial}{\partial p_k}\left(\frac{\partial U}{\partial q_k}\right) = 0 \qquad k = 1, 2, \ldots, s$$

donc, la formule (5) nous donne

$$V_t = V_0$$

c'est-à-dire le théorème classique de Liouville.

Remarque 2° : Le théorème 1 nous montre que dans l'espace des phases, le courant généré par un système mécanique non conservatif est une transformation qui ne conserve pas la mesure et donc le théorème de récurrence de H. Poincaré, en général, n'est pas valable, c'est-à-dire, dans la Mécanique statistique non conservative le paradoxe de E. Zermelo, en général, n'est pas valable. Le théorème 1 constitue une justification physique pour les théorèmes ergodiques pour les opérateurs qui ne conservent pas la mesure ([2], [21]).

§ 4. ÉVOLUTION DE LA DENSITÉ DE PROBABILITÉ DANS L'ESPACE DES PHASES

Si le nombre des points matériels qui constituent un système mécanique est très grand, il est impossible de déterminer avec précision l'état du système à un moment bien déterminé. Au lieu de la question : quel sera l'état du système au moment t, nous posons la question suivante : quelle sera la probabilité qu'au moment t le point représentatif du système, dans l'espace des phases, appartienne à un ensemble donné dans l'espace Γ ? En admettant qu'au moment t_0, nous avons dans l'espace des phases une densité de probabilité (de présence du point représentatif du système mécanique), nous voulons voir comment change, dans le temps, cette densité de probabilité.

THÉORÈME 2 : *Si l'on connaît la valeur de la densité de probabilité à un moment initial t_0 dans un point initial déterminé, la valeur de cette densité de probabilité à un moment final t quelconque, au point obtenu par le déplacement du point initial le long de sa trajectoire dans l'espace des phases, sera fournie par la relation*

$$\rho_t(q(q_0, p_0, t_0, t),\ p(q_0, p_0, t_0, t)) = \rho_{t_0}(q_0, p_0)\, e^{-\sum\limits_{k=1}^{s}\int_{t_0}^{t}\frac{\partial Q_k}{\partial p_k}\, du} \tag{8}$$

Démonstration : Grâce au courant, tous les points du domaine D_0 au moment t_0 vont au domaine D_t au moment t et donc la probabilité que le point représentatif se trouve au moment t_0, dans le domaine D_0 est égale avec la probabilité que le point représentatif du système se trouve au moment t dans le domaine D_t, c'est-à-dire

$$\int_{D_t} \rho_t(q, p)\, dq\, dp = \int_{D_0} \rho_{t_0}(q_0, p_0)\, dq_0\, dp_0 .$$

Mais

$$\int_{D_t} \rho_t(q, p)\, dq\, dp = \int_{D_0} \rho_t\,(q(q_0, p_0, t_0, t), p(q_0, p_0, t_0, t))\,\Delta\, dq_0\, dp_0 .$$

Alors

$$\rho_t(q(q_0, p_0, t_0, t), p(q_0, p_0, t_0, t)) = \rho_{t_0}(q_0, p_0)\,\Delta^{-1} =$$

$$= \rho_{t_0}(q_0, p_0)\, e^{-\sum\limits_{k=1}^{s}\int_{t_0}^{t}\frac{\partial Q_k}{\partial p_k}\, du} \qquad \text{q.e.d.}$$

Remarque. Dans le cas conservatif

$$\frac{\partial Q_k}{\partial p_k} = 0 \qquad (k = 1, 2, \ldots, s)$$

donc, la densité de probabilité se conserve dans le temps

$$\rho_t(q(q_0, p_0, t_0, t), p(q_0, p_0, t_0, t)) = \rho_{t_0}(q_0, p_0). \tag{9}$$

§ 5. DÉTERMINATION DE LA DENSITÉ DE PROBABILITÉ AU MOMENT INITIAL

A l'échelle macroscopique, l'état d'un système mécanique microscopique est défini par un petit nombre de paramètres, mais à l'échelle microscopique cet état est défini par un nombre énorme de paramètres. Entre les paramètres macroscopiques et ceux microscopiques il y a certaines relations, dans le sens que la connaissance de l'état microscopique implique la connaissance de l'état macroscopique correspondant. La réciproque n'est pas vraie et il existe une large variété d'états microscopiques compatibles avec un état macroscopique donné.[1] Alors, si nous avons une fonction $f = f(q, p)$ qui dépend de l'état microscopique du système, quand une certain état macroscopique est donné, la valeur correspondante de la fonction f n'est pas uniquement déterminée, c'est-à-dire, une telle fonction d'état f est une variable aléatoire. Tous les paramètres qui définissent l'état macroscopique d'un système (volume, pression, etc.) sont fonctions qui dépendent de l'état microscopique du système et qui sont observables à l'échelle macroscopique. Du point de vue microscopique, nous admettons que toutes ces fonctions d'état, observables à l'échelle macroscopique, ont des valeurs parfaitement déterminées, quand l'état macroscopique du système est donné. Cependant, du point de vue microscopique, elles sont variables aléatoires, n'ayant pas, chacune, une valeur unique, déterminée. Cette contradiction entre la description microscopique et la description macroscopique d'un système s'élucide, en Mécanique statistique, en admettant que les grandeurs observables à l'échelle macroscopique sont variables aléatoires avec une loi de répartition, de telle sorte que les grandes déviations de ces variables aléatoires de valeurs moyennes respectives sont peu probables. Ce qu'on appelle, à l'échelle macroscopique, la valeur de la grandeur observable, coïncide pratiquement avec la valeur moyenne de la variable aléatoire respective.

La formule (8) nous donne la loi d'évolution de la densité de probabilité dans l'espace des phases. Mais reste ouvert le problème de la détermination de la densité de probabilité au moment initial t_0. Pourquoi intervient cette densité de probabilité au moment initial? Au moment initial t_0 nous déterminons les valeurs moyennes au moment t_0 d'un certain nombre de fonctions d'état attachées au système mécanique. Pratiquement, ces mesurages sont toujours insuffisants pour déterminer avec précision l'état du système au moment t_0. Après E. T. Jaynes [12], nous considérons comme densité de probabilité au moment initial t_0, la densité de probabilité qui rend maximum l'incertitude compatible avec nos connaissances au moment t_0 (les valeurs moyennes au moment t_0 d'un certain nombre de fonctions d'état). La densité de probabilité qui correspond au maximum de l'entropie (comme mesure de l'incertitude) a la propriété importante qu'elle n'ignore aucune possibilité. Avec ce principe du maximum de l'entropie, si l'on connaît la valeur moyenne de l'énergie du système, supposée constante dans le temps (le cas conservatif), E. T. Jaynes [12][2] a obtenu la distribution canonique dans l'espace des phases et a fondé la Thermodynamique des états d'équilibre, sans utilisation des équations de mouvement (dans le cas conservatif, la densité de probabilité se conserve dans le temps) ou d'autres suppositions supplémentaires. Avec

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[1] Ces considérations sont valables aussi pour un système mécanique mégascopique examiné à l'échelle macroscopique.

[2] Les considérations de E. T. Jaynes pour le cas discret, peuvent être généralisées pour le cas continu (voir [14], [15]).

le principe du maximum de l'entropie, nous déterminons la distribution probabilistique plus large, compatible avec ce que nous connaissons, grâce aux mesurages effectués à l'échelle macroscopique, à un certain moment t_0.

Supposons donc qu'au moment t_0 nous connaissons la valeur moyenne $<f>_{t_0}$ d'une fonction d'état quelconque f,

$$<f>_{t_0} = \int_\Gamma f(q_0, p_0, t_0)\, \rho_{t_0}(q_0, p_0)\, dq_0\, dp_0 . \tag{10}$$

Déterminons la densité de probabilité ρ_{t_0}, au moment t_0, qui fait maximum l'entropie

$$H(\rho_{t_0}) = -\int_\Gamma \rho_{t_0}(q_0, p_0) \log \rho_{t_0}(q_0, p_0)\, dq_0\, dp_0 \tag{11}$$

en tenant compte que nous avons la condition (10) et que ρ_{t_0} étant une dénsité de probabilité

$$\int_\Gamma \rho_{t_0}(q_0, p_0)\, dq_0\, dp_0 = 1. \tag{12}$$

En utilisant la méthode des multiplicateurs de Lagrange, nous obtenons

$$\rho_{t_0}(q_0, p_0) = e^{-\lambda - \alpha f(q_0, p_0, t_0)} .$$

En notant

$$\Phi_{t_0}(\alpha) \doteq \int_\Gamma e^{-\alpha f(q_0, p_0, t_0)}\, dq_0\, dp_0$$

nous avons

$$\rho_{t_0}(q_0, p_0) = \frac{1}{\Phi_{t_0}(\alpha)} e^{-\alpha f(q_0, p_0, t_0)} . \tag{13}$$

Si au moment t_0 nous connaissons les valeurs moyennes d'un nombre m de fonctions d'état $f_1, f_2, \ldots, f_m$, en suivant la même méthode, nous trouvons pour la densité de probabilité au moment t_0 l'expression

$$\rho_{t_0}(q_0, p_0) = e^{-\lambda - \sum_{k=1}^{m} \alpha_k f_k(q_0, p_0, t_0)} \tag{14}$$

où les constantes se déterminent par les égalités

$$\lambda = \log \Phi_{t_0}(\alpha_1, \alpha_2, \ldots, \alpha_m) \tag{15}$$

$$<f_k>_{t_0} = -\frac{\partial \log \Phi_{t_0}(\alpha_1, \alpha_2, \ldots, \alpha_m)}{\partial \alpha_k} \qquad (k = 1, 2, \ldots, m) \tag{16}$$

où nous avons noté

$$\Phi_{t_0}(\alpha_1, \alpha_2, \ldots, \alpha_m) = + \int_{\Gamma} e^{-\sum_{k=1}^{m} \alpha_k f_k(q_0, p_0, t_0)} \, dq_0 \, dp_0 . \tag{17}$$

D'après les relations (8) et (14) il résulte que si au moment t_0 nous connaissons m valeurs moyennes $< f_k >_{t_0} (k = 1, 2, \ldots, m)$ alors, la densité de probabilité au moment t $(t > t_0)$ a l'expression

$$\rho_t(q(q_0, p_0, t_0, t), p(q_0, p_0, t_0, t)) = e^{-\lambda - \sum_{i=1}^{m} \alpha_i f_i(q_0, p_0, t_0) - \sum_{k=1}^{s} \int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} du} \tag{18}$$

où les constantes λ, α_1, $\alpha_2, \ldots, \alpha_m$ se déterminent par les égalités (15), (16).

§ 6. LE PROCESSUS STOCHASTIQUE CORRESPONDANT

En ce qui concerne le courant dans l'espace des phases, qui décrit l'évolution du système mécanique, le caractère aléatoire est intervenu dans le mode suivant : le processus est subordonné au système des équations quasi-canoniques (3), univoquement si les conditions initiales sont données mais même ces conditions initiales sont aléatoires. Il existe alors une distribution probabilistique dans l'état initial du système, et cette distribution est propagée dans le temps d'après la relation (8). Nous avons donc un processsus stochastique de type Markoff dégénéré, avec la densité de probabilité initiale $\rho_{t_0}(q_0, p_0)$ et avec la densité de probabilité de passage du point (q_0, p_0) au moment t_0, dans le point (q, p) au moment t $(t > t_0)$, donné par

$$\rho_{t_0, t}(q_0, p_0; q, p) = \begin{cases} 1 & \text{si} \quad q = q(q_0, p_0, t_0, t), \quad p = p(q_0, p_0, t_0, t) \\ 0 & \text{si} \quad q \neq q(q_0, p_0, t_0, t) \text{ ou } p \neq p(q_0, p_0, t_0, t) \end{cases}$$

où $q(q_0, p_0, t_0, t)$ et $p(q_0, p_0, t_0, t)$ représentent les solutions du système des équations quasi-canoniques (3) avec les conditions initiales q_0, p_0 au moment t_0. La densité de probabilité évolue dans le temps, selon la formule (8).

§ 7. LES ÉQUATIONS PHÉNOMÉNOLOGIQUES

Les variables macroscopiques satisfont des équations phénoménologiques qui sont des équations différentielles de type déterministique, en déterminant l'avenir si les conditions initiales sont données. Se pose alors le problème de la justification microscopique (si nous avons un système microscopique) ou mégascopique (si nous avons un système mégascopique) des équations phénoménologiques établies à l'échelle macroscopique.

Supposons maintenant que nous avons une seule variable macroscopique f. Sa valeur au moment t est $<f>_t$, c'est-à-dire

$$<f>_t = \int_\Gamma f \rho_t \,\mathrm{d}v$$

où nous avons noté, pour simplifier l'écriture, avec dv l'élément de volume dans Γ. Nous avons d'après (8)

$$\frac{\mathrm{d}<f>_t}{\mathrm{d}t} = \int_\Gamma \left[\frac{\mathrm{d}f}{\mathrm{d}t}\rho_t + f\frac{\mathrm{d}\rho_t}{\mathrm{d}t}\right]\mathrm{d}v = \int_\Gamma \frac{\mathrm{d}f}{\mathrm{d}t}\rho_t \,\mathrm{d}v - \sum_{k=1}^{s}\int_\Gamma f\rho_t \frac{\partial Q_k}{\partial p_k}\mathrm{d}v$$

donc

$$\frac{\mathrm{d}<f>_t}{\mathrm{d}t} = <\frac{\mathrm{d}f}{\mathrm{d}t}>_t - \sum_{k=1}^{s} <f\frac{\partial Q_k}{\partial p_k}>_t =$$

$$= <\frac{\mathrm{d}f}{\mathrm{d}t} - f\sum_{k=1}^{s}\frac{\partial Q_k}{\partial p_k}>_t = <\alpha(f)>_t\text{[3]}.$$

Si nous avons r variables macroscopiques (paramètres macroscopiques) alors, leur variation en fonction de temps sera

$$\frac{\mathrm{d}<f_j>_t}{\mathrm{d}t} = <\frac{\mathrm{d}f_j}{\mathrm{d}t} - f_j\sum_{k=1}^{s}\frac{\partial Q_k}{\partial p_k}>_t = <\alpha_j(f_j)>_t \qquad (j = 1, 2, \ldots, r).$$

Considérons maintenant l fonctions de ces r variables macroscopiques

$$F_i(t) = F_i(<f_1>_t, <f_2>_t, \ldots, <f_r>_t) \qquad (i=1, 2, \ldots, l)$$

---

[3] Si nous pouvons décomposer $\alpha(f)$ dans la série avec le centre dans $<f>_t$:

$$\alpha(f) = \alpha(<f>_t) + (f - <f>_t)\,\alpha'(<f>_t) + \frac{1}{2}(f - <f>_t)^2\alpha''(<f>_t) + \cdots$$

et si nous omettons les termes en commençant par la dérivée de deuxième ordre, nous avons

$$\frac{\mathrm{d}<f>_t}{\mathrm{d}t} = \alpha(<f>_t).$$

Cette équation est l'équation phénoménologique pour $<f>_t$ comme fonction de t.
Si $\alpha(t)$ a la forme

$$\alpha(f) = -Cf \qquad (C = \text{const.})$$

alors

$$\frac{\mathrm{d}<f>_t}{\mathrm{d}t} = -C<f>_t$$

et donc

$$<f>_t = <f>_{t_0}e^{-C(t-t_0)}$$

Alors, nous avons pour les flux de ces grandeurs

$$J_i = \frac{\mathrm{d}F_i}{\mathrm{d}t} = \sum_{j=1}^{r} \frac{\partial F_i}{\partial <f_j>_t} \cdot \frac{\mathrm{d}<f_j>_t}{\mathrm{d}t} =$$

$$= \sum_{j=1}^{r} \frac{\partial F_i}{\partial <f_j>_t} \cdot <\alpha_j(f_j)>_t = \sum_{j=1}^{r} L_{ij} X_j \qquad (i = 1, 2, \ldots, l)$$

où nous avons noté avec

$$L_{ij} = \frac{\partial F_i}{\partial <f_j>_t} \qquad (i = 1, 2, \ldots, l; j = 1, 2, \ldots, r)$$

$$X_j = <\alpha_j(f_i)>_t \qquad (j = 1, 2, \ldots, r).$$

§ 8. ÉVOLUTION VERS L'ÉTAT D'ÉQUILIBRE

Nous disons que le système mécanique tend vers l'équilibre si pour chaque $\varepsilon > 0$ et chaque $(q_0, p_0) \in \Gamma$ tel que $0 < \rho_{t_0}(q_0, p_0) < +\infty$ il existe le nombre réel $T = T(\varepsilon, q_0, p_0)$ tel que si $t' > T$, $t'' > T$, nous avons

$$|\rho_{t'}(q(q_0, p_0, t_0, t'), p(q_0, p_0, t_0, t')) -$$
$$- \rho_{t''}(q(q_0, p_0, t_0, t''), p(q_0, p_0, t_0, t''))| < \varepsilon.$$

Théorème 3 : *Si pour chaque* $q_0 = q(t_0)$, $p_0 = p(t_0)$ *les intégrales*

$$\int_{t_0}^{\infty} \frac{\partial Q_k}{\partial p_k} \mathrm{d}u < +\infty \qquad (k = 1, 2, \ldots, s) \tag{19}$$

sont convergentes et il existe une constante $M > 0$ *telle que pour chaque* $t > t_0$ *et* $q_0 = q(t_0)$, $p_0 = p(t_0)$

$$-\int_{t_0}^{t} \frac{\partial Q_k}{\partial p_k} \mathrm{d}u < M \qquad (k = 1, 2, \ldots, s) \tag{20}$$

alors, le système mécanique tend vers l'équilibre.

Démonstration : De l'hypothèse (19), il résulte que pour chaque $\delta > 0$ et $q_0 = q(t_0)$, $p_0 = p(t_0)$ il existe $T = T(\delta, q_0, p_0)$ tel que si $t' > T$ $t'' > T$ nous avons

$$\left| \sum_{k=1}^{s} \int_{T}^{t'} \frac{\partial Q_k}{\partial p_k} \mathrm{d}u - \sum_{k=1}^{s} \int_{T}^{t''} \frac{\partial Q_k}{\partial p_k} \mathrm{d}u \right| < \delta.$$

C'est-à-dire, pour chaque $\varepsilon > 0$ et $(q_0, p_0) \in \Gamma$ tel que $0 < \rho_{t_0}(q_0, p_0) < +\infty$ il existe le nombre $T = T(\varepsilon, q_0, p_0)$ tel que si $t' > T, t'' > T$ nous avons

$$\left| e^{-\sum_{k=1}^{s} \int_{T}^{t'} \frac{\partial Q_k}{\partial p_k} \mathrm{d}u} - e^{-\sum_{k=1}^{s} \int_{T}^{t''} \frac{\partial Q_k}{\partial p_k} \mathrm{d}u} \right| < \frac{\varepsilon}{\rho_{t_0}(q_0, p_0) e^{sM}} .$$

Si nous tenons compte de la loi d'évolution de la densité de probabilité (8), vu que les intégrales (20) sont uniformément bornées, il résulte que pour chaque $\varepsilon > 0$ et $q_0 = q(t_0)$, $p_0 = p(t_0)$ tels que $0 < \rho_{t_0}(q_0, p_0) < +\infty$ il existe $T = T(\varepsilon, q_0, p_0)$ tel que si $t' > T$, $t'' > T$ nous avons

$$\begin{aligned} & |\rho_{t'}(q(q_0, p_0, t_0, t'),\ p(q_0, p_0, t_0, t')) - \\ & \qquad - \rho_{t''}(q(q_0, p_0, t_0, t''),\ p(q_0, p_0, t_0, t''))| = \\ & = \rho_{t_0}(q_0, p_0)\, e^{-\sum_{k=1}^{s} \int_{t_0}^{T} \frac{\partial Q_k}{\partial p_k} du} \left| e^{-\sum_{k=1}^{s} \int_{T}^{t'} \frac{\partial Q_k}{\partial p_k} du} - e^{-\sum_{k=1}^{s} \int_{T}^{t''} \frac{\partial Q_k}{\partial p_k} du} \right| \leqslant \\ & \leqslant \rho_{t_0}(q_0, p_0)\, e^{sM} \frac{\varepsilon}{\rho_{t_0}(q_0, p_0)\, e^{sM}} = \varepsilon \qquad \text{q. e. d.} \end{aligned}$$

§ 9. VARIATION DE L'ENTROPIE MICROSCOPIQUE OU MÉGASCOPIQUE

Considérons l'entropie microscopique (si nous avons un système microscopique) ou mégascopique (si nous avons un système mégascopique),

$$\mathrm{H}(t) = -\int_\Gamma \rho_t \log \rho_t \, dv = - < \log \rho_t >_t .$$

Nous avons

$$\begin{aligned} \frac{d\mathrm{H}}{dt} &= -\int_\Gamma (\log \rho_t + 1) \frac{d\rho_t}{dt} dv = \\ &= \int_\Gamma (\log \rho_t + 1) \left(\sum_{k=1}^{s} \frac{\partial Q_k}{\partial p_k} \right) \rho_t \, dv = < (\log \rho_t + 1) \sum_{k=1}^{s} \frac{\partial Q_k}{\partial p_k} >_t . \end{aligned}$$

C'est-à-dire, l'évolution de l'entropie est une conséquence directe du caractère non conservatif des forces généralisées. Dans le cas conservatif

$$\frac{\partial Q_k}{\partial p_k} = 0 \qquad (k = 1, 2, \ldots, s)$$

et alors

$$\frac{d\mathrm{H}}{dt} = 0$$

c'est-à-dire

$$\mathrm{H} = \text{const.}$$

§ 10. THÉORÈME H DE L. BOLTZMANN [4]

Soit $\mathcal{S}$ un système mécanique microscopique avec un nombre quelconque de degrés de liberté et soit Γ l'espace des phases correspondant. Supposons que du point de vue macroscopique, le système admette N

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[4] Voir [9].

états et soient $\omega_1, \omega_2, \ldots, \omega_N$ les ensembles d'états microscopiques compatibles avec ces états macroscopiques, invariables dans le temps, de sorte qu'on ait

$$\Gamma = \bigcup_{k=1}^{N} \omega_k$$

avec la condition d'exclusivité

$$\omega_i \cap \omega_j = \emptyset \qquad (i \neq j\,;\; i, j = 1, 2, \ldots, N)$$

due à la supposition que l'état microscopique détermine complètement l'état macroscopique correspondant.

Soit maintenant une suite de temps

$$t_0 < t_1 < t_2 < \ldots < t_k < t_{k+1} < \ldots$$

Dans l'espace Γ, le courant défini par les équations du mouvement et qui représente l'évolution du système, est une application biunivoque de Γ sur Γ. Dans l'intervalle (t_k, t_{k+1}) chaque point de Γ vient en un autre point bien déterminé. Par l'effet de ce passage ; a) les points qui appartiennent à ω_j au moment t_k se répartissent entre les ensembles $\omega_1, \omega_2, \ldots \omega_N$ au moment t_{k+1}, b) chaque point est occupé à chaque moment. Alors, le passage du point représentatif du système de l'ensemble ω_j dans l'ensemble ω_i, c'est-à-dire le passage du système de l'état macroscopique qui correspond à l'ensemble ω_j, à l'état macroscopique qui correspond à l'ensemble ω_i, est réalisé avec une certaine probabilité :

$$0 \leqslant p_{t_k, t_{k+1}}(\omega_i \mid \omega_j) \leqslant 1.$$

Ces probabilités de passage, pour $i, j = 1, 2, \ldots, N$, dépendent de l'intervalle (t_k, t_{k+1}). Le courant dans l'espace des phases étant une application biunivoque de l'espace Γ sur Γ, les probabilités ainsi définies vérifient les relations fondamentales

$$\sum_{i=1}^{N} p_{t_k, t_{k+1}}(\omega_i \mid \omega_j) = 1\,; \qquad \sum_{j=1}^{N} p_{t_k, t_{k+1}}(\omega_i \mid \omega_j) = 1 \tag{21}$$

quels que soient $k = 0, 1, 2, \ldots$; $i = 1, 2, \ldots, N$; $j = 1, 2, \ldots, N$.

Si, au moment t_k, les probabilités que le point représentatif appartienne aux ensembles $\omega_1, \omega_2, \ldots, \omega_N$ respectifs, c'est-à-dire les probabilités des états macroscopiques correspondants, sont

$$p_{t_k}(\omega_i) \geqslant 0 \qquad (i = 1, 2, \ldots, N)$$

à la condition

$$\sum_{i=1}^{N} p_{t_k}(\omega_i) = 1 \tag{22}$$

alors, au moment suivant t_{k+1}, les probabilités de ces états seront

$$p_{t_{k+1}}(\omega_i) = \sum_{j=1}^{N} p_{t_k}(\omega_j)\, p_{t_k, t_{k+1}}(\omega_i \mid \omega_j) \qquad (i = 1, 2, \ldots, N). \tag{23}$$

Désignons par H_{t_k} l'entropie des états macroscopiques $\omega_1, \omega_2, \ldots, \omega_N$ au moment t_k. On aura

$$\mathrm{H}_{t_k} = - \sum_{i=1}^{N} p_{t_k}(\omega_i) \log p_{t_k}(\omega_i) \tag{24}$$

et nous démontrons le théorème fondamental suivant :

THÉORÈME 4 (*Théorème H de L. Boltzmann*) : *L'entropie augmente avec le temps, c'est-à-dire*

$$\mathrm{H}_{t_k} \leqslant \mathrm{H}_{t_{k+1}} \qquad (k = 0, 1, 2, \ldots).$$

Démonstration. Nous utilisons deux inégalités connues : Si

$$\pi_{ij} \geqslant 0, \quad \sum_{i=1}^{m} \pi_{ij} = 1, \quad p_i \geqslant 0, \quad \sum_{i=1}^{m} p_i = 1, \qquad (i, j = 1, 2, \ldots, m)$$

alors[5]

$$\prod_{i=1}^{m} (p_i)^{\pi_{ij}} \leqslant \sum_{i=1}^{m} \pi_{ij} p_i . \tag{25}$$

Si

$$\sum_{i=1}^{m} p_i = \sum_{i=1}^{m} q_i = 1, \quad p_i \geqslant 0, \quad q_i = \geqslant 0 \quad (i = 1, 2, \ldots, m)$$

alors[6]

$$- \sum_{i=1}^{m} q_i \log q_i \leqslant - \sum_{i=1}^{m} q_i \log p_i . \tag{26}$$

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[5] D'après l'inégalité de Jensen, si $y = f(x)$ est une fonction convexe sur l'intervalle $[a, b]$; $x_1, x_2, \ldots, x_m$ sont des valeurs quelconques de l'argument, qui appartiennent à l'intervalle $[a, b]$ et ne sont pas toutes égales entre elles, et $q_1, q_2, \ldots, q_m$ sont m nombres positifs avec la somme égale à 1, nous avons

$$\sum_{i=1}^{m} q_i f(x_i) \leqslant f\left(\sum_{i=1}^{m} q_i x_i\right).$$

Soit maintenant $y = \log x$. Alors

$$\sum_{i=1}^{m} q_i \log x_i \leqslant \log \left(\sum_{i=1}^{m} q_i x_i\right) \tag{27}$$

donc

$$\prod_{i=1}^{m} (x_i)^{q_i} \leqslant \sum_{i=1}^{m} q_i x_i .$$

[6] Si dans l'inégalité (27) nous posons

$$x_1 = \frac{p_1}{q_1}, \quad x_2 = \frac{p_2}{q_2}, \quad \ldots, \quad x_m = \frac{p_m}{q_m}$$

où

$$p_k \geqslant 0 \quad (k = 1, 2, \ldots, m) ; \quad \sum_{k=1}^{m} p_k = 1$$

nous obtenons

$$- \sum_{k=1}^{m} q_k \log q_k \leqslant - \sum_{k=1}^{m} q_k \log p_k .$$

D'après (21)—(26) on obtient immédiatement les inégalités suivantes [7] :

$$\begin{aligned} \mathrm{H}_{t_{k+1}} &= -\sum_{i=1}^{N} p_{t_{k+1}}(\omega_i)\log p_{t_{k+1}}(\omega_i) = \\ &= -\sum_{i=1}^{N}\sum_{j=1}^{N} p_{t_k}(\omega_j)\, p_{t_k\,.\,t_{k+1}}(\omega_i \mid \omega_j)\log p_{t_{k+1}}(\omega_i) = \\ &= -\sum_{j=1}^{N} p_{t_k}(\omega_j)\log\left(\prod_{i=1}^{N}[p_{t_{k+1}}(\omega_i)]^{p_{t_k\,.\,t_{k+1}}(\omega_i \mid \omega_j)}\right) \geqslant \\ &\geqslant -\sum_{j=1}^{N} p_{t_k}(\omega_j)\log\left(\sum_{i=1}^{N} p_{t_k\,.\,t_{k+1}}(\omega_i \mid \omega_j)\, p_{t_{k+1}}(\omega_i)\right) \geqslant \\ &\geqslant -\sum_{j=1}^{N} p_{t_k}(\omega_j)\log p_{t_k}(\omega_j) = \mathrm{H}_{t_k} \qquad \text{q.e.d.} \end{aligned}$$

Donc, l'entropie macroscopique évolue dans un sens unique

$$\mathrm{H}_{t_0} \leqslant \mathrm{H}_{t_1} \leqslant \ldots \leqslant \mathrm{H}_{t_k} \leqslant \mathrm{H}_{t_{k+1}} \leqslant \ldots \leqslant \log N.$$

Il existe donc une limite

$$\lim_{k\to\infty} \mathrm{H}_{t_k} = \mathrm{H}_\infty \leqslant \log N$$

ce qui démontre l'évolution du système vers un état d'équilibre macroscopique.

Remarque : L'analogie de la situation considérée ici avec celle d'une chaîne de systèmes de transmission de l'information par un même ensemble de signaux $\omega_1, \omega_2, \ldots, \omega_N$ et avec une perturbation donnée, pour chaque intervalle de temps, par une matrice doublement stochastique (voir [8]), est évidente.

§ 11. COMPLÉMENTS

a) L'espace des phases et le courant attaché à un système mécanique non conservatif constituent un espace à mesure, qui se modifie dans le temps. L'espace de base Γ et les ensembles mesurables $\mathfrak{B}_{2s}$ sont les mêmes, mais la mesure se modifie dans le temps. Une seule variable aléatoire, définie sur cet espace à mesure qui varie dans le temps, définit un vrai processus stochastique dans le sens usuel.

b) Dans la Mécanique statistique présentée ici, nous avons supposé que le mouvement est uniquement déterminé, mais les conditions initiales sont aléatoires. Nous pouvons considérer, cependant, que les équations de

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[7] Voir aussi [4], p. 14, mais sans aucune liaison avec la Mécanique statistique, ou avec la propagation de l'entropie dans le temps.

mouvement sont des équations stochastiques, c'est-à-dire que les forces ont un caractère aléatoire. Dans ce cas, la probabilité intervient tant dans les conditions initiales que dans l'évolution proprement dite du système matériel considéré. Dans ce cas, le théorème H démontré au § 10 reste valable.

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Institut de Mathématiques de l'Académie de la République Socialiste de Roumanie, Bucarest.

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Statistical Mechanics of Nonconservative Systems.

P. CALDIROLA

Istituto di Scienze Fisiche dell'Università - Milano

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Summary. — The statistical mechanics of a large class of systems subject to nonconservative forces is developed. In particular some fundamental theorems concerning the properties of phase space are extended and the formula of the classical Boltzmann distribution is generalized for such a class of nonconservative systems. Finally formulas for dissipative systems which are an immediate generalization of Bose-Einstein and Fermi-Dirac statistical distributions are established.

1. – Some authors have, lately, endeavoured to outline the statistical mechanics of nonconservative systems (1). We have the impression, however, that the formulation given to the problem in their papers is not the most suitable to display the characteristics of these systems, and, moreover, that some of their results are not directly and easily applicable even to the simplest cases of real physical interest, such as, for example, an ensemble of particles subject to ordinary friction forces. We think that a more suitable and direct approach to the statistical mechanics of nonconservative systems exists. Such an approach is based on the Lagrangian and Hamiltonian theory of a certain class of systems subject to nonconservative forces, theory that we developed many years ago with the aim to arriving at the quantum-mechanical laws of motion of these systems (*).

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(1) S. GUIASU: *Compt. Rend.*, **216**, 1179 (1965); S. GUIASU: *Rend. Acad. Lincei.* **39**, 447 (1966).

(*) Including the dissipative forces in the Hamiltonian to describe the motion of molecules is rather artificial, for the concept of dissipation is an average effect of the collisions between particles interacting through conservative forces. In a truly fundamental theory the dissipation should not be injected in the Hamiltonian, but it should come out of the microscopic theory.

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As is well known (²), the dynamical behaviour of a Lagrangian system characterized by the generalized co-ordinates $q_1 \dots q_s$, with a kinetic energy $T = \frac{1}{2}\sum_{h,k}^{s} a_{hk}\dot{q}_h\dot{q}_k$ (the coefficients a_{hk} may depend on the q_r) and subject to forces with generalized components $Q_h(q_1 \dots q_s;\ \dot{q}_1 \dots \dot{q}_s;\ t)$, is governed by the Lagrangian equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_r} - \frac{\partial L}{\partial q_r} = 0 \qquad (r = 1, 2, \dots, s)\,, \tag{1}$$

where $L = T + V$ is the Lagrangian function of the system and $V(q_1 \dots q_s;\ \dot{q}_1 \dots \dot{q}_s;\ t)$ is the potential function from which the Q_r's can be derived according to

$$Q_r = \frac{\partial V}{\partial q_r} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial V}{\partial \dot{q}_r}\right). \tag{2}$$

This potential function has the form

$$V = \sum_{0}^{1}{}_{n} \sum_{1}^{s}{}_{r} f_{nr}\, \dot{q}^n\,. \tag{3}$$

where f_{nr} are arbitrary functions of q_r and t.

From (3) one obtains in the case of the single particle with the cartesian co-ordinates x, y, z:

$$V = -\Phi + \boldsymbol{A}\cdot\boldsymbol{v}\,,$$

$$\boldsymbol{F} = -\operatorname{grad}\Phi - \frac{\partial \boldsymbol{A}}{\partial t} + \boldsymbol{v} \times \operatorname{rot}\boldsymbol{A}\,,$$

where Φ and A are functions of x, y, z, and t. All the forces, of which the components depend only on the q_r, $\dot{q}_r$ and t and which can be derived from a potential function of the aforesaid type, are only the Q_r which can be deduced from (3) by means of eq. (2).

When, instead, the system is subject to generalized forces $Q_h(q_1 \dots q_s;\ \dot{q}_1 \dots \dot{q}_s;\ t)$ that cannot be derived from a potential, it is still possible (³) to put the equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_h}\right) - \frac{\partial T}{\partial q_h} = \frac{\partial V}{\partial q_h} + Q_h(q_1 \dots q_s;\ \dot{q}_1 \dots \dot{q}_s;\ t)\,, \tag{4}$$

in a Lagrangian form, if one performs the time-transformation

$$\tau = \Psi(t) \tag{5}$$

(²) G. Racah: *Rend. Acad. Lincei*, 25, 223 (1937); P. Caldirola: *Rend. Ist. Lomb. Scienze*, 72, 379 (1939).

(³) P. Caldirola: *Nuovo Cimento*, 18, 393 (1941).

from which one obtains immediately

$$dt = \varphi(t)\,d\tau \qquad \text{where} \qquad \varphi(t) = 1/\dot{T}(t)\,,$$

provided the Q_r have the form

$$Q_r = f(t)\sum_1^s{}_k\, a_{rk}\dot{q}_k \tag{6}$$

and

$$\varphi(t) = C\exp\left[\int f(t)\,dt\right]. \tag{7}$$

Here C is a numerical constant which, by assuming suitable initial conditions, may be taken as equal to 1. In this case, in fact, eqs. (4) take the form

$$\frac{d}{d\tau}\left(\frac{\partial L^*}{\partial \dot{q}_j^*}\right) - \frac{\partial L^*}{\partial q_r} = 0\,, \tag{8}$$

where

$$L^* = T^* + V^*\,, \tag{9}$$

with $\dot{q}_r^*$, T^*, and V^* defined by

$$\dot{q}_r^* = \frac{dq_r}{d\tau} = \dot{q}_r\varphi(t)\,, \qquad T^* = T\varphi(t)^2\,, \qquad V^* = V\varphi(t)^2\,. \tag{10}$$

If we now introduce the Hamiltonian

$$H^* = \sum_1^s{}_r \frac{\partial L^*}{\partial \dot{q}_r^*} - L^*\,, \tag{11}$$

and the conjugate momenta

$$p_r^* = \frac{\partial L^*}{\partial \dot{q}_r^*}\,, \tag{12}$$

the equations of motion of the system take the Hamiltonian form

$$\frac{d}{d\tau}p_r^* = \frac{\partial H^*}{\partial q_r}\,, \qquad \frac{d}{d\tau}q_r = -\frac{\partial H^*}{\partial p_r^*}\,, \tag{13}$$

where

$$H^* = H^*(q_1 \ldots q_s;\, p_1^* \ldots p_s^*;\, \tau)\,.$$

Our system will allow for an integral of motion that is the generalization of energy for conservative systems, *i.e.* we shall have

$$H^* = W\,,$$

where W is a constant, if the condition

$$\frac{\partial V^*}{\partial \tau} = 0\,,$$

is satisfied, *i.e.* if V has the form

$$V = U(q_1 \dots q_s)/\varphi(t)^2\,. \tag{14}$$

Note that, in the case of the single particle subject only to the friction force $\boldsymbol{F} = -\lambda m \boldsymbol{v}$, one obtains

$$\varphi(t) = \exp[\lambda t]$$

and consequently

$$H^* = T^* = T\exp[2\lambda t] = p^{*2}/2m\,, \qquad V^* = V = 0\,, \qquad p^* = p\exp[\lambda t]\,;$$

in this case, furthermore

$$p^2\exp[2\lambda t]/2m = W$$

is an integral of motion.

2. – The Hamiltonian form in which we have cast the equations of motion for the class of nonconservative systems which we have already considered enables us to extend to such systems the theorems established by Liouville for conservative systems.

Let us begin with the theorem of conservation of extension in phase. The generalized form of this theorem may be stated in the following way:

« Let us consider the totality of the representative points that, at time $t = 0$, occupy a given domain $D_0^* = D_0$ of the phase-space Γ^* (Γ^* is defined as the phase-space the co-ordinates of which are the $q_i^* = q_i$'s and the p_i^*).

Let us now follow the movement of these points along their trajectories in phase space: the totality of the positions they occupy at time t constitutes a domain D_t^*, the volume of which V_t^* is equal to the volume V_0 of D_0, *i.e.* $V_t^* = V_0$: that is to say, we have

$$\int\limits_{D_t} \mathrm{d}q_1 \dots \mathrm{d}q_s\, \mathrm{d}p_1^* \dots \mathrm{d}p_s^* = \int\limits_{D_0} \mathrm{d}q_1^0 \dots \mathrm{d}q_s^0\, \mathrm{d}p_1^0 \dots \mathrm{d}p_s^0\,.$$

Remembering that $p_r^* = p_r\varphi(t)$, we obtain immediately

$$\int_{D_t} \mathrm{d}q_1 \dots \mathrm{d}q_s \mathrm{d}p_1 \dots \mathrm{d}p_s = \varphi(t)^{-s} \int_{D_0} \mathrm{d}q_1^0 \dots \mathrm{d}q_s^0 \mathrm{d}p_1^0 \dots \mathrm{d}p_s^0 . \tag{15}$$

We find, thus, that the extension of the domain occupied in the ordinary phase-space Γ by the representative points of our dissipative system, continues to decrease, tending to zero when $t \to \infty$.

Let us now consider the theorem of conservation of density in phase: for the systems we have been examining, we may write:

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \varrho^* = \frac{\partial \varrho^*}{\partial \tau} + [\varrho^*, H^*] ,$$

where ϱ^* is the density in the space Γ^*. Supposing that at time $t = t_0$ the density $\varrho_0^* = \varrho_0$ is uniform over all the domain $D_0^* = D_0 \subset \Gamma^*$, so that $[\varrho_0^*, H_0^*] = 0$, we obtain $\partial\varrho^*/\partial\tau = 0$, *i.e.* ϱ^* remains constant during all the time-evolution of the representative points of the system.

That is, we have

$$\varrho_\tau^*(q_1 \dots q_s;\ p_1^* \dots p_s^*) = \varrho_0(q_1^0 \dots q_s^0;\ p_1^0 \dots p_s^0) ,$$

from which we obtain

$$\varrho_t(q_1 \dots q_s;\ p_1 \dots p_s) = \varrho_0(q_1^0 \dots q_s^0;\ p_1^0 \dots p_s^0)\, \varphi(t)^s . \tag{16}$$

This equation shows us that the density of the representative points in the region of phase-space which they occupy, increases continually. As an obvious consequence of these last two theorems, we obtain furthermore that

$$\int_{D_t} \varrho_t(q_1 \dots q_r;\ p_1 \dots p_s)\, \mathrm{d}q_1 \dots \mathrm{d}q_s \mathrm{d}q_1 \dots \mathrm{d}p_s =$$
$$= \int_{D_0} \varrho_0(q_1^0 \dots q_s^0;\ p_1^0 \dots p_s^0)\, \mathrm{d}q_1^0 \dots \mathrm{d}q_s^0 \mathrm{d}p_1^0 \dots \mathrm{d}p_s^0 .$$

This result expresses the fact that the number of representative points in phase-space remains constant.

3. – The possibility of deducing the fundamental laws of statistical mechanics from the equations of motion of an ensemble of systems, is based, in classical physics, on the validity of a suitable ergodic theorem, that allows us to

substitute the microcanonical averages in phase-space for the time averages (⁴). The most satisfactory formulation of the ergodic theorem seems to be that of Birkhoff, which, on the basis of the results of the two preceding Sections, may be extended to the class of nonconservative systems which we have been examining.

For these systems, Birkhoff's ergodic theorem may be stated as follows: « Let us consider an isolated system with an unspecified number of degrees of freedom, subject to nonconservative forces; the average with respect to the time parameter τ (average over a dynamical trajectory in the phase-space with co-ordinates q and p^*) of any function f of the points of phase-space $\Gamma^*\delta$ that is integrable according to Lebesgue, defined by $\lim\limits_{\theta\to\infty}(1/\theta)\int_0^\theta f(P_\tau)\,\mathrm{d}\tau$, exists, and does not depend on the initial time. Moreover if, and only if, the dynamical system is metrically transitive, that is to say, if and only if, the surface σ^* of the « Hamiltonian » (that we suppose to be an integral of the equations of motion $\mathrm{d}H^*/\mathrm{d}\tau = 0$) cannot be decomposed into two sets of points σ_1^*, σ_2^* both with a positive measure, and both invariant with respect to the motion of the system, the average with respect to the aforesaid parameter is equal, apart from a set of points representing the initial states of the system (initial phases) with Lebesgue measure zero, to the microcanonical average over Γ^*. That is to say, we have

$$\lim_{\theta\to\infty}\int_0^\theta f[q(\tau),\,p^*(\tau)]\,\mathrm{d}\tau = \frac{\int_{\sigma^*} f(q,\,p^*)\,\mathrm{d}\sigma^*}{\int_{\sigma^*}\mathrm{d}\sigma^*}\,,$$

where $\mathrm{d}\sigma^*$ is the invariant microcanonical measure of the surface element of σ^*.

Starting from this theory we can then deduce, in a way which is completely analogous to that used for the conservative systems, the canonical distribution law for an ensemble (gas) of systems (particles) subject to dissipative forces.

It follows:

$$\mathrm{d}N = \frac{\exp[-\beta H^*(q,\,p^*)]\,\mathrm{d}q_1\ldots\mathrm{d}q_s\,\mathrm{d}p_1^*\ldots\mathrm{d}p_s^*}{\int\exp[-\beta H^*(q,\,p^*)]\,\mathrm{d}q_1\ldots\mathrm{d}q_s\,\mathrm{d}p_1^*\ldots\mathrm{d}p_s^*}\,,$$

where β is still a universal constant.

Recalling, then, the espressions $H^* = H\varphi(t)^2$, $p^* = p\varphi(t)$ and defining

$$\beta_t = \beta\varphi(t)^2\,, \tag{17}$$

(⁴) I. E. FARQUHAR: *Ergodic Theory in Statistical Mechanics* (London, 1964) (see particularly Sect. 3 and Sect. 4).

we obtain

$$\mathrm{d}N = \frac{\exp[-\beta_t H(q, p)]\,\mathrm{d}q_1 \dots \mathrm{d}q_s \mathrm{d}p_1 \dots \mathrm{d}p_s}{\int \exp[-\beta_t H(q, p)]\,\mathrm{d}q_1 \dots \mathrm{d}q_s \mathrm{d}p_1 \dots \mathrm{d}p_s}\,. \tag{18}$$

This relationship is an obvious generalization of Boltzmann's well-known distribution law for conservative systems.

Remembering expression (7) of $\varphi(t)$ we see that the number of particles with energy $H(q, p) = \varepsilon$ decreases continually as t increases; this is due to the fact that friction forces tend to diminish and ultimately annul the energy of every single particle. The final state of the ensemble ($t \to \infty$) will be a state of zero total energy.

The physical meaning of the substitution of β_t for β in (18) is easily perceived.

Let us call T_0 the initial temperature of the thermostat and consequently of our gas (before the dissipative forces begin to work). We will, therefore, have $\beta = 1/kT_0$. Starting from $t = 0$ the temperature of the gas, instead of remaining constant, decreases continually according to the law $T = T_0\varphi(t)^2$ and the gas assumes at every instant the equilibrium distribution corresponding to the temperature T.

Note, furtmermore, that if we increase adiabatically the temperature T_t of the thermostat, according to the law $T_t = T_0\varphi(t)^{-2}$, the gas continues to have the Boltzmann distribution corresponding to the constant temperature T_0.

From the physical point of view, the most interesting case to which we can apply the results we have obtained, is that of the gas of free particles subject to the friction forces $-\lambda m v$.

Using the formulas of the last Section we obtain the generalization of Maxwell's distribution law for this case

$$\mathrm{d}N = \frac{2N}{\sqrt{\pi}}\beta_t^{\frac{3}{2}} \exp[-\beta_t \varepsilon]\sqrt{\varepsilon}\,\mathrm{d}\varepsilon\,, \tag{19}$$

with

$$\beta_t = \frac{1}{kT_0} \exp[-2\lambda t]\,. \tag{20}$$

On the basis of what we found for the more general case, the interpretation of these results is immediate (*).

(*) Note that, so far, we have assumed that the dissipated energy associated with the nonconservative forces has not been reabsorbed in any way by the thermostat. If, instead, this were not case (and if the reabsorption were complete), Boltzmann's distribution would remain invaried. This, for instance, happens in the case of an electron gas immersed in a thermostat constituted by neutral molecules. The existence of friction forces forces deriving from the collision of the electrons with the molecules does not alter the Boltzmann distribution assumed by the electron gas, the temperature of which remains constantly equal to the initial temperature of the neutral

We could, moreover, develop without any difficulty the statistical thermodynamics of our gas subject to energy dissipation due to friction forces.

It seems more doubtful whether it is possible to find—apart from the case of the gas of free particles subject to friction forces—other cases of real physical interest that can be dealt with by means of the theory we have developed. This is due to the fact that if we want the Hamiltonian H^* to be a constant of motion, the potential V must depend on t in a very special and perhaps even artificial way.

We can, however, give as a second example the case of a system of linear oscillators subject, not only to the friction force, but also to an attractive force $-k\exp[-2\lambda t]x$. For such an oscillator we have

$$H = \frac{p^2}{2m} + \frac{k}{2}\exp[-2\lambda t]x^2\,,$$

and the Hamiltonian

$$H^* = H\exp[2\lambda t] = \frac{p^{*2}}{2m} + \frac{k}{2}x^2$$

is still an integral of the equations of motion. For a system of oscillators of this type, Boltzmann's generalized distribution formula, which we have found in this Section, holds good.

4. – The results obtained above, can be extended even to the quantum-mechanical case. We must first of all note that the Hamiltonian formulation for the nonconservative systems outlined in Sect. 1 of this paper, allows us to effect the quantization of these systems through a process which is the obvious generalization (5) of the usual process by which we pass from classical to quantum mechanics. Starting, therefore, from the Hamiltonian $H^*(q_r, p_r^*)$ we shall obtain the corresponding quantistic operator by substituting the cano-

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molecular gas. We can, on the other hand, deduce this result directly by solving the system of Boltzmann equations for the electronic and molecular distributions in the hypothesis of a Lorentz gas, for which the loss of energy is due to the elastic collisions of electrons with molecules. The dynamical friction occurring in the equation of mean electron motion for a Lorentz gas is a typical illustration of a dissipative effect which can be calculated in a kinetic theory, as mentioned in the footnote of p. 171.

(5) see CALDIROLA (3). For other contributions to the quantization of nonconservative systems see: E. KANAI: *Progr. Theor. Phys.*, 3, 440 (1948); E. H. KERNER: *Can. Journ. Phys.*, 36, 371 (1958); K. W. H. STESEN: *Proc. Phys. Soc.*, 72, 1027 (1958); G. VALENTINI: *Rend. Ist. Lomb. Scienze*, 95, 255 (1958); P. G. SONA: *Energia Nucleare*, 13, 318 (1966) has recently studied a more extensive class of nonconservative systems from the point of view both of classical, mechanics and of quantum mechanics.

nical variables q_r and p_r^* with the Hermitian operators defined by the usual commutation rules:

$$[q_r, p_r^*] = i\hbar\delta_{rs} .$$

In the q representation and in the Schrödinger picture, we, therefore, obtain the following quantum-mechanical evolution equation

$$i\hbar\frac{\partial\psi}{\partial\tau} = \mathscr{H}^*\left(q_r, -i\hbar\frac{\partial}{\partial q_r}; \tau\right)\psi . \tag{21}$$

Given, then, an ensemble of systems (such as a gas of particles), subject to nonconservative forces, of the type we examined, and admitting for this ensemble, the existence of the integral of the Hamiltonian H^*, thanks to the validity of suitable ergodic theorems which are an obvious extension of the ergodic quantum-mechanical theorems (⁶) for systems subject only to the action of conservative forces, it is then possible to substitute the time averages (with respect to τ) with suitable microcanonical quantum-mechanical averages over the states contained in a H^*-shell, to which, we suppose, our ensemble of systems belong.

It is then easy to establish statistical distribution formulas for nonconservative systems which are an immediate generalization of the well known formulas of Bose-Einstein and of Fermi-Dirac. We, in fact, obtain

$$\bar{n}_r = \frac{g_r}{\exp\left[(\alpha + \beta.\,\varepsilon_r) \pm 1\right]}, \tag{22}$$

where, as in the classical case, we have put $\beta_t = \beta\varphi(t)^2$ (in the case of friction forces it is still $\varphi(t) = \exp[-2\lambda t]$). We see, therefore, how the behaviour of dissipative systems of the class studied in this paper, can be deduced from that of the corresponding conservative systems in a way analogous to that in which we pass in classical statistical mechanics from conservative to nonconservative systems.

(⁶) I. E. FARQUHAR (⁴) (see especially Sect. 8).

RIASSUNTO

Viene studiata la Meccanica Statistica di una certa classe di sistemi soggetti a forze dissipative. In particolare si estendono alcuni fondamentali teoremi relativi a proprietà dello spazio delle fasi e si generalizza la formula di distribuzione classica di Boltzmann. Si mostra infine l'estensione dei risultati ottenuti al caso della meccanica quantistica generalizzando le formule di Fermi-Dirac e Bose-Einstein.

Статистическая механика неконсервативных систем.

Резюме (*). — Изучается статистическая механика большого класса систем, подверженных действию неконсервативных сил. В частности, выводятся некоторые фундаментальные теоремы, касающиеся свойств фазового пространства и обобщается формула классического распределения Больцмана для такого класса неконсервативных систем. Наконец, устанавливаются формулы для диссипативных систем, которые являются непосредственным обобщением статистических распределений Бозе-Эйнштейна и Ферми-Дирака.

(*) *Переведено редакцией.*

P. ROMAN, *et al.*
21 Settembre 1969
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A Lie-Admissible Model for Dissipative Plasmas (*).

P. ROMAN and R. M. SANTILLI
Department of Physics, Boston University - Boston, Mass.

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1. – In the present note we introduce a model for dissipative plasmas constructed in terms of an elementary generalization of well-known basic equations for plasma physics to dissipative conditions.

For this purpose, let us first recall the role of Hamiltonian mechanics for deriving the Liouville equation of a conservative system.

We consider an n-component system in phase space represented by the Hamiltonian $H(q_k, p_k)$, the density $\varrho(q_k, p_k, t)$ and the velocity $V \equiv (dq_k/dt, dp_k/dt)$, where $k = 1, 2, \ldots, n$. On account of the property

$$\nabla\cdot V \equiv \frac{\partial}{\partial q_k}\frac{dq_k}{dt} + \frac{\partial}{\partial p_k}\frac{dp_k}{\partial t} = \frac{\partial^2 H}{\partial q_k \partial p_k} - \frac{\partial^2 H}{\partial p_k \partial q_k} = 0\,, \tag{1}$$

where summation over repeated indices is assumed, and by defining the Poisson bracket for any pair of functions $A(q_k, p_k)$ and $B(q_k, p_k)$ according to

$$[A, B]_p = \frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial q_k}\,, \tag{2}$$

the Liouville equation for our system is given by

$$\frac{\partial \varrho}{\partial t} + V\cdot\nabla\varrho = \frac{\partial \varrho}{\partial t} + [\varrho\cdot H]_p = 0\,. \tag{3}$$

From eqs. (1) and (2) we clearly see the basic role of Hamiltonian mechanics for deriving eq. (3). This implies as a consequence that the Liouville equation (3) possesses well-defined limits of validity, since Hamiltonian mechanics is applicable in its general formulation to conservative (or holonomic) systems and is extendible only to a few

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(1) In connection with the limits of validity of Hamiltonian mechanics see, for instance, H. GOLDSTEIN: *Classical Mechanics* (Reading, Mass., 1965).

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specific dissipative (or nonholonomic) systems (¹). For instance, when there is a dissipative condition which cannot be expressed in terms of a generalized potential, Hamiltonian mechanics is not longer valid, and the problem of the same basic procedure for deriving an explicit form of the Liouville equation has not been fully clarified yet (²).

2. – In a recent paper (³), an algebraic criterion for selecting a generalization of Hamiltonian mechanics for dissipative systems has been introduced. This criterion can be essentially summarized as follows. The Poisson bracket (2) can be considered, from an algebraic viewpoint, as an abstract product

$$A\cdot B=[A,B]_p\,, \tag{4}$$

which defines a Lie algebra L. If one considers a dissipative framework, then a generalization of Hamiltonian mechanics generally implies an enlargment of the basic product according to an extended bracket

$$A\circ B=(A,B) \tag{5}$$

which in principle defines no longer a Lie algebra.

The above criterion for selecting enlarged procedures restricts the algebras defined by (5) to the so-called Lie-admissible algebras. These are nonassociative algebras U with abstract product $A\circ B$ such that the attached algebras U^-, which are the same vector spaces as U, but with the new product

$$[A,B]_U=A\circ B-B\circ A\,, \tag{6}$$

are Lie algebras.

More explicitly, the above algebraic criterion restricts the possibile generalized formulations by means of the condition on the enlarged bracket

$$(A,B)-(B,A)=c[A,B]_p\,, \tag{7}$$

where c is a scalar ($\neq 0$ and $\neq \infty$) with respect to q_k and p_k.

Some features of this selectivity criterion are:

1) The Hamiltonian procedure itself satisfies the requirements as basic formulation since

$$[A,B]_p-[B,A]_p=2[A,B]_p\,. \tag{8}$$

2) The generalized procedure reduces to the Hamiltonian mechanics when the system becomes conservative, since a Lie-admissible algebra can contract itself to a Lie algebra (⁴).

(²) For a large bibliography on the generalizations of the Hamilton and Lagrange formulations since 1873 see, W. D. MacMillan: *Dynamics of rigid bodies* (New York, 1936).

(³) R. M. Santilli: *Dissipativity and Lie-admissible algebras*, Coral Gables preprint no. CTS/M/67/2. To appear in *Meccanica* (April 1969).

(⁴) R. M. Santilli: *Suppl. Nuovo Cimento*, **6**, 1225 (1968).

3) A well-defined content of a system in a conservative condition can be preserved for its extension to dissipative conditions since the original Lie algebra invariance L is « imbedded » (⁵) in the enlarged algebra U.

Among the generalizations of the Hamiltonian mechanics for dissipative systems satisfying the above restriction we consider the so-called pseudo-Hamiltonian mechanics (⁶) which, in terms of two-parameter formulation can be introduced by means of the equations (³)

$$\begin{cases} \dot{q}_k = \lambda \dfrac{\partial H}{\partial p_k}, \\ \dot{p}_k = \mu \dfrac{\partial H}{\partial q_k} + f_k, \end{cases} \qquad k = 1, 2, \ldots, \mu, \tag{9}$$

where λ and μ are free parameters ($\neq 0$ and $\neq \infty$) independent of q_k and p_k, and f_k are the components of the external forces.

A physical interpretation of the parameters λ and μ can be introduced as follows. Consider a (discrete) conservative system described by the Lagrangian and Hamiltonian

$$\begin{cases} L = T(\dot{q}) - V(q), \\ H = T(p) + V(q), \end{cases} \qquad p = \frac{\partial L}{\partial q}, \tag{10}$$

where, as usual, T and V represent respectively the kinematic and potential energies. Suppose that the system for a given period of time becomes dissipative under the action of an external force. Then the kinetic and potential energies generally vary and we can write as true Lagrangian and Hamiltonian for the dissipative conditions

$$\begin{cases} L_D = T_D(q) - V_D(q) + \text{external terms}, \\ H_D = T_D(p) + V_D(q) + \text{external terms}. \end{cases} \tag{11}$$

The above quantities can always be written in terms of the original kinetic and potential energies as

$$\begin{cases} L_D = \lambda T(\dot{q}) + \mu V(q) + \cdots, \\ H_D = \lambda T(p) - \mu V(q) + \cdots, \end{cases} \tag{12}$$

where the quantities

$$\lambda = \frac{T_D}{T}, \qquad \mu = -\frac{V_D}{V} \tag{13}$$

represent the variations of the kinetic and potential energies with respect to the corresponding values for conservative conditions and can be considered, generally, as functions of q, $\dot{q}$, and t, *e.g.* $\lambda = \lambda(\dot{q}, t)$ and $\mu = \mu(q, t)$.

Suppose now, as a « perturbative approach », that either the variations (13) of T and of V are small enough to be approximated by constants, or that the true varia-

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(⁵) R. M. SANTILLI: *Nuovo Cimento*, **51** A, 570 (1967).

(⁶) R. J. DUFFIN: *Arch. Rational Mech. Anal.*, **9**, 309 (1962).

tions (13) can be approximated by some suitable chosen averages in phase space. Then, because of the independence (⁷) of λ and μ from q, $\dot{q}$, and t, the pseudo-Lagrange equations are given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L_D}{\partial \dot{q}_k} - \frac{\partial L_D}{\partial q_k} = \lambda \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_k} + \mu \frac{\partial L}{\partial q_k} = f_k\,, \qquad k = 1, 2, \dots, \mu\,, \tag{14}$$

and the pseudo-Hamiltonian equations (9) follow as

$$\begin{cases} \dot{q}_k = \dfrac{\partial H_D}{\partial p_k} = \lambda \dfrac{\partial H}{\partial p_k} & \left(p_k = \dfrac{\partial L_D}{\partial q_k} = \lambda \dfrac{\partial L}{\partial q_k}\right), \\ \dot{p}_k = -\dfrac{\partial H_D}{\partial p_k} + f_k = \mu \dfrac{\partial H}{\partial q_k} + f_k\,. & k = 1, 2, \dots, \mu\,. \end{cases} \tag{15}$$

In this formulation the total time derivative of any function $F(q_k, p_k, t)$ is given by

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\partial F}{\partial t} + \left(\lambda \frac{\partial F}{\partial q_k}\frac{\partial H}{\partial p_k} + \mu \frac{\partial H}{\partial q_k}\right) \qquad (\text{for } f_k = 0)\,. \tag{16}$$

By recalling that we are in a dissipative condition, the total energy is not conserved and its variation in time is represented by

$$\frac{\mathrm{d}H_D}{\mathrm{d}t} = (\lambda + \mu)\frac{\partial H}{\partial q_k}\frac{\partial H}{\partial p_k} \neq 0\,, \qquad \text{for } \lambda \neq -\mu\,. \tag{17}$$

Finally, from (16), the generalized bracket is given by

$$(A, B) = \lambda \frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} + \mu \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial p_k}\,. \tag{18}$$

where A and B are any functions of q_k and of p_k.

We clearly see that pseudo-Hamiltonian mechanics satisfies the above selectivity criterion since the algebra $[U(\lambda, \mu)]^-$ characterized by the product (18) is a Lie algebra on account of the property (⁸)

$$(A, B) - (B, A) = (\lambda - \mu)[A, B]_p\,. \tag{19}$$

(⁷) In this formulation the «isotropy» of the dissipativity in phase space is expressed by the independence of the λ and μ parameters on the degrees of freedom. A further extension of the formulation for anisotropic conditions can be investigated by associating different parameters λ_k and μ_k (with $k = 1, 2, \dots, n$) with each pair of canonical variables q_k and p_k.

(⁸) Let us also note that from an algebraic viewpoint only one parameter is essential, since the algebra $U(\lambda, \mu)$ characterized by the product (18) is isomorphic to the so-called isotropic algebra with product

$$(A * B) = \frac{\partial A}{\partial q_k} * \frac{\partial B}{\partial p_k} + \frac{1}{\varepsilon}\frac{\partial B}{\partial q_k} * \frac{\partial A}{\partial p_k}\,,$$

where

$$\frac{\partial A}{\partial q_k} * \frac{\partial B}{\partial p_k} = \lambda \frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k}\,, \qquad \frac{\partial B}{\partial q_k} * \frac{\partial A}{\partial p_k} = \lambda \frac{\partial B}{\partial q_k}\frac{\partial A}{\partial p_k}\,,$$

and $\varepsilon = \lambda/\mu$. Thus, from an algebraic viewpoint, the two-parameter formulation (9) is equivalent to the Duffin formulation (⁶).

Furthermore, the procedure itself reduces to Hamiltonian mechanics when the parameters λ and μ obtain the values $+1$ and -1, respectively.

An interesting aspect of this generalized procedure is that the true Hamiltonian H for a conservative region is formally preserved in a dissipative region, where it assumes the name of pseudo-Hamiltonian, since the dissipativity of the system is represented by the parameters involved in the formulation.

Pseudo-Hamiltonian mechanics has been introduced for representing some dissipative electrical network and for describing small motions of dissipative systems about a position of static equilibrium (^{6}). It has been also used for introducing a model of dissipative field theory by performing an extension to continuous system (^{3}), for whose purpose the above selectivity criterion was derived.

In the following we shall consider the above « perturbative approach » where λ and μ are constants.

3. – In connection with plasma physics, pseudo-Hamiltonian mechanics could be of some interest either for investigating plasma in dissipative conditions because of exchange of energy with an external system (*e.g.* an electric or a magnetic field), or for investigating partial regions of globally conservative plasmas with internal exchange of energy (or of momentum or of angular momentum), whenever the dissipativity does not allow the use of Hamiltonian mechanics (*e.g.* when the dissipative forces are not expressible in terms of generalized potentials (^{1}).)

Let us consider a dissipative plasma according to one of the above conditions. The generalization of the Liouville equation in terms of pseudo-Hamiltonian mechanics is given by

$$\frac{\partial \varrho}{\partial t} + (\varrho, H) + (\lambda + \mu)\varrho \frac{\partial^2 H}{\partial q_k\, \partial p_k} = C\,, \tag{20}$$

where (ϱ, H) is now the bracket (18), the third term in the l.h.s. comes from the contribution of $\nabla \cdot V$ which is now no longer zero as in (1), and C is a collision term.

Let the pseudo-Hamiltonian H be of linear velocity force type, *i.e.*

$$\frac{\partial^2 H}{\mathrm{d}q_k\, \partial p_k} = K\,, \tag{21}$$

with K a constant. Then, by (20) and by computing the total time derivative of ϱ we get (for $C = 0$)

$$\varrho = \varrho_0 \exp[-At]\,, \tag{22}$$

where $A = K(\lambda + \mu)$. Thus, under the above conditions, the particle density in phase space is no longer constant, but it decreases or increases in time corresponding to $K(\lambda + \mu) > 0$ or $K(\lambda + \mu) < 0$, respectively. For $\lambda = -\mu = 1$, *i.e.* when the pseudo-Hamiltonian mechanics reduces to the Hamiltonian mechanics, we recover the constant behavior in time of ϱ for conservative conditions.

Let us consider a collision term of the form

$$C = -\frac{\varrho - \varrho_0}{t_c}\,, \tag{23}$$

where ϱ_0 is the equilibrium distribution and t_c is the relaxation time. Then the generalized Fokker-Planck equation in terms of pseudo-Hamiltonian mechanics is given by

$$\frac{\partial \varrho}{\partial t} + \boldsymbol{V}\cdot\nabla_q \varrho + \boldsymbol{F}\cdot\nabla_p \varrho = -\frac{X\varrho - \varrho_0}{t_c}, \tag{24}$$

where

$$\boldsymbol{V} = \dot{\boldsymbol{q}}, \qquad \boldsymbol{F} = \dot{\boldsymbol{p}}, \qquad X = 1 + t_c K(\lambda + \mu). \tag{25}$$

If the above equation refers to an electron gas under the action of an electric field $\boldsymbol{E}$, then for small deviations from the equilibrium configuration we can write

$$\varrho = \frac{1}{X}\varrho_0 - \frac{t_c}{X^2}(\boldsymbol{V}\cdot\nabla_q \varrho_0 + e\boldsymbol{E}\cdot\nabla_p \varrho_0), \tag{26}$$

so that to first order, by assuming ϱ_0 to be independent of q_k, we have

$$\varrho = \frac{1}{X}\varrho_0 - \frac{t_c}{X^2} e\boldsymbol{E}\cdot\nabla_p \varrho_0 . \tag{27}$$

Under the above assumptions, the electric current and the conductivity tensor defined for conservative conditions by

$$J_K = -\frac{e^2 t_c}{m} E_i \int V_K \frac{\partial \varrho_0}{\partial V_i} \tag{28}$$

and

$$T_{ij} = -\frac{e^2 t_c}{m} \int V_i \frac{\partial \varrho_0}{\partial V_i}\, dv, \tag{29}$$

respectively, will become in our dissipative framework

$$J_k = \frac{e^2 t_c m_0}{m X_2} E_k, \tag{30}$$

$$T_{ij} = \frac{e^2 t_c m_0}{m X^2} \delta_{ij}, \tag{31}$$

where we have assumed a Maxwell distribution.

This result illustrates, in the case of our example, how the parameters λ and μ of the formalism influence the physical quantities of the system. More explicitly, these quantities represent a decrease (increase) of the electric current and of the conductivity tensor with respect to the corresponding quantities of a conservative condition when $Kt_c(\lambda + \mu) > 1$ (< 1). Thus the parameters of the formulation can be used to determine the best fit for physically established values of $\boldsymbol{J}$ and of T_{ij}. Of course, when the parameters are contracted to the values $\lambda = -\mu = 1$, then all the corresponding expressions for conservative conditions are recovered.

Let us also note that our « perturbative approach » seems to be compatible with the considered example of an elementary dissipative plasma, since also for the conservative formulation the solutions corresponding to (24) are calculated for small deviations from the equilibrium configuration.

In a similar way, other equations for a nonrelativistic or a relativistic plasma can be extended to a dissipative condition either according to the above « perturbative approach » or by means of more general procedures.

In any case, when a dissipative condition appears in a region of a plasma and the true Lagrangian L_C and Hamiltonian H_D are conceived in such a way as to represent the variations of the kinetic and potential energies according to (12), then the Liouville equation of the system will be of the form given by expression (20) when λ and μ are independent of q_k and p_k.

Conceivably, further investigations of the above model may be interesting. For instance, one could study the possible connections between the instabilities of a given region of a plasma and the exchange of energy, momentum or angular momentum between the considered region and the rest of the system.

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Apports de chaleur et mécanique dissipative.

J. FRONTEAU

Faculté des Sciences, Laboratoire de Physique - Tananarive

(ricevuto il 15 Ottobre 1970)

Summary. — The assumption of a dissipative model for heat transfers is introduced and the coherence of some of its consequences is shown.

1. – Introduction.

Du fait de la mécanique statistique et de la mécanique quantique, le formalisme proprement (*) hamiltonien est aujourd'hui omniprésent en physique. Ceci signifie que le physicien contemporain postule que toute interaction élémentaire, quel qu'en soit d'ailleurs le niveau, moléculaire, atomique, nucléaire ou subnucléaire, est un phénomène non-dissipatif. Dans ces conditions, la notion de dissipation n'a de sens que pour les interactions macroscopiques, que l'on comprend comme des phénomènes statistiques. Quelques auteurs ont cependant tenté, depuis peu, de faire sortir la physique et surtout la mécani-

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(*) On désigne ici par formalisme « proprement » hamiltonien la traditionnelle mécanique hamiltonienne des systèmes conservatifs, par opposition aux formalismes qui en dérivent et qui traitent les systèmes dissipatifs soit en introduisant et en conservant un terme de force dissipatif dans les équations d'Hamilton (¹), soit en effectuant un changement de variable portant sur le temps (²), soit encore en introduisant deux paramètres caractéristiques de la dissipation (³).

(¹) S. GUIAŞU: *Rend. Accad. Naz. Lincei*, **39**, 447 (1965).

(²) P. CALDIROLA: *Nuovo Cimento*, **46** B, 172 (1966).

(³) P. ROMAN and R. M. SANTILLI: *Lett. Nuovo Cimento*, **2**, 449 (1969).

que statistique (1-10), de ce cadre peut-être trop étroit que constitue le formalisme proprement hamiltonien. Le présent article va dans ce sens: l'auteur essaie d'y décrire les apports de chaleur à l'aide d'un modèle dissipatif.

Le modèle mécanique classique de la chaleur ne couvre, à proprement parler, que le premier principe de la thermodynamique. On ne peut pousser plus loin le modèle mécanique qu'en surajoutant une statistique. à l'évolution *non-dissipative* de chaque molécule. Le présent article tente de développer d'une autre façon le modèle mécanique de la chaleur. Il s'agit de comprendre l'entropie et le second principe sans qu'il soit a priori besoin d'une statistique, mais en postulant pour chaque molécule une *mécanique dissipative.* A long terme le but serait de ramener la thermodynamique à la dynamique en réduisant les concepts d'apports de *travail* et de *chaleur* à ceux d'apports *hamiltonien* et *non-hamiltonien* d'énergie mécanique, la variation d'entropie étant liée au caractère non-hamiltonien des apports de chaleur.

L'outil fondamental de la méthode sera le théorème d'évolution des volumes dans l'espace des conditions initiales d'un système différentiel quelconque (nous l'appellerons théorème de Liouville « vrai ») (11-13) qui généralise le cas particulier traditionnel de la conservation des volumes dans l'espace des phases de la mécanique hamiltonienne.

Le modèle dissipatif présenté ci-dessous est évidemment le plus simple qu'on puisse imaginer. Notre but est d'essayer de montrer, dans une première étape, que ce modèle est compatible avec les résultats classiques de la thermodynamique. On limitera l'étude au cas du gaz parfait, c'est-à-dire d'un ensemble de particules ponctuelles, identiques et sans interaction. Ce gaz sera à l'état propre non relativiste, c'est-à-dire que les vitesses des particules seront toutes faibles devant c.

2. – Le modèle dissipatif proposé.

Nous postulerons que tout apport de chaleur peut être représenté par une force de la forme

$$F = \alpha m v$$

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(4) S. GUIAŞU: *Compt. Rend. Ac. Sc. Roum.*, **12**, 1087 (1962).

(5) F. FER: *Compt. Rend.*, **260**, 3873 (1965).

(6) F. FER: *Compt. Rend.*, **260**, 4159 (1965).

(7) J. FRONTEAU: *L'entropie et la physique moderne*, CERN, rapport interne MPS/Int. MU/EP 66-5 (1966).

(8) S. GUIAŞU: *Rev. Roum. Math. Pures Appl.*, **11**, 541 (1966).

(9) F. FER: *Compt. Rend.*, **265**, 205 (1967).

(10) F. FER: *Compt. Rend.*, **265**, 289 (1967).

(11) J. LIOUVILLE: *Journ. Math. Pures Appl.*, **3**, 342 (1838).

(12) C. G. J. JACOBI: *Vorlesungen über Dynamik, Oeuvres (complément)* (Berlin, 1884), p. 92.

(13) J. FRONTEAU: *Le théorème de Liouville et le problème général de la stabilité*, CERN, 65-38 (1965).

agissant sur chaque particule (de masse au repos constante m); α est une constante (*), positive ou négative suivant le signe de l'« apport » de chaleur. Par la suite, de telles forces seront dites « forces calorifiques ». Dans l'expression de ces forces, $\boldsymbol{v}$ est la vitesse par rapport au référentiel K_0 dans lequel le gaz est au repos macroscopique (le centre de masse du gaz y est fixe).

Insistons sur le fait que le modèle proposé ci-dessus n'est évidemment qu'une hypothèse dont l'auteur ne prétend pas établir d'un coup la validité; il s'agit seulement d'attirer l'attention du lecteur sur quelques conséquences de cette hypothèse.

3. – Application des théorèmes généraux de la dynamique classique.

3·1. *Théorème du centre de gravité.*

$$\left(\sum m\right)\frac{\mathrm{d}V_G}{\mathrm{d}t} = \sum F = \sum \alpha m v = \alpha \sum m v \, .$$

Or, P désignant une particule quelconque,

$$\sum mGP = 0 \qquad \text{(définition du centre de masse } G) \, .$$

En dérivant dans K_0, il vient

$$\sum mv = 0 \, , \qquad \sum F = 0 \, .$$

Ainsi, le mouvement du centre de gravité n'est nullement affecté par l'existence des forces calorifiques; l'apport de chaleur ne modifie pas sa vitesse. Remarquons en passant que ce résultat est conforme à la position d'Arzeliès quant à la transformation relativiste des grandeurs thermodynamiques (cf. (14). Introduction, page XXVII, ou page 671).

3·2. *Théorème du moment cinétique.*

$$\frac{\mathrm{d}\sigma_G}{\mathrm{d}t} = \sum M_G^t F \, .$$

Pour les forces calorifiques,

$$\sum M_G^t F = \alpha \sum GP \wedge mv = \alpha \sigma_G \, .$$

(*) A quelques détails près, le modèle conduit aux mêmes résultats si l'on remplace la constante α par une fonction $\alpha(t)$ commune à toutes les particules.

(14) H. ARZELIÈS: *Thermodynamique relativiste et quantique* (Paris, 1968).

En intégrant, il vient:

$$\sigma_G = (\sigma_G)_i \exp[\alpha t] \qquad \text{(l'indice } i \text{ caractérise l'instant initial)} .$$

Le moment cinétique macroscopique du gaz reste nul s'il l'était au début de l'apport de chaleur.

3'3. *Théorème des forces vives.*

$$\begin{aligned} \mathrm{d}\Big(\sum E_{\text{cin}}\Big) &= \sum \mathrm{d}E_{\text{cin}} = \sum \delta\mathscr{T} = \sum \boldsymbol{F}\cdot\boldsymbol{v}\,\mathrm{d}t , \\ \sum \boldsymbol{F}\cdot\boldsymbol{v}\,\mathrm{d}t &= \sum \alpha m\boldsymbol{v}\cdot\boldsymbol{v}\,\mathrm{d}t = \alpha\Big(\sum mv^2\Big)\mathrm{d}t . \end{aligned}$$

En intégrant, il vient

$$\sum E_{\text{cin}} = \Big(\sum E_{\text{cin}}\Big)_i \exp[2\alpha t] .$$

L'énergie cinétique du système varie (exponentiellement) sans pour qu'autant le centre de gravité se déplace, et sans pour qu'autant apparaisse un moment cinétique d'ensemble.

4. – Application du théorème du viriel.

$$\sum \tfrac{1}{2}mv^2 = -\tfrac{1}{2}\sum \boldsymbol{F}\cdot\boldsymbol{GP} = -\varphi ,$$

$$\varphi = \varphi_{\text{pression}} + \varphi_{\text{cal}} \qquad \text{(pour un gaz parfait, } \varphi_{\text{int}} \equiv 0) .$$

Calculons le viriel des forces calorifiques

$$\varphi_{\text{cal}} = \frac{1}{2}\sum \alpha m\boldsymbol{v}\cdot\boldsymbol{GP} = \frac{\alpha}{4}\frac{\mathrm{d}}{\mathrm{d}t}\Big[\sum m(\boldsymbol{GP})^2\Big] .$$

La théorie du viriel postule, du fait de l'équilibre statistique du gaz, que $\sum m(\boldsymbol{GP})^2$ est une constante. En conséquence

$$\varphi_{\text{cal}} = 0 .$$

Les résultats classiques découlant de la théorie du viriel ne sont donc pas modifiés par l'introduction des forces calorifiques. Entre autre, pour un gaz parfait, on a à tout instant

$$\sum E_{\text{cin}} = -\varphi_{\text{pression}} = \tfrac{3}{2}PV .$$

5. – Introduction de l'entropie fine [cf. (7)].

Considérons l'équation du mouvement de chaque particule du gaz soumis aux forces calorifiques

$$m\gamma = \alpha m v\,,$$

c'est-à-dire, en ramenant le système au premier ordre,

$$\mathrm{d}X/\mathrm{d}t = X' \qquad \mathrm{d}X'/\mathrm{d}t = \alpha X'\,, \qquad\qquad X = (x, y, z)\,,$$

Introduisons le jacobien

$$J = \frac{D(x, y, z, x', y', z)}{D(x_i, y_i, z_i, x'_i, y'_i, z'_i)}\,,$$

l'indice i caractérisant l'instant origine, et définissons l'entropie fine par la relation

$$S_f = K \log |J| \qquad (K \text{ constante de Boltzmann})\,.$$

On sait que le jacobien J commande l'évolution temporelle des volumes dans l'« espace des conditions initiales » à 6 dimensions x, y, z, x', y', z'. L'*entropie fine sera donc une mesure de cette évolution.*

Appliquons maintenant le théorème de Liouville vrai (11-13) au système différentiel considéré ci-dessus:

$$\frac{\mathrm{d}}{\mathrm{d}t} \log |J| = \text{divergence du second membre du système ramené au premier ordre,}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \log |J| = \frac{\partial x'}{\partial x} + \frac{\partial y'}{\partial y} + \frac{\partial z'}{\partial z} + \frac{\partial(\alpha x')}{\partial x'} + \frac{\partial(\alpha y')}{\partial y'} + \frac{\partial(\alpha z')}{\partial z'}\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \log |J| = 3\alpha\,;$$

or (cf. Subsec. 3·3)

$$\frac{\mathrm{d}E_{\text{cin}}/\mathrm{d}t}{E_{\text{cin}}} = 2\alpha\,,$$

d'où

$$\frac{\mathrm{d}}{\mathrm{d}t} \log |J| = \frac{3}{2}\,\frac{\mathrm{d}E_{\text{cin}}/\mathrm{d}t}{E_{\text{cin}}}\,,$$

ou encore

$$\mathrm{d}S_f = \frac{3}{2} K \frac{\mathrm{d}E_{\text{cin}}}{E_{\text{cin}}}\,.$$

En définissant l'entropie comme une grandeur extensive, il vient

$$\mathrm{d}S = \sum \mathrm{d}S_j\,,$$
$$\mathrm{d}S = \frac{3}{2}K\sum\frac{\mathrm{d}E_{\text{cin}}}{E_{\text{cin}}}\,.$$

Insistons sur le fait que les variations d'énergie cinétique considérées ici sont dues aux forces calorifiques.

6. – Passage à l'entropie macroscopique.

6·1. *Introduction de la réversibilité.* – Soit θ la température cinétique du gaz, c'est-à-dire, à un facteur près, l'énergie cinétique moyenne des particules. Notons qu'il s'agit de la température du gaz, et non de celle d'une source extérieure (cf. à ce propos (14), p. 682).

Considérons maintenant un apport dQ de chaleur, que nous interpréterons à l'aide de forces calorifiques, et cherchons à quelles conditions, θ et dQ étant donnés, la fonction dS définie ci-dessus passe par un extremum.

Les N particules constituant le gaz étant affectées d'un indice j, posons

$$E_j = (E_{\text{cin}})_j\,,\qquad X_j = (\mathrm{d}E_{\text{cin}})_j\,.$$

Avec ces notations,

$$\frac{2}{3K}\,\mathrm{d}S = \sum_j\left(\frac{\mathrm{d}E_{\text{cin}}}{E_{\text{cin}}}\right)_j = \sum_j\frac{X_j}{E_j} = F(X_j, E_j)\,.$$

Le problème de l'extremum de dS revient à trouver les conditions d'extremum de la fonction $F(X_j, E_j)$ sachant que:

$$f(X_j) = \sum_j X_j = \mathrm{d}Q \quad \text{constante donnée}\,,$$
$$g(E_j) = \sum_j E_j = N\theta \quad \text{constante donnée}\,.$$

Appliquons la méthode des multiplicateurs de Lagrange; λ et μ étant deux paramètres auxiliaires, les X_j et les E_j caractérisant l'extremum sont définis par la compatibilité des équations suivantes:

$$\left\{\begin{aligned}&\frac{\partial F}{\partial X_j}+\lambda\frac{\partial f}{\partial X_j}+\mu\frac{\partial g}{\partial X_j}=0\,,\\&\frac{\partial F}{\partial E_j}+\lambda\frac{\partial f}{\partial E_j}+\mu\frac{\partial g}{\partial E_j}=0\,,\end{aligned}\right.\qquad j=1,\ldots,N,$$

c'est-à-dire:

$$\left\{\begin{aligned} &\frac{1}{E_j}+\lambda=0\,,\\ &-\frac{X_j}{E_j^2}+\mu=0\,, \end{aligned}\right. \Rightarrow \left\{\begin{aligned} &E_j=-\frac{1}{\lambda}\,,\\ &X_j=\frac{\mu}{\lambda^2}\,. \end{aligned}\right.$$

Les conditions d'extremum sont donc

$$\begin{aligned} &(E_{\text{cin}})_1 \;= (E_{\text{cin}})_2 \;= (E_{\text{cin}})_3 \;= \dots = (E_{\text{cin}})_N\,,\\ &(\mathrm{d}E_{\text{cin}})_1 = (\mathrm{d}E_{\text{cin}})_2 = (\mathrm{d}E_{\text{cin}})_3 = \dots = (\mathrm{d}E_{\text{cin}})_N\,. \end{aligned}$$

La condition $(E_{\text{cin}})_1 = (E_{\text{cin}})_2 = \dots = (E_{\text{cin}})_N$ définit l'état d'équilibre parfait. Tout apport de chaleur tel que $(\mathrm{d}E_{\text{cin}})_1 = (\mathrm{d}E_{\text{cin}})_2 = \dots = (\mathrm{d}E_{\text{cin}})_N$ fait passer à un état d'équilibre arbitrairement voisin. La transformation est réversible, et l'on vient de retrouver que dans ce cas dS connaît un extremum.

6·2. *Calcul de* dQ/θ *pour un apport de chaleur réversible* (cas de la transformation à volume constant).

$$\begin{aligned} &\mathrm{d}Q = \sum \mathrm{d}E_{\text{cin}} &&(\mathrm{d}E_{\text{cin}} \text{ dues aux forces calorifiques})\,,\\ &K\theta = \tfrac{2}{3}\bar{E}_{\text{cin}} &&(K \text{ constante de Boltzmann})\,, \end{aligned}$$

$$\frac{\mathrm{d}Q}{\theta} = \frac{\sum \mathrm{d}E_{\text{cin}}}{(2/3K)\,\bar{E}_{\text{cin}}} = \frac{3}{2}\,K\,\frac{\sum \mathrm{d}E_{\text{cin}}}{\bar{E}_{\text{cin}}}\,.$$

La transformation étant *réversible* au sens défini ci-dessus,

$$\bar{E}_{\text{cin}} = E_{\text{cin}} \quad \text{et} \quad (\mathrm{d}E_{\text{cin}})_1 = (\mathrm{d}E_{\text{cin}})_2 = \dots = (\mathrm{d}E_{\text{cin}})_N\,,$$

d'où

$$\frac{\mathrm{d}Q}{\theta} = \frac{3}{2}\,K\,\frac{N\,\mathrm{d}E_{\text{cin}}}{E_{\text{cin}}} = \frac{3}{2}\,KN\,\frac{\mathrm{d}E_{\text{cin}}}{E_{\text{cin}}} = N\,\mathrm{d}S_f\,,$$

$$\frac{\mathrm{d}Q}{\theta} = \frac{3}{2}\,KN\,\mathrm{d}(\log E_{\text{cin}}) = \mathrm{d}S\,.$$

On retrouve bien que dQ/θ est intégrable dans le cas d'une transformation réversible.

6·3. *La fonction H de Boltzmann.* — La mécanique statistique définit la moyenne $\bar{\Phi}$ de toute fonction Φ à l'aide d'intégrales étendues à l'espace des phases, c'est-à-dire, puisque les particules du gaz parfait sont identiques (même masse m), étendues à l'espace x, y, z, x', y', z'. Désignons par ϱ la densité de population de cet espace.

$$\bar{\Phi} = \frac{\int \Phi \varrho \, \mathrm{d}v}{\int \varrho \, \mathrm{d}v} = \frac{\int \Phi \varrho \, \mathrm{d}v}{N} ;$$

N, nombre de particules, est une constante.

Appliquons cette moyenne à l'entropie fine S_f [cf. (7)]

$$\bar{S}_f = \frac{1}{N} \int S_f \varrho \, \mathrm{d}v .$$

Or, $\varrho = \varrho_i / |J|$ (i caractérise l'instant initial),

$$S_f = K \log |J| ,$$

d'où

$$\bar{S}_f = \frac{K}{N} \int \varrho \log \frac{\varrho_i}{\varrho} \, \mathrm{d}v ,$$

$$\bar{S}_f = -\frac{K}{N} \int \varrho \log \varrho \, \mathrm{d}v + \frac{K}{N} \int \varrho \log \varrho_i \, \mathrm{d}v .$$

En postulant une densité initiale uniforme,

$$\frac{K}{N} \int \varrho \log \varrho_i \, \mathrm{d}v = \frac{K \log \varrho_i}{N} \int \varrho \, \mathrm{d}v = K \log \varrho_i = \text{const} ,$$

d'où

$$\bar{S}_f = -\frac{K}{N} \int \varrho \log \varrho \, \mathrm{d}v + \text{const} .$$

On reconnaît la fonction H de Boltzmann $H = \int \varrho \log \varrho \, \mathrm{d}v$; retenons

$$H = -\frac{N}{K} \bar{S}_f + \text{const} .$$

7. – Invariance relativiste de l'entropie fine.

Soient $K_0(x_0 y_0 z_0)$ et $K(xyz)$ deux référentiels en translation uniforme l'un par rapport à l'autre le long de l'axe des z. Le gaz est au repos macroscopique par rapport à K_0.

Posons

$$v_e = \text{vitesse de } K_0/K \qquad \text{(vitesse d'entraînement)},$$

$$\beta_e = \frac{v_e}{c},$$

$$\gamma_e = \frac{1}{\sqrt{1-\beta_e^2}}.$$

La transformation de Lorentz s'écrit

$$\begin{aligned} t &= \gamma_e\left[t_0 + \beta_e \frac{z_0}{c}\right], \\ z &= \gamma_e\,[z_0 + \beta_e c t_0], \\ y &= y_0, \\ x &= x_0. \end{aligned}$$

(L'indice 0 caractérise les grandeurs définies dans K_0. Ce sera l'indice i qui caractérisera tout état initial.)

Posons $\lambda = \gamma_e$, $\mu = \gamma_e \beta_e c$, $\nu = \gamma_e \beta_e / c$, $k = \gamma_e$. Il vient

$$\begin{aligned} x &= x_0, \\ y &= y_0, \\ z &= \lambda z_0 + \mu t_0, \\ t &= \nu z_0 + k t_0, \end{aligned} \qquad \begin{vmatrix} \lambda & \mu \\ \nu & k \end{vmatrix} = 1.$$

Prenons les différentielles

$$\begin{aligned} \mathrm{d}x &= \mathrm{d}x_0, \\ \mathrm{d}y &= \mathrm{d}y_0, \\ \mathrm{d}z &= \lambda\,\mathrm{d}z_0 + \mu\,\mathrm{d}t_0, \\ \mathrm{d}t &= \nu\,\mathrm{d}z_0 + k\,\mathrm{d}t_0, \end{aligned}$$

d'où

$$\begin{aligned} \mathrm{d}x/\mathrm{d}t &= \frac{\mathrm{d}x_0}{\nu\,\mathrm{d}z_0 + k\,\mathrm{d}t_0}, \\ \mathrm{d}y/\mathrm{d}t &= \frac{\mathrm{d}y_0}{\nu\,\mathrm{d}z_0 + k\,\mathrm{d}t_0}, \\ \mathrm{d}z/\mathrm{d}t &= \frac{\lambda\,\mathrm{d}z_0 + \mu\,\mathrm{d}t_0}{\nu\,\mathrm{d}z_0 + k\,\mathrm{d}t_0}. \end{aligned}$$

Nous retiendrons ces résultats sous la forme suivante:

$$
\begin{aligned}
x &= x_0\,,\\
y &= y_0\,,\\
z &= \lambda z_0 + \mu t_0\,,\\
\dot{x} &= \frac{x'_0}{k+\nu z'_0}\,,\\
\dot{y} &= \frac{y'_0}{k+\nu z'_0}\,,\\
\dot{z} &= \frac{\mu+\lambda z'_0}{k+\nu z'_0}\,,
\end{aligned}
$$

(Les trois dernières relations ont été obtenues en divisant les deux termes des seconds membres précédents par dt_0. Dans ces conditions, le signe ˙ représente la dérivée par rapport à t et le signe $'$ la dérivée par rapport à t_0.)

Calculons les dérivées partielles et écrivons un jacobien qui nous sera utile par la suite

$$
\frac{D(x\,y\,z\,\dot{x}\,\dot{y}\,\dot{z})}{D(x_0 y_0 z_0 x'_0 y'_0 z'_0)} =
\begin{vmatrix}
1 & 0 & 0 & 0 & 0 & 0\\
0 & 1 & 0 & 0 & 0 & 0\\
0 & 0 & \lambda & 0 & 0 & 0\\
0 & 0 & 0 & \dfrac{1}{k+\nu z'_0} & 0 & -\dfrac{\nu x'_0}{(k+\nu z'_0)^2}\\
0 & 0 & 0 & 0 & \dfrac{1}{k+\nu z'_0} & -\dfrac{\nu y'_0}{(k+\nu z'_0)^2}\\
0 & 0 & 0 & 0 & 0 & \dfrac{1}{(k+\nu z'_0)^2}
\end{vmatrix},
$$

c'est-à-dire, en développant,

$$
\frac{D(x\,y\,z\,\dot{x}\,\dot{y}\,\dot{z})}{D(x_0 y_0 z_0 x'_0 y'_0 z'_0)} = \frac{\lambda}{(k+\nu z'_0)^4}\,;
$$

or

$$
\begin{aligned}
k + \nu z'_0 &= \gamma_e\left[1 + \beta_e \frac{z'_0}{c}\right],\\
\lambda &= \gamma_e\,,
\end{aligned}
$$

d'où

$$\frac{D(x\,y\,z\,\dot{x}\,\dot{y}\,\dot{z})}{D(x_0 y_0 z_0 x'_0 y'_0 z'_0)} = \frac{1}{\gamma_e^3[1+\beta_e(z'_0/c)]^4}\,.$$

Le gaz étudié étant dans un état propre non relativiste, on a $z'_0 \ll c$. Avec cette hypothèse, on obtient

$$\frac{D(x\,y\,z\,\dot{x}\,\dot{y}\,\dot{z})}{D(x_0 y_0 z_0 x'_0 y'_0 z'_0)} \simeq \frac{1}{\gamma_e^3}\,.$$

Pour simplifier les expressions, introduisons la notation

$$\frac{D(x)}{D(x_0)} = \frac{D(x\,y\,z\,\dot{x}\,\dot{y}\,\dot{z})}{D(x_0 y_0 z_0 x'_0 y'_0 z'_0)}\,.$$

Il vient, l'indice i caractérisant l'instant initial dans chacun des référentiels K_0 et K,

$$\frac{D(x)}{D(x_i)} \equiv \frac{D(x)}{D(x_0)}\cdot\frac{D(x_0)}{D(x_{0i})}\cdot\frac{D(x_{0i})}{D(x_i)}\,,$$

$$\frac{D(x)}{D(x_i)} \simeq \frac{1}{\gamma_e^3}\cdot\frac{D(x_0)}{D(x_{0i})}\cdot\gamma_e^3 \qquad \text{(puisque l'entraînement est uniforme),}$$

d'où

$$\frac{D(x)}{D(x_i)} \simeq \frac{D(x_0)}{D(x_{0i})}\,.$$

Passons aux entropie fines

$$S_f = K \log \frac{D(x)}{D(x_i)}\,, \qquad (S_f)_0 = K \log \frac{D(x_0)}{D(x_{0i})}\,.$$

Il vient en définitive

$$S_f \simeq (S_f)_0 \qquad\qquad (\text{pour } z'_0 \ll c)\,.$$

Remarque: Pour obtenir une invariance rigoureuse (gaz relativiste ou non) il suffirait de généraliser la notion d'entropie fine à l'aide du jacobien de l'espace $(x_\mu u_\mu)$ à 8 dimensions, $D(x_\mu u_\mu)/D(x_{\mu i} u_{\mu i})$. En effet, on démontre que

$$\frac{D(x_\mu u_\mu)}{D(x_{\mu_0} u_{\mu_0})} = 1 \qquad\qquad (\text{cf. } (^{14}) \text{ page } 310)\,.$$

Il ne resterait donc qu'à terminer le raisonnement comme pour l'espace à 6 dimensions.

8. - Evolution vers l'équilibre.

Jusqu'à présent nous avons étudié les échanges de chaleur avec l'extérieur. Considérons maintenant l'évolution vers l'équilibre, en l'absence de tout échange avec l'extérieur, les échanges d'énergie entre particules du gaz étant dus à des forces calorifiques.

Considérons deux particules du gaz, P_1 at P_2 et supposons $(E_{\text{cin}})_2 > (E_{\text{cin}})_1$. Notons plus simplement $E_2 > E_1$. Pour parvenir à la même énergie (évolution vers l'équilibre parfait) les deux particules échangeront une energie $\mathrm{d}E = (E_2 - E_1)/2$, d'où la variation des deux entropies fines

$$\mathrm{d}S_{f1} = \frac{3}{2} K \frac{\mathrm{d}E}{E_1}, \qquad \mathrm{d}S_{f2} = \frac{3}{2} K \frac{(-\mathrm{d}E)}{E_2},$$

d'où enfin $\mathrm{d}S = \mathrm{d}S_{f1} + \mathrm{d}S_{f2} > 0$.

L'entropie d'un système isolé ne peut que croître (ou rester constante quand l'équilibre est atteint).

* * *

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● RIASSUNTO (*)

Si introduce un modello dissipativo per il trasferimento di calore e si dimostra la coerenza di alcune conseguenze ottenute con esso.

(*) *Traduzione a cura della Redazione.*

Перенос тепла и диссипативная механика.

Резюме (*). — Вводится предположение диссипативной модели для переноса тепла и показывается согласованность некоторых следствий этой модели.

(*) *Переведено редакцией.*

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DIE VERALLGEMEINERTE LIOUVILLE-GLEICHUNG

G. GERLICH

Lehrstuhl B für Theoretische Physik der Technischen Universität Braunschweig,
Braunschweig, Deutschland

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Synopsis

The generalized Liouville equation is obtained, if the differential equation for the distribution function of a physical system is deduced without assuming that Liouville's theorem is applicable. The entropy of such distribution functions is determined. If one admits frictional forces, which are proportional to the velocity, the entropy decreases in the course of time, although, considering irreversible processes, the entropy of a distribution function usually increases. The damped harmonic oscillator and the consequences for the derivation of the n-time BBGKY hierarchy are briefly discussed.

1. *Einleitung.* Die verallgemeinerte Liouville-Gleichung wird hergeleitet, ohne daß der Satz von Liouville herangezogen wird. Da häufig zwischen dem Satz von Liouville und der Liouville-Gleichung kein Unterschied gemacht wird, soll zuerst der Zusammenhang zwischen beiden dargelegt werden. Dies läßt sich am einfachsten durchführen, wenn man sich nicht gleich auf physikalische Systeme bezieht, sondern die Situation mit dem in der Theorie der stochastischen Prozesse üblichen Sprachgebrauch beschreibt.

Wir betrachten eine vom reellen Parameter t (der Zeit) abhängige Schar von Abbildungen (Transformationen) des reellen n-dimensionalen Raums R^n in sich

$$x^i = h^i((x_0^1, \dots, x_0^n), t), \qquad i = 1, 2, \dots, n, \tag{1}$$

wofür abkürzend

$$x = h(x_0, t) \tag{2}$$

geschrieben werden soll. Die Transformationen (2) sollen umkehrbar und zweimal stetig partiell nach allen Variablen differenzierbar sein bis auf Punkte vom L-B-Maß Null. Diese Ausnahmepunktmenge soll unabhängig von t sein, und es soll ausgeschlossen sein, daß solche singulären Punkte bei (2) für ein gewisses t übergehen in nichtsinguläre Punkte und umgekehrt.

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Diese Schar von Abbildungen kann man als stochastischen Prozeß betrachten: Die Klasse der L–B-meßbaren Teilmengen des R^n bezeichnen wir mit $\boldsymbol{B}$, und für die Variable x_0 definieren wir durch eine L-B-Dichte $f(x_0)$ im R^n ein Wahrscheinlichkeitsmaß $\boldsymbol{P}$. Die σ-Algebra für die Variable x sei ebenfalls die Klasse $\boldsymbol{B}$. Ist die durch (2) gegebene Schar von Abbildungen für jeden Wert des Parameters t $\boldsymbol{B}$–$\boldsymbol{B}$-meßbar, ist durch (2) eine Schar von Zufallsvariablen definiert, die man einen stochastischen Prozeß nennt (zur Definition des stochastischen Prozesses siehe z. B. Bauer[1]). In der Theorie der stochastischen Prozesse versucht man Verteilungen der Variablen x zu endlich vielen Zeiten zu bestimmen, insbesondere aber für eine Zeit. Diese letztgenannte Verteilungsdichte von x zur Zeit t soll $f_1(x, t)$ genannt werden. Will man dann den Erwartungswert einer Funktion g von x zur Zeit t bestimmen, geschieht dies mit $f_1(x, t)$ durch

$$\langle g\,(x(t))\rangle = \int g(x) f_1(x, t)\, \mathrm{d}x, \tag{3}$$

wobei dx das L–B-Maß im R^n der Variablen x kennzeichnet. Mit der Verteilungsdichte $f(x_0)$ und (2) lautet der Erwartungswert (3)

$$\langle g\,(x(t))\rangle = \int g(h\,(x_0, t)) f(x_0)\, \mathrm{d}x_0 . \tag{4}$$

Betrachtet man (2) als eine von einem Parameter t abhängige Variablentransformation von x_0 nach x, die für $t = t_0$ die identische Transformation sein soll, dann gehört zu dieser Transformation eine Funktionaldeterminante J, die als Determinante von $\partial h^i/\partial x_0^k$ im allgemeinen eine Funktion von x_0 und t ist:

$$J(x_0, t) = \mathrm{Det}\left(\frac{\partial h^i}{\partial x_0^k}\right). \tag{5}$$

Mit der zu (2) gehörenden Umkehrtransformation

$$x_0 = h^{-1}\,(x, t) \tag{6}$$

kann man aus f und J die Funktionen $\tilde{f}$ und $\tilde{J}$ bilden:

$$\tilde{f}(x, t) = f(h^{-1}\,(x, t)), \qquad \tilde{J} = J\,(h^{-1}\,(x, t), t). \tag{7}$$

Damit läßt sich (4) durch eine Transformation der Integrationsvariablen in die Form (3) bringen

$$\int g(h\,(x_0, t))\, f(x_0)\, \mathrm{d}x_0 = \int g(x)\, \tilde{f}\, \tilde{J}^{-1}\, \mathrm{d}x. \tag{8}$$

Die gesuchte Verteilungsdichte f_1 ist also gegeben durch

$$f_1(x, t) = \tilde{J}^{-1}\, \tilde{f}(x, t) \tag{9}$$

Mit dem Satz von Liouville erhält man $J = \tilde{J} = 1$, also $f_1 = \tilde{f}$, und eine Differentialgleichung für $\tilde{f}$ ist automatisch eine Differentialgleichung für f_1, die man die Liouville-Gleichung nennt. Ohne die Voraussetzungen für den Satz von Liouville soll die Differentialgleichung für f_1 hergeleitet werden. Dies ist die verallgemeinerte Liouville-Gleichung.

2. *Die Herleitung der verallgemeinerten Liouville-Gleichung.* Die verallgemeinerte Liouville-Gleichung erhält man, wenn die Transformationen (2) die von den Anfangswerten x_0 abhängigen Lösungen eines Systems gewöhnlicher Differentialgleichungen sind

$$\dot{x}^i = K^i\left((x^1, \ldots, x^n), t\right), \qquad i = 1, 2, \ldots, n. \tag{10}$$

Dies wird abkürzend geschrieben als

$$\dot{x}^i = K^i(x, t). \tag{11}$$

Die Umformungen beruhen auf der folgenden Überlegung: Es sei g eine beliebige (differenzierbare) Funktion von x_0 und t, dann läßt sich mit der Transformation (6) eine Funktion $\tilde{g}$ von x und t definieren, für die gilt

$$\tilde{g}(x, t) = g\left(h^{-1}(x, t), t\right), \tag{12}$$

$$\tilde{g}\left(h(x_0, t), t\right) = g(x_0, t). \tag{13}$$

Hierfür erhält man mit der Kettenregel und mit

$$\frac{\partial h^i(x_0, t)}{\partial t} = K^i\big|_{x = h(x_0, t)}, \tag{14}$$

bei Verwendung der Summationskonvention

$$\begin{aligned} \frac{\partial}{\partial t} g(x_0, t) &= \frac{\partial}{\partial t} \tilde{g}\left(h(x_0, t), t\right) \\ &= \left.\frac{\partial \tilde{g}}{\partial t}\right|_{x = h(x_0, t)} + \left.\frac{\partial h^i}{\partial t} \frac{\partial \tilde{g}}{\partial x^i}\right|_{x = h(x_0, t)} = \left(\frac{\partial \tilde{g}}{\partial t} + K^i \frac{\partial \tilde{g}}{\partial x^i}\right)_{x = h(x_0, t)}. \end{aligned} \tag{15}$$

Dies kann man auch als Gleichung in den Variablen x und t lesen, wenn man sich die Variable x_0 mit (6) ersetzt denkt

$$\left.\frac{\partial}{\partial t} g(x_0, t)\right|_{x_0 = h^{-1}(x, t)} = K^i \frac{\partial \tilde{g}}{\partial x^i} + \frac{\partial \tilde{g}}{\partial t}. \tag{16}$$

Da $\tilde{f}$ gebildet wird aus einer Funktion $f(x_0)$, die unabhängig von t ist, erhält man aus (16) für $\tilde{f}$ die Differentialgleichung

$$\frac{\partial \tilde{f}}{\partial t} + K^i \frac{\partial \tilde{f}}{\partial x^i} = 0. \tag{17}$$

Multipliziert man diese Gleichung mit $\tilde{J}^{-1}$, ergibt sich

$$\begin{aligned} &\tilde{J}^{-1} \frac{\partial \tilde{f}}{\partial t} + \tilde{J}^{-1} K^i \frac{\partial \tilde{f}}{\partial x^i} \\ &\quad = \frac{\partial}{\partial t} (\tilde{J}^{-1} \tilde{f}) + K^i \frac{\partial}{\partial x^i} (\tilde{J}^{-1} \tilde{f}) - \tilde{f} \left(\frac{\partial}{\partial t} \tilde{J}^{-1} + K^i \frac{\partial}{\partial x^i} \tilde{J}^{-1} \right) = 0, \end{aligned} \tag{18}$$

bzw.

$$\frac{\partial}{\partial t} f_1 + K^i \frac{\partial}{\partial x^i} f_1 + f_1 \left(\frac{\partial \ln \tilde{J}}{\partial t} + K^i \frac{\partial}{\partial x^i} \ln \tilde{J} \right) = 0. \tag{19}$$

Mit (16) folgt hieraus

$$\frac{\partial}{\partial t} f_1 + K^i \frac{\partial}{\partial x^i} f_1 + f_1 \left. \frac{\partial \ln J}{\partial t} \right|_{x_0 = h^{-1}(x,\, t)} = 0. \tag{20}$$

Wenn man in der letzten Gleichung den Faktor bei f_1 aus (11) bestimmen kann, ohne ihn mit der Transformation (2) berechnen zu müssen, ist (20) die verallgemeinerte Liouville-Gleichung.

Sind die Ableitungen von $h^k(x_0, t)$ nach x_0^i und t vertauschbar, erhält man mit (14), der Kettenregel und den Rechenregeln für Determinanten

$$\frac{\partial}{\partial t} \ln J(x_0, t) = \left. \frac{\partial K^i}{\partial x^i} \right|_{x = h(x_0,\, t)}. \tag{21}$$

Die Umformungen, die zu dieser Gleichung führen, sind die gleichen, die beim Beweis des Satzes von Liouville durchgeführt werden (vgl. z. B. Chintschin[2]), Khilmi[3])).

Die bei (2) genannten Differenzierbarkeitsforderungen sind nötig, um die Vertauschbarkeit der Ableitungen von h nach x_0^i und t zu sichern. Mit den vorne genannten Einschränkungen ist es dafür hinreichend, die 2mal stetige Differenzierbarkeit von $K^i(x, t)$ nach x^j und t zu fordern (vgl. z. B. Kamke[4])). Die ausgeschlossene Punktmenge vom Maß Null soll sich nach Voraussetzung im Laufe der Zeit nicht ändern und ist durch $K^i(x, t)$ gegeben. Bei dem so eingeschränkten

$K^i(x, t)$ sind die Voraussetzungen für den Eindeutigkeitssatz von Lösungen für Systeme gewöhnlicher Differentialgleichungen erfüllt. Deshalb sind auch die Lösungen von (11) umkehrbar eindeutige Transformationen von x_0 auf x, wie es bei (2) vorausgesetzt wurde.

Setzt man (21) in (20) ein, erhält man die verallgemeinerte Liouville-Gleichung

$$\frac{\partial f_1}{\partial t} + K^i \frac{\partial}{\partial x^i} f_1 + f_1 \frac{\partial K^i}{\partial x^i} = 0, \tag{22}$$

die man auch in der Form

$$\frac{\partial f_1}{\partial t} + \frac{\partial}{\partial x^i} (K^i f_1) = 0, \tag{23}$$

schreiben kann. Die übliche Liouville-Gleichung läßt sich auch in der Form (23) schreiben, doch wird für sie $\partial K^i/\partial x^i = 0$ vorausgesetzt.

3. *Berechnung von J und $\tilde{J}$ in Spezialfällen.* Für die Umkehrbarkeit der Transformation (2) ist notwendig, daß J ungleich Null ist. Dies ist nach dem Satz von Liouville sicher erfüllt, da dann sogar J gleich eins ist. Aber auch ohne den Satz von Liouville, d.h. mit einer Abschwächung der Voraussetzung $\partial K^i/\partial x^i = 0$ läßt sich zeigen, daß J ungleich Null ist. Außerdem wird in manchen Anwendungen des Satzes von Liouville weniger benötigt, daß $J = \tilde{J} = 1$ ist, sondern es würde in diesen Fällen reichen, J oder $\tilde{J}$ überhaupt zu kennen, ohne vorher die Differentialgleichungen (11) lösen zu müssen. Dies ist nicht nur mit den Voraussetzungen des Satzes von Liouville, sondern auch im folgenden Spezialfall gegeben. Setzt man nämlich voraus, daß $\partial K^i/\partial x^i$ höchstens eine Funktion der Zeit t und nicht eine Funktion von x ist, erhält man für (21)

$$\frac{\partial}{\partial t} \ln J(x_0, t) = \left. \frac{\partial K^i}{\partial x^i} \right|_{x = h(x_0, t)} = c(t). \tag{24}$$

Diese Differentialgleichung läßt sich integrieren

$$\ln J(x_0, t) = \int_{t_0}^{t} c(t')\,\mathrm{d}t' + g(x_0). \tag{25}$$

Da für t gegen t_0 ln J gleich 0 werden muß, gilt

$$g(x_0) = 0. \tag{26}$$

Also ist J nur eine Funktion der Zeit

$$J(x_0, t) = \exp\left(\int_{t_0}^{t} c(t')\,\mathrm{d}t'\right). \tag{27}$$

die für jedes endliche t ungleich Null ist. Als Spezialfall folgt aus dieser Rechnung der Satz von Liouville: Mit $c(t) = 0$ ist $J = 1$, woraus sich die Invarianz des Maßes für alle t bei der Transformation (2) ergibt. Da nach (27) J nur eine Funktion von t ist, ist auch $\tilde{J}$ nur eine Funktion von t, also gilt

$$J = \tilde{J} = \exp\left(\int_{t_0}^{t} c(t')\,\mathrm{d}t'\right). \tag{28}$$

In dem Fall (24) sind also J und $\tilde{J}$ bekannt, auch wenn man nicht explizit die Lösungen (2) des Systems (11) kennt.

4. *Die Entropie der Verteilungsdichte* f_1. Die Funktion $c(t)$ spielt bei der zeitlichen Änderung der Entropie der Verteilungsdichte f_1 eine besondere Rolle. Die Entropie der Verteilungsdichte f_1 ist gegeben durch

$$S_t = -\int f_1 \ln f_1 \,\mathrm{d}x. \tag{29}$$

Mit (9) kann man dies schreiben als

$$S_t = -\int \tilde{J}^{-1}\tilde{f} \ln(\tilde{J}^{-1}\tilde{f})\,\mathrm{d}x = -\int \tilde{J}^{-1}\tilde{f} \ln \tilde{f}\,\mathrm{d}x + \int \tilde{J}^{-1}\tilde{f} \ln \tilde{J}\,\mathrm{d}x. \tag{30}$$

Führt man hier die Variablentransformation (2) durch, folgt

$$S_t = -\int f(x_0) \ln f(x_0)\,\mathrm{d}x_0 + \int f(x_0) \ln J\,\mathrm{d}x_0, \tag{31}$$

was man schreiben kann als

$$S_t = S_0 + \langle \ln J \rangle. \tag{32}$$

Mit der Voraussetzung (24) erhält man

$$S_t = S_0 + \int_{t_0}^{t} c(t')\,\mathrm{d}t'. \tag{33}$$

Die zeitliche Änderung der Entropie der Verteilung f_1 ist also gegeben durch die zeitliche Veränderung von $\langle \ln J \rangle$ und im Spezialfall (24) durch $c(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t} S_t = c(t). \tag{34}$$

Mit den Voraussetzungen des Satzes von Liouville ist $c(t)$ und damit die zeitliche Änderung von S_t gleich Null.

Betrachtet man als Beispiel ein System von N Massenpunkten, auf die neben üblichen konservativen Kräften noch Reibungskräfte der Art

$$(1/m)\,K = -\alpha v \tag{35}$$

wirken, ist

$$\frac{\partial K^i}{\partial x^i} = -3N\alpha. \tag{36}$$

Auch in dem etwas allgemeineren Fall, wenn die Werte α für die Teilchen verschieden sind, ist dies eine negative Konstante. Deshalb nimmt die Entropie der Verteilung $f_1(x, t)$ ab, während bei irreversiblen Prozessen normalerweise die Entropie einer Verteilung zunimmt. Dies ist kein Widerspruch zum zweiten Hauptsatz, da der Entropiesatz der Thermodynamik nicht einfach als Zunahme der Entropie einer Verteilung ausgesprochen werden kann. Man kann das Wesentliche schon bei einem einfachen Beispiel, dem gedämpften harmonischen Oszillator, erkennen: Hierfür lautet die verallgemeinerte Liouville-Gleichung

$$\frac{\partial f_1}{\partial t} + v\,\frac{\partial f_1}{\partial x} - (\alpha v + \beta x)\,\frac{\partial f_1}{\partial v} - \alpha f_1 = 0. \tag{37}$$

Die charakteristischen Differentialgleichungen dieser partiellen Differentialgleichung erster Ordnung

$$\frac{\mathrm{d}t}{\mathrm{d}s} = 1, \qquad \frac{\mathrm{d}x}{\mathrm{d}s} = v, \qquad \frac{\mathrm{d}v}{\mathrm{d}s} = -\alpha v - \beta x, \qquad \frac{\mathrm{d}f_1}{\mathrm{d}s} = \alpha f_1 \tag{38}$$

sind mit der zweidimensionalen Anfangsmannigfaltigkeit

$$t = 0, \qquad x = x_0, \qquad v = v_0, \qquad f_1 = f(x_0, v_0) \tag{39}$$

zu lösen. Eliminiert man mit der ersten Differentialgleichung in der üblichen Weise den Parameter s und löst mit

$$f_1 = f(x_0, v_0)\,\mathrm{e}^{\alpha t} \tag{40}$$

die letzte Differentialgleichung, bleiben nur noch die Differentialgleichungen des gedämpften harmonischen Oszillators. Mit $\omega = (\beta - \frac{1}{4}\alpha^2)^{\frac{1}{2}}$ lauten die Lösungen

$$x = \mathrm{e}^{-\frac{1}{2}\alpha t}\left[\left(\cos\omega t + \frac{\alpha}{2\omega}\sin\omega t\right)x_0 + \frac{1}{\omega}\sin\omega t\; v_0\right], \tag{41}$$

$$v = \mathrm{e}^{-\frac{1}{2}\alpha t}\left[\left(\frac{\alpha^2}{4\omega} + \omega\right)\sin\omega t\; x_0 + \left(\cos\omega t - \frac{\alpha}{2\omega}\sin\omega t\right)v_0\right], \tag{42}$$

deren Transformationsdeterminante $(\partial x/\partial x_0)(\partial v/\partial v_0) - (\partial x/\partial v_0)(\partial v/\partial x_0)$ in Übereinstimmung mit (28), (9) und (40) gegeben ist durch $e^{-\alpha t}$. Die nach den Parametern x_0, v_0 aufgelösten Lösungen

$$x_0 = e^{\frac{1}{2}\alpha t}\left[\left(\cos\omega t - \frac{\alpha}{2\omega}\sin\omega t\right)x - \frac{1}{\omega}\sin\omega t\, v\right], \tag{43}$$

$$v_0 = e^{\frac{1}{2}\alpha t}\left[\left(\frac{\alpha^2}{4\omega} + \omega\right)\sin\omega t x + \left(\cos\omega t + \frac{\alpha}{2\omega}\sin\omega t\right)v\right] \tag{44}$$

müssen in (40) eingesetzt werden. Wählt man als Verteilung $f(x_0, v_0)$ eine Gaußverteilung

$$f(x_0, v_0) \sim \exp(-c_1 x_0^2 - c_2 v_0^2), \tag{45}$$

sieht man, daß sich beim Einsetzen von (43) und (44) die Breite der Verteilung mit $e^{-\frac{1}{2}\alpha t}$ verändert, also abnimmt. Ohne den Faktor $\tilde{J}^{-1} = e^{\alpha t}$ in (40) würde diese Verringerung der Breite zu einer Abnahme der Gesamtwahrscheinlichkeit führen. In Übereinstimmung mit (34) und (36) nimmt also die Entropie der Verteilungsdichte f_1 ab, was die anschaulich klare Tatsache beschreibt, daß im Laufe der Zeit mit immer größerer Sicherheit die Werte x und v des gedämpften harmonischen Oszillators in der Umgebung der Null liegen.

5. *Folgerungen für die n-Zeiten BBGKY-Hierarchie.* In der statistischen Mechanik wird der bei (2) definierte stochastische Prozeß, der gar nicht so sehr „zufällig" ist, als Hilfskonstruktion verwendet, um andere stochastische Prozesse zu beschreiben, die verglichen mit (2) wirklich „zufällig" sind. Dies geschieht in der Weise, daß als Bildbereich nicht der gesamte R^n, sondern nur ein Teilraum niedrigerer Dimension verwendet wird, dessen Variablen mit x^r gekennzeichnet werden sollen. Die Schar von Zufallsvariablen ist dann

$$x^r = h^r(x_0, t), \tag{46}$$

wobei x_0 die Variablen des Gesamtsystems zur Zeit t_0 und x^r die Variablen des Teilsystems zur Zeit t sind. In Ref. 5 ist bei Verwendung des Satzes von Liouville die BBGKY-Hierarchie für die n-Zeiten Verteilungen solcher Prozesse hergeleitet worden. Bei den meisten dort durchgeführten Umformungen wurde weniger $J = 1$, als vielmehr überhaupt die Kenntnis von J oder $\tilde{J}$ benötigt. Solche Umformungen sind also auch im Spezialfall (24) möglich. Der Ausgangspunkt für die Aufstellung der n-Zeiten BBGKY-Hierarchie ist eine Distributionsdifferentialgleichung. Die hierfür nötigen Überlegungen lassen sich anhand einer weiteren Herleitung der verallgemeinerten Liouville Gleichung erläutern.

Die Funktion f_1 kann man mit einer δ Distribution f^* in der Form schreiben

$$f_1(x, t) = \tilde{J}^{-1}\tilde{f}(x, t) = \int \tilde{J}^{-1}(x', t)\,\delta(x - x')\tilde{f}(x', t)\,\mathrm{d}x'$$

$$= \int \delta(x - h(x_0, t))\,f(x_0)\,\mathrm{d}x_0 = \int f^* f(x_0)\,\mathrm{d}x_0. \tag{47}$$

Mit der Kettenregel und (14) erhält man aus

$$\frac{\partial}{\partial t}\int f^* g(x)\,\mathrm{d}x = \frac{\partial}{\partial t}\,g(h(x_0, t)) = \frac{\partial h^i}{\partial t}\,\frac{\partial g}{\partial x^i}\bigg|_{x=h(x_0,t)}$$

$$= K^i\,\frac{\partial g}{\partial x^i}\bigg|_{x=h(x_0,t)} = \left[\frac{\partial}{\partial x^i}(K^i g) - g\,\frac{\partial K^i}{\partial x^i}\right]_{x=h(x_0,t)}$$

$$= -\int g(x)\,K^i\,\frac{\partial}{\partial x^i}\,\delta(x - h(x_0, t))\,\mathrm{d}x$$

$$-\int g(x)\,\frac{\partial K^i}{\partial x^i}\,\delta(x - h(x_0, t))\,\mathrm{d}x \tag{48}$$

eine Differentialgleichung für f^*, die äußerlich so aussieht wie die verallgemeinerte Liouville Gleichung (22). Multipliziert man die Differentialgleichung für f^* mit $f(x_0)$ und integriert über x_0, ergibt sich die verallgemeinerte Liouville-Gleichung. Zur Aufstellung der n-Zeiten BBGKY-Hierarchie muß die Differentialgleichung für $\delta(x^r - h^r(x_0, t))$ aufgestellt werden. Die nötigen Umformungen unterscheiden sich von (48) nur dadurch, daß statt der Ableitungen nach allen Variablen von x nur die Ableitungen nach den Variablen x^r des Teilraums vorkommen. Deshalb ist klar, daß auch die n-Zeiten BBGKY-Hierarchie aufgestellt werden kann, wenn nicht der Satz von Liouville gilt und insbesondere auch wenn das Gesamtsystem nicht mit einer Hamiltonfunktion beschrieben werden kann.

Herrn Professor E. Richter danke ich für die vielen anregenden Gespräche.

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Vers une description non conservative de l'évolution en physique

Jean Fronteau
Départment de Physique
Université d'Orléans
45045 Orléans Cedex, France

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Abstract

The objective of this paper is to outline some applications of nonconservative forces in physics, with particular reference to thermodynamics.

After some generalities on particle optics, the author points out that the fundamental tool in this field, namely Liouville's theorem, has a much wider bearing than is currently believed, applicable indeed as it is to any dynamical system, conservative or not.

The importance of the Jacobian of evolution, which governs the time evolution of the measure in the dynamical space studied, leads the author to justify the introduction of the concept of "fine entropy" associated to any particle of the system. He shows in fact how this notion allows us to build, on a dissipative basis (purely dissipative to begin with) a thermodynamical theory of evolutive phenomena. He insists on the necessity, for him, to consider the evolutive aspect of phenomena as primordial, with regards to the probabilistic aspect.

A short incursion into Quantum Mechanics lays once again insistance on the necessity to study evolution wherever it appears. The author comes finally back to "fine Thermodynamics" and shows that it admits a relativistic covariant extension, compatible with macroscopic relativistic Thermodynamics.

The connection between the physical ideas presented in this work and recent studies on strong nonconservative interactions is indicated in the Foreword.

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Avant-propos.

Ce mémoire résume huit années de l'histoire d'une idée, et j'ai beaucoup hésité à l'écrire. En effet, il comporte une part d'autobiographie ; or ceci n'est pas un genre à la mode chez les Scientifiques puisque, bien au contraire, leur style s'est fait, ces dernières années, de plus en plus impersonnel. Aggravée souvent par l'usage d'une langue véhiculaire étrangère, cette dépersonnalisation de l'exposé est presque devenue le garant de l'objectivité scientifique ; on comprend donc, d'entrée de jeu, que toute forme de publication autobiographique risque de susciter bien des critiques. Ainsi, pourquoi faire un livre sur un sujet qui n'est pas traité complètement ? Les publications dans les revues scientifiques ne sont-elles pas suffisantes ? Au plan purement scientifique, pour les résultats acquis, il est clair que quelques articles suffisent. Cependant, si l'objectif est de décrire sur le vif le cheminement incertain d'une idée, ce livre a sans doute sa justification. L'écueil pédagogique est évident : l'exposé ne sera pas assez didactique ; on ne trouvera ici que des résultats fragmentaires regroupés autour d'un thème encore trop philosophique. Mon espoir serait pourtant d'amener le lecteur à dépasser ces imperfections techniques pour atteindre l'idée qui, à mon sens, est la chose importante que je dois essayer de faire partager. Autre écueil possible : celui des citations et des références. Le sujet que nous allons aborder ensemble est vaste ; il touche plusieurs domaines scientifiques traditionnels dont je ne pourrai présenter ni les résultats classiques ni les acquisitions récentes. J'espère que le lecteur saura reconnaître que ce n'est pas là procédé pour minimiser les travaux des autres. Voilà pour les références scientifiques. Reste le problème des remarques d'ordre autobiographique. Se battre pour faire admettre une idée suscite des soutiens inestimables et des oppositions parfois sévères, réactions qui sont toutes très importantes pour le chercheur. Il faudra donc que j'en fasse état, mais j'essaierai de le faire de façon aussi anonyme que possible. Il serait dommage de soulever ici des querelles de personnes.

Boissy-la-Rivière, août 1974.

I

Mécanique et Thermodynamique

Dans ce premier chapitre, je vais définir le problème qui me préocupe, et j'utiliserai à cet effet un langage presque dépourvu de mathématique afin d'essayer d'élargir quelque peu l'audience de l'exposé. J'espère que ceux qui tiennent à la forme mathématique ne seront cependant pas rebutés par ce chapitre, promesse leur étant faite que, dans la suite du livre, ils trouveront la justification rigoureuse — ainsi que le développement chronologique — des idées exposées.

Je vais beaucoup parler de la Thermodynamique et, puisque mon but est d'en présenter une vue nouvelle, il me faudra souligner l'intérêt d'une telle tentative par comparaison avec la pensée classique. On pourrait donc se proposer de faire tout d'abord une critique serrée et détaillée de la Thermodynamique traditionnelle, mais cela nous mènerait très loin et risquerait d'être vite fastidieux. J'emprunterai donc une autre voie, laquelle consistera à décrire cette sorte d'insatisfaction que j'ai toujours ressentie en présence de la formulation classique de la Thermodynamique et de la Mécanique statistique, et ce livre s'adressera surtout à ceux qui auront ressenti quelque chose de semblable.

L'objectif est de jeter un pont entre la Mécanique et la Thermodynamique ou — plus exactement — un nouveau pont, puisque tel est déjà le rôle de la Mécanique statistique. Il s'agit en fait de redonner au mot "thermodynamique" son sens étymologique, les phénomènes calorifiques étant décrits par une dynamique de I chaleur, de même que les phénomènes non calorifiques -par exemple le mouvement des planètes- sont décrits par la Dynamique classique. Dans une Mécanique nouvelle, englobant Mécanique classique et Thermodynamique, devrait évidemment figurer une grandeur du type entropie qui permettrait de distinguer les phénomènes calorifiques de ceux qui ne le sont pas. Nous allons montrer tout d'abord que la Mécanique traditionnelle porte en germe l'idée que nous venons d'énoncer.

La Mécanique classique étudie au premier chef le mouvement de ce qu'elle appelle les "points matériels", c'est-à-dire des mobiles qui ne sont pas trop petits (sinon la Mécanique quantique entre en scène), qui ne sont pas trop rapides (sinon c'est la Mécanique relativiste qui intervient), et qui ne tournent pas sur eux-mêmes. Le lecteur sait qu'on représente ces points matériels par des points géométriques affectés d'une masse. Etudier le mouvement de tels objets pose d'emblée le grave problème de la définition expérimentale du temps et de la masse, mais nous supposerons ici que cette difficulté est résolue. Nous saurons donc mesurer des positions, des temps et des masses. Ceci étant admis, qu'est-ce que comprendre la dynamique d'un mouvement ? Il s'agit depuis Newton, après avoir mesuré la variation temporelle de la position du mobile, de pouvoir la retrouver par le calcul en intégrant une équation différentielle de type imposé , à savoir :

$$m\frac{d^2\vec{Y}}{dt^2} = \vec{\mathcal{F}} \,, \qquad (1)$$

la force $\vec{\mathcal{F}}$ étant la traduction mathématique de l'influence du monde extérieur sur le point matériel de masse m , dont la position à l'instant t est $\vec{Y}$. La forme de $\vec{\mathcal{F}}$, elle, n'est pas imposée a priori. C'est l'intuition du physicien qui l'incite à essayer telle ou telle fonction $\vec{\mathcal{F}}$ afin de retrouver par le calcul, à l'aide de ce modèle, tel mouvement qu'il aura mesuré auparavant. L'exemple nous a été donné par Newton qui a imaginé, puis vérifié, la forme qu'il fallait donner à $\vec{\mathcal{F}}$ pour comprendre les lois du mouvement des planètes. Ceci est bien connu, de même que l'introduction de la notion d'énergie en Mécanique ; en multipliant la relation (1) par une variation infinitésimale de la position, on obtient l'égalité suivante, dont les deux membres ont la nature physique de ce qu'on est convenu d'appeler énergie :

$$\left(m\frac{d^2\vec{Y}}{dt^2}\right) . \, d\vec{Y} = \vec{\mathcal{F}} \, . \, d\vec{Y} \qquad (2)$$

Le membre de droite découle de l'influence du monde extérieur ; on l'interprétera donc comme l'énergie fournie par l'extérieur, δE^e , alors que le membre de gauche sera interprété comme l'énergie reçue par le mobile, δE^r. Cette double image satisfait le besoin de conservation inhérent à l'esprit de l'homme, puisque la relation (2) prend la forme :

$$\delta E^r = \delta E^e \quad , \tag{3}$$

qui consiste à dire qu'à chaque instant le mobile absorbe l'énergie que lui fournit le monde extérieur.

Paradoxalement, la difficulté provient de ce que, jusqu'à présent, les physiciens n'ont eu besoin que de modèles mécaniques relativement simples, lesquels ont permis d'écrire la conservation de l'énergie sous une forme apparemment plus plaisante mais sûrement moins générale que (3). Cette formulation restrictive a ses origines dans les travaux de Newton lui-même puisque, pour étudier la dynamique des planètes, il a suffi de choisir une force $\vec{\mathcal{F}}$ qui ne dépendait que de la position $\vec{Y}$ et qui, de plus, en dépendait de façon particulièrement pratique, à savoir comme le gradient d'une certaine fonction :

$$\vec{\mathcal{F}}(\vec{Y}) = -\text{grad}\ \Phi(\vec{Y}). \tag{4}$$

Par la suite, il s'est avéré que la plupart des problèmes que les physiciens ont abordés avec l'esprit mécaniste ont été résolus à l'aide de modèles du type précédent. Avec la restriction (4), les deux membres de la relation (3) deviennent intégrables $\left[\delta E^r = d\left(\frac{1}{2}\, m\, V^2\right) \ , \ \delta E^e = -\, d\, \Phi\right]$, ce qui signifie qu'il n'est plus nécessaire d'envisager la conservation de l'énergie à chaque instant, en suivant le mobile pas à pas, mais qu'on peut maintenant la considérer globalement, entre deux instants bien différents, et ce indépendamment du détail du trajet suivi. En introduisant le concept d'énergie cinétique, $E_{cin} = \frac{1}{2}\, m\, V^2$, on en arrive ainsi à la relation :

$$(E_{cin})_2 - (E_{cin})_1 = -\left[\Phi_2 - \Phi_1\right] \quad , \tag{5}$$

ce qui signifie toujours que l'énergie absorbée par le mobile est égale à l'énergie perdue par le monde extérieur dans son interaction avec ledit mobile. Malheureusement, le cas particulier (5) a fini par détrôner l'expression générale (3), l'usage faisant de (5) le vrai principe de conservation de l'énergie mécanique. Du même coup, c'est la Mécanique restreinte caractérisée par (4) et (5) que l'Histoire a baptisée Mécanique conservative; définition que nous admettrons d'ailleurs, pour nous conformer à l'usage, et malgré l'équivoque qu'elle entretient. Si l'on se souvient enfin que la formulation la plus élégante de la mécanique conservative reste, aux yeux des physiciens, celle qui a été proposée par Hamilton, on comprend le rôle de premier plan que joue le formalisme hamiltonien dans la Science contemporaine.

Il faut remarquer, cependant, que les mécaniciens ne s'en sont pas toujours tenus à la dynamique conservative définie ci-dessus. En effet, par exemple, pour comprendre le mouvement d'une particule électrisée passant dans l'entrefer d'un aimant, on a dû représenter le rôle du champ magnétique par une force $\vec{\mathcal{F}}$ dépendant de la vitesse de la particule, et non seulement de sa position. Mais il s'agissait encore d'un cas très particulier, la force en question n'apportant pas d'énergie, de telle sorte que le phénomène avait pu être absorbé par le formalisme hamiltonien. Mais il y a eu les fusées, et il a bien fallu comprendre leur dynamique, ce qui a exigé qu'on fasse appel à un modèle de type $\vec{\mathcal{F}} = (\vec{w}-\vec{v})\frac{dm}{dt}$, où $\vec{v}$ est la vitesse de la fusée et $\vec{w}$ la vitesse des gaz éjectés. Or, ce modèle, qui contient entre autres un terme parallèle à la vitesse du mobile, est de nature radicalement nouvelle, en ce sens que ce n'est pas un modèle conservatif. De toute façon, il y a toujours eu le problème des mobiles freinés par des frottements (par exemple, la pierre qui tombe en chute libre dans l'air, et non dans le vide), et les mécaniciens ont été amenés, pour en comprendre la dynamique, à introduire des modèles non conservatifs, dépendant de la vitesse ou de son carré. Or, puisque l'expérience prouve que le frottement "dissipe" l'énergie mécanique sous forme de chaleur (tel est le terme consacré par l'usage), les mécaniciens ont donc admis depuis fort longtemps qu'il existait un lien entre les modèles non conservatifs et les phénomènes calorifiques. Et pourtant cette idée n'avait jamais été exploitée à fond, d'où le besoin que nous avons ressenti de développer la mécanique dissipative ou, si l'on préfère, la mécanique non conservative, avec l'intention de l'associer à la science de la chaleur, c'est-à-dire à la Thermodynamique.

Traditionnellement, et malgré le modèle dynamique des frottements dont on vient de parler, l'étude de la chaleur n'appartient pas à la Mécanique. Obligés, pour comprendre les phénomènes calorifiques, de créer des concepts nouveaux, les physiciens ont du même coup créé une science nouvelle, la Thermodynamique. D'emblée cette science s'est définie à l'échelle macroscopique. Cela signifie que les objets dont elle étudie le comportement sont des systèmes, c'est-à-dire des ensembles d'objets microscopiques qu'elle renonce à individualiser. Ainsi, un gaz enfermé dans une enceinte constitue un système qu'il s'agit d'étudier globalement, sans se soucier du mouvement des diverses molécules du gaz. La Mécanique, elle, aurait considéré chaque molécule comme un point matériel à étudier individuellement. Malgré cette différence importante, c'est la Mécanique qui a fourni à la Thermodynamique son premier postulat, à savoir le principe de conservation de l'énergie :

$$\delta E^r = \delta E^e \quad . \tag{6}$$

A tout instant, le système considéré reçoit l'énergie que lui fournit le monde extérieur. Puisque la Mécanique, qui pourtant -on l'a vu- avait abordé le problème de la dissipation par frottement, n'avait pu expliquer les apports de chaleur, le premier rôle de la Thermodynamique devait donc être d'assumer cette notion nouvelle en la distinguant de l'énergie mécanique. Expérimentalement, on savait faire la distinction. Il fallait donc d'abord introduire des notations pour rendre compte des mesures ; δQ serait la chaleur fournie par l'extérieur, et $\delta\mathcal{T}$ l'apport d'énergie mécanique, d'où la forme thermodynamique de la conservation de l'énergie :

$$\delta E^r = \delta Q + \delta\mathcal{T} \quad . \tag{7}$$

Il reste à souligner que les thermodynamiciens, qui ont admis l'intégrabilité de $\delta E^r, (\delta E^r = dU)$, ont su se préserver du leurre de l'intégrabilité de la forme différentielle δQ , lequel eût entraîné la Thermodynamique dans une dégénérescence "conservative" du type (5).

L'expérience ayant prouvé que, même s'ils sont égaux en grandeur, un apport de chaleur et un apport d'énergie mécanique ne sont pas équivalents, il fallait pouvoir représenter par un nombre cette différence de nature. C'est la raison pour laquelle Clausius a introduit le quotient $\frac{\delta Q}{T}$, que nous appellerons l'apport d'entropie :

$$\delta S^e = \frac{\delta Q}{T} \quad , \tag{8}$$

T représentant la température absolue. Lorsqu'un système reçoit de l'énergie, seule la partie calorifique de ce transfert entraîne un apport d'entropie. La distinction devenait ainsi radicale entre δQ et $\delta\mathcal{T}$. Si maintenant le système évolue longtemps, et qu'on se propose de calculer l'apport total d'entropie correspondant, il faut considérer les variations instantanées successives, en suivant pas à pas la transformation. Heureusement, il existe un cas idéal où le calcul se simplifie. C'est le cas de ces évolutions très spéciales que la Thermodynamique a baptisées transformations réversibles, et qu'on a définies comme des processus infiniment lents, suites continues d'états d'équilibre, c'est-à-dire d'états qui seraient à tout jamais stables si le système était isolé du monde extérieur. Pour une évolution de ce type, la forme différentielle $\frac{\delta Q}{T}$ devient intégrable, et dès lors, on peut calculer par une banale soustraction l'apport total d'entropie entre deux états ε_1 et ε_2. La lettre S représentant la fonction entropie, cela s'écrit:

$$(9) \qquad \underset{\text{réversible}}{\left(\int_{\varepsilon_1}^{\varepsilon_2} \frac{\delta Q}{T}\right)} = S_2 - S_1 \quad .$$

En fait, ce cas n'est qu'une idéalisation, toute évolution vraie étant plus ou moins irréversible. Le second principe de la Thermodynamique consiste à reconnaître que les faits imposent toujours, pour une transformation irréversible, que l'apport total d'entropie soit inférieur à la variation correspondante calculée dans le cas idéal de la réversibilité :

$$(10) \qquad \underset{\text{irréversibie}}{\left(\int_{\varepsilon_1}^{\varepsilon_2} \frac{\delta Q}{T}\right)} < \underset{\text{réversible}}{\left(\int_{\varepsilon_1}^{\varepsilon_2} \frac{\delta Q}{T}\right)} = S_2 - S_1$$

Les physiciens ont toujours été intrigués par ce second principe et ses implications philosophiques, l'univers devant évoluer irréversiblement, selon ce principe, vers un état d'équilibre qui ne pourrait être que sa mort. Ils ont donc étudié de très près les deux relations (9) et (10), mais il semble qu'ils aient négligé le problème que pose la forme même du quotient $\frac{\delta Q}{T}$. Et pourtant ce quotient, que rien ne rattache directement aux autres concepts de la Physique et de la Mécanique, a quelque chose d'hétéroclite et d'un peu gênant. C'est cette constatation qui a porté l'auteur à rechercher une origine mécanique au $\frac{\delta Q}{T}$ de la Thermodynamique.

Chercher dans la Mécanique les racines de la Thermodynamique n'est pas une idée nouvelle, puisque tel est le rôle que s'est assigné -et avec succès- la Mécanique statistique : dans cet esprit, tout système de la Thermodynamique est conçu comme un ensemble de points matériels au sens de la Mécanique, et il s'agit de retrouver les principes de la Thermodynamique à partir des lois de la Mécanique et des théorèmes de Probabilités régissant le comportement de systèmes constitués d'une multitude de points matériels. La Mécanique statistique n'a pas rencontré de difficultés particulières à propos de la conservation de l'énergie. En effet, puisque c'est une loi qui, d'après la Mécanique, est valable pour chaque élément du système, on conçoit facilement qu'on la retrouve pour le système entier. La Mécanique statistique s'est donc attachée à interpréter le second principe de la Thermodynamique, c'est-à-dire la double relation (10). C'est à cet effet que Boltzmann a introduit sa fonction H, que nous noterons ici H^B. Pour mémoire, et pour souligner la difficulté du problème sans entrer pour autant dans des détails qui seraient inutiles dans ce chapitre, rappelons quelle est l'allure de cette fonction définie par une intégrale portant sur une certaine densité de probabilité ρ :

$$H^B = \int_\Gamma \rho \,\mathrm{Log}\, \rho \quad dX \tag{11}$$

Boltzmann a ensuite démontré que cette fonction H^B et la fonction entropie des thermodynamiciens, S, avaient un certain nombre de propriétés en commun, lesquelles ont justifié l'audacieuse et géniale assimilation que Boltzmann a faite de ces deux grandeurs, à un coefficient de proportionnalité près :

$$S = - k \, H^B \tag{12}$$

Malheureusement, le fait que deux grandeurs aient certaines propriétés communes n'implique pas que ces grandeurs soient identiques. Aussi, même si l'idée de Boltzmann est exacte -comme nous nous appliquerons à le prouver dans les chapitres qui suivent- , une identification sur la seule base de propriétés communes laisse le chercheur un peu insatisfait. C'est pourquoi nous allons essayer d'expliquer, sur une même base mécanique, la double forme que la Physique a donnée à la notion d'entropie : pourquoi ce quotient $\frac{\delta Q}{T}$, pourquoi cette fonction H^B , et pourquoi cette relation (12) entre les deux aspects de l'entropie ? Bref, notre livre est une tentative pour habiliter la Mécanique à traiter un problème qui, actuellement, n'est pas de son ressort, à savoir les échanges de chaleur. Le prix à payer -à notre avis- est de sortir de la Mécanique conservative et d'accepter une certaine classe de forces $\vec{\mathcal{F}}$ dépendant des vitesses. Notons qu'on s'en tiendra à une dynamique de points matériels, les mobiles en rotation sur eux-mêmes n'ayant pas encore été introduits dans la théorie.

III

Le théorème de Liouville

X étant un vecteur à n composantes réelles

$X \in \mathbb{R}^n \quad , \quad X = (x^{(1)}, x^{(2)}, \ldots\ldots\ldots\ldots x^{(n)}),$

F une fonction à valeurs dans $\mathbb{R}^n$

$F = (f^{(1)}, f^{(2)}, \ldots\ldots\ldots\ldots f^{(n)}),$

et t une variable réelle qui, très souvent, représentera le temps, un système différentiel du premier ordre s'écrit

$$(1) \qquad \frac{dX}{dt} = F(X,t)$$

c'est-à-dire, en projection sur les n axes de la base choisie pour $\mathbb{R}^n$,

$$\begin{cases} \dfrac{dx^{(1)}}{dt} = f^{(1)}(x^{(1)}, x^{(2)}, \ldots\ldots\ldots\ldots x^{(n)}, t) \\ \dfrac{dx^{(2)}}{dt} = f^{(2)}(x^{(1)}, x^{(2)}, \ldots\ldots\ldots\ldots x^{(n)}, t) \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \dfrac{dx^{(n)}}{dt} = f^{(n)}(x^{(1)}, x^{(2)}, \ldots\ldots\ldots\ldots x^{(n)}, t) \end{cases} .$$

On sait que l'importance des systèmes différentiels du premier ordre tient à ce que tout système différentiel, d'ordre quelconque, peut être transformé en un système du premier ordre qui lui est équivalent. Ceci étant dit, nous nous proposons de rappeler un théorème très important qui a été démontré par Liouville en 1838.[1]

Plaçons-nous dans le cas (très courant) où le système [1] admet pour tout t une solution unique

$$X_t = X(X_o,t) \quad ,$$

X_o représentant les conditions initiales

$$X_o = X(X_o,0) \quad ,$$

et considérons le déterminant fonctionnel

$$J_t = \frac{D[X_t]}{D[X_o]} = \frac{D[X(X_o,t)]}{D[X_o]} = J(X_o,t) \quad .$$

Le théorème de Liouville porte sur la dérivée de ce jacobien J_t:

$$\frac{d\,J_t}{dt} = \lim_{h \to 0} \frac{J_{t+h} - J_t}{h} \quad .$$

Grâce à la relation suivante, qui nécessite qu'on exprime X_{t+h} en fonction de X_t,

$$J_{t+h} = \frac{D[X_{t+h}]}{D[X_o]} = \frac{D[X_{t+h}]}{D[X_t]} \cdot \frac{D[X_t]}{D[X_o]} = \frac{D[X_{t+h}]}{D[X_t]} \cdot J_t \quad ,$$

la définition de J_t devient :

$$\frac{d\,J_t}{dt} = \lim_{h \to 0} J_t \frac{\frac{D[X_{t+h}]}{D[X_t]} - 1}{h}$$

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[1] *J. LIOUVILLE. Journal de Math. pures et appliquées* *3*, *342 (1838)*

ou :

$$\frac{d\,J_t}{dt} = J_t \lim_{h \to 0} \frac{\dfrac{D\left[X_{t+h}\right]}{D\left[X_t\right]} - 1}{h} \quad .$$

Pour exprimer X_{t+h} en fonction de X_t et calculer le déterminant $\frac{D\left[X_{t+h}\right]}{D\left[X_t\right]}$, h étant un accroissement arbitrairement petit, utilisons le développement de X_{t+h} en ne gardant que les deux premiers termes (la suite du calcul montrera que cela suffit) :

$$X_{t+h} = X_t + h\,\frac{dX_t}{dt} \quad .$$

X_t étant solution du système différentiel [1], il vient :

$$X_{t+h} = X_t + h\,F\left[X_t,\ t\right] \quad .$$

Prenons le temps d'écrire ceci en projection sur les axes de $\mathbb{R}^n$:

$$\begin{aligned}
x_{t+h}^{(1)} &= x_t^{(1)} + h\,f^{(1)}\left[x_t^{(1)},\ x_t^{(2)},\ \ldots\ldots\ldots\ x_t^{(n)},\ t\right] \\
x_{t+h}^{(2)} &= x_t^{(2)} + h\,f^{(2)}\left[x_t^{(1)},\ x_t^{(2)},\ \ldots\ldots\ldots\ x_t^{(n)},\ t\right] \\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\
x_{t+h}^{(n)} &= x_t^{(n)} + h\,f^{(n)}\left[x_t^{(1)},\ x_t^{(2)},\ \ldots\ldots\ldots\ x_t^{(n)},\ t\right]
\end{aligned}$$

Il vient alors :

$$\frac{D\left[X_{t+h}\right]}{D\left[X_t\right]} = \begin{vmatrix}
\dfrac{\partial x_{t+h}^{(1)}}{\partial x_t^{(1)}} & \dfrac{\partial x_{t+h}^{(1)}}{\partial x_t^{(2)}} & \ldots\ldots\ldots & \dfrac{\partial x_{t+h}^{(1)}}{\partial x_t^{(n)}} \\
\dfrac{\partial x_{t+h}^{(2)}}{\partial x_t^{(1)}} & \dfrac{\partial x_{t+h}^{(2)}}{\partial x_t^{(2)}} & \ldots\ldots\ldots & \dfrac{\partial x_{t+h}^{(2)}}{\partial x_t^{(n)}} \\
\ldots\ldots & \ldots\ldots & \ldots\ldots\ldots & \ldots\ldots \\
\dfrac{\partial x_{t+h}^{(n)}}{\partial x_t^{(1)}} & \dfrac{\partial x_{t+h}^{(n)}}{\partial x_t^{(2)}} & \ldots\ldots\ldots & \dfrac{\partial x_{t+h}^{(n)}}{\partial x_t^{(n)}}
\end{vmatrix}$$

c'est-à-dire :

$$\frac{D\left[X_{t+h}\right]}{D\left[X_t\right]} = \begin{vmatrix} 1 + h \dfrac{\partial f^{(1)}}{\partial x_t^{(1)}} \left[X_t, t\right] ; & h \dfrac{\partial f^{(1)}}{\partial x_t^{(2)}} \left[X_t, t\right] & \ldots\ldots & h \dfrac{\partial f^{(1)}}{\partial x_t^{(n)}} \left[X_t, t\right] \\ h \dfrac{\partial f^{(2)}}{\partial x_t^{(1)}} \left[X_t, t\right] ; & 1 + h \dfrac{\partial f^{(2)}}{\partial x_t^{(2)}} \left[X_t, t\right] & \ldots\ldots & h \dfrac{\partial f^{(2)}}{\partial x_t^{(n)}} \left[X_t, t\right] \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ h \dfrac{\partial f^{(n)}}{\partial x_t^{(1)}} \left[X_t, t\right] ; & h \dfrac{\partial f^{(n)}}{\partial x_t^{(2)}} \left[X_t, t\right] & \ldots\ldots & 1 + h \dfrac{\partial f^{(n)}}{\partial x_t^{(n)}} \left[X_t, t\right] \end{vmatrix}$$

En négligeant les termes en h d'ordre supérieur à 1, il reste :

$$\frac{D\left[X_{t+h}\right]}{D\left[X_t\right]} = 1 + h \sum_{\ell=1}^{n} \frac{\partial f^{(\ell)}}{\partial x_t^{(\ell)}} \left[X_t, t\right] .$$

On reconnaît la divergence du champ de vecteurs F, d'où :

$$\frac{D\left[X_{t+h}\right]}{D\left[X_t\right]} = 1 + h \operatorname{div} F \left[X_t, t\right] .$$

L'expression de la dérivée $\frac{d J_t}{dt}$ devient alors :

$$\frac{dJ_t}{dt} = J_t \lim_{h \to 0} \frac{h \operatorname{div} F \left[X_t, t\right]}{h} = J_t \operatorname{div} F \left[X_t, t\right] .$$

Nous retiendrons ce résultat sous la forme

$$\boxed{\frac{d}{dt} \operatorname{Log} J_t = \operatorname{div} F}$$

C'est le théorème de Liouville.

On remarque tout de suite que, si la divergence est identiquement nulle, J est une constante. On calcule alors la valeur de cette constante à l'instant initial, et l'on trouve :

$$J_o = J(X_o, 0) = \frac{D\left[X(X_o, o)\right]}{D\left[X_o\right]} = \frac{D\left[X_o\right]}{D\left[X_o\right]} = 1$$

Ainsi, une divergence identiquement nulle implique $J_t \equiv 1$; or la réciproque est évidente. On retiendra donc l'équivalence de ces deux propriétés :

$$\boxed{\mathrm{div}\ F \equiv 0 \Longleftrightarrow J_t \equiv 1}$$

Le lecteur aura déjà fait le rapprochement entre ce jacobien J_t identiquement égal à 1 (pour div $F \equiv 0$) et le fameux déterminant des matrices optiques qui, lui aussi, est toujours égal à 1. En effet, en optique corpusculaire, les traces projetées sont déterminées —— souvenons-nous du cas du champ magnétique quadrupolaire —— par des équations différentielles du second ordre dans lesquelles ne figure pas la dérivée première $\frac{dz}{ds}$, c'est-à-dire des équations de la forme

$$\frac{d^2z}{ds^2} + K(s)\, z = 0,$$

où K(z) est une fonction de s qui dépend du champ considéré. Cette équation est équivalente au système suivant, où z et z' sont alors deux variables indépendantes :

$$\begin{cases} \dfrac{dz}{ds} = z' \\ \dfrac{d}{ds}(z') = -K(s)\, z \end{cases}$$

Calculons la divergence.

$$\mathrm{div}\ F = \frac{\partial}{\partial z}(z') + \frac{\partial}{\partial z'}\left[-K(s)z\right] \quad .$$

z et z' étant indépendants, la divergence est identiquement nulle, ce qui implique $J_s \equiv 1$. Or, le système étant linéaire, sa solution s'écrit :

$$\begin{bmatrix} z_s \\ z'_s \end{bmatrix} = \begin{pmatrix} A_s & B_s \\ C_s & D_s \end{pmatrix} \begin{bmatrix} z_o \\ z'_o \end{bmatrix}$$

et le jacobien J_s, d'après sa définition

$$J_s = \frac{D\left[z_s\ ,\ z'_s\right]}{D\left[z_o\ ,\ z'_o\right]} \quad ,$$

est justement égal au déterminant de la matrice optique. L'affaire est réglée.

J'ai affirmé, il y a quelques lignes, que la dérivée $\frac{dz}{ds}$ ne figurait pas dans les équations différentielles des trajectoires projetées de l'optique corpusculaire. Autrement dit, il n'y apparaît pas de terme de frottement, lequel serait en $\frac{dz}{ds}$; c'est qu'en effet la dynamique des particules chargées soumises à un champ magnétique est une dynamique conservative. Cette remarque nous amène tout naturellement à la formulation hamiltonienne de la Mécanique, selon laquelle le mouvement de tout système dynamique conservatif est régi par les équations

$$\left\{\begin{array}{l} \dfrac{dq^{(\ell)}}{dt} = \dfrac{\partial \mathcal{H}}{\partial p^{(\ell)}} \\[2ex] \dfrac{dp^{(\ell)}}{dt} = - \dfrac{\partial \mathcal{H}}{\partial q^{(\ell)}} \end{array}\right. \qquad \ell = 1,\ 2 \ \ldots\ldots\ldots\ L,$$

dans lesquelles les $q^{(\ell)}$ sont les L paramètres repérant la configuration du système, et les $p^{(\ell)}$ les L moments conjugués, $H = \mathcal{H}(p^{(\ell)}, q^{(\ell)}, t)$ étant l'hamiltonien du système matériel considéré. Or ces équations d'Hamilton constituent un système de 2 L équations différentielles du premier ordre. La divergence associée se calcule très simplement;

$$\operatorname{div} F = \sum_{\ell=1}^{L} \left[\frac{\partial}{\partial q^{(\ell)}} \left(\frac{\partial \mathcal{H}}{\partial p^{(\ell)}}\right) + \frac{\partial}{\partial p^{(\ell)}} \left(- \frac{\partial \mathcal{H}}{\partial q^{(\ell)}}\right)\right] \quad ,$$

et l'on trouve 0 identiquement. Le jacobien correspondant est donc toujours égal à 1.

$$\boxed{\begin{array}{l}\text{Toute formulation}\\ \text{hamiltonienne}\end{array} \quad \Longrightarrow \quad \frac{D\left[p_t^{(\ell)}\ ,\ q_t^{(\ell)}\right]}{D\left[p_o^{(\ell)}\ ,\ q_o^{(\ell)}\right]} \equiv 1}$$

Nous aurons beaucoup à dire sur le résultat précédent. Commençons par son interprétation géométrique. Notons Γ l'espace $\mathbb{R}^n$, et appelons $\mathcal{D}$ tout domaine compact de Γ . La solution $X_t = X(X_o, t)$ du système différentiel [1] est une application φ_t

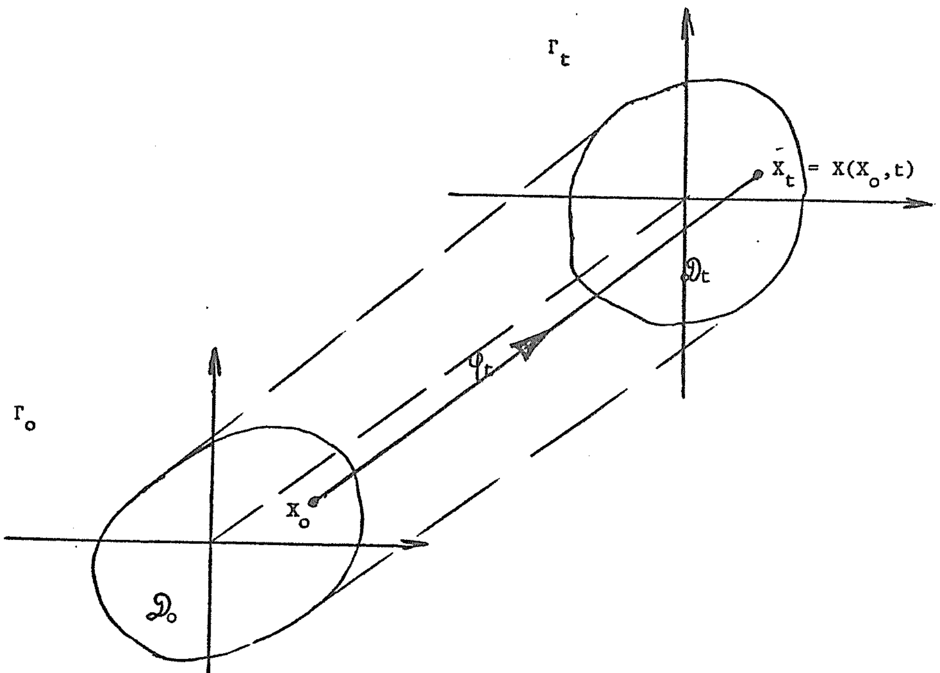
$$X_o \xrightarrow{\varphi_t} X_t$$

qu'on appelle flot, ou évolution temporelle, et qui transforme Γ et $\mathcal{D}$ point par point :

$$\Gamma_o \xrightarrow{\varphi_t} \Gamma_t$$

$$\mathcal{D}_o \xrightarrow{\varphi_t} \mathcal{D}_t \quad .$$

Puisqu'il n'est pas question de représenter les n dimensions de $\mathbb{R}^n$, dessinons Γ comme s'il s'agissait d'un plan. Nous obtenons alors le schéma suivant, qui est la reproduction de celui qui a été utilisé au chapitre précédent pour représenter la marche d'un faisceau de particules.



La mesure de $\mathcal{D}_t$ (son hypervolume, dans $\mathbb{R}^n$) est l'intégrale :

$$\mathcal{M}es\,(\mathcal{D}_t) = \int_{\mathcal{D}_t} dX_t ,$$

où dX_t est l'élément d'hypervolume $dX_t = dx_t^{(1)}\,dx_t^{(2)}\,dx_t^{(3)}\,\ldots\ldots\ldots\,dx_t^{(n)}$.

L'application φ_t définit un changement de variables, t étant alors un paramètre ;

$$X_t = X\,[X_o, t] .$$

Passons aux variables X_o. L'intégrale devient, d'après Jacobi,

$$\mathcal{M}es\,(\mathcal{D}_t) = \int_{\mathcal{D}_o} \frac{D\,[X_t]}{D[X_o]}\,dX_o ,$$

et le jacobien de la transformation est justement le déterminant de Liouville $J_t = J(X_o, t)$.

$$\mathcal{M}es\,(\mathcal{D}_t) = \int_{\mathcal{D}_o} J(X_o, t)\,dX_o .$$

Ainsi, c'est le jacobien de Liouville qui régit la variation temporelle de la mesure dans Γ. Nous retiendrons ceci sous forme différentielle :

$$\boxed{dX_t = J_t\,dX_o} .$$

En conséquence,

$$\boxed{J_t \equiv 1 \quad \Longrightarrow \quad \mathcal{M}es\,(\mathcal{D}_t) \equiv \mathcal{M}es\,(\mathcal{D}_o)}$$

c'est-à-dire que, pour un système conservatif, les domaines $\mathcal{D}$ gardent une mesure constante bien qu'ils se déforment lorsque le temps s'écoule.

On reconnaît la propriété énoncée au chapitre précédent pour les surfaces fermées représentant un faisceau, mais elle est devenue maintenant une propriété de caractère extrêmement général, qui est l'une des bases de la mécanique statistique traditionnelle.

Avant d'aborder au chapitre suivant la critique de l'usage restrictif que l'on fait d'ordinaire du théorème de Liouville, il reste à formuler deux remarques. Nous noterons d'abord que l'invariance de la mesure de $\mathfrak{D}_t$ par le flot φ_t est un théorème de conservation plus large que la conservation de l'énergie totale du système. En effet, on a $\mathcal{M}es(\mathfrak{D}_t) \equiv \mathcal{M}es(\mathfrak{D}_o)$ dès qu'un hamiltonien H existe pour l'ensemble des forces agissant sur le système, lors même que le champ de forces varie avec le temps, ce qui entraîne $H = \mathcal{H}(p^{(\ell)}, q^{(\ell)}, t) \neq$ Cste. Il s'ensuit en général une ambiguïté sur le sens du mot "conservatif", lequel peut être utilisé lorsque c'est H, ou lorsque c'est la mesure des domaines $\mathfrak{D}$, que le mouvement conserve. Nous le définirons ici par l'invariance de la mesure de tout $\mathfrak{D}$. En notant par $\not{H}$ la non-existence d'un hamiltonien pour l'ensemble des forces, nous résumerons la situation par le tableau suivant, dans lequel les qualificatifs "dissipatif" et "non conservatif" sont définis synonymes. Par la suite, si nous avons besoin de distinguer le signe du phénomène, nous parlerons de "dissipation" lorsqu'il y aura perte d'énergie, et d' "anti-dissipation" lorsqu'il y aura absorption d'énergie sous forme non hamiltonienne.

$H = \mathcal{H}(p^{(\ell)}, q^{(\ell)})$	$H = C^{ste}$	$\mathcal{M}es(\mathfrak{D}) = C^{ste}$	systèmes conservatifs
$H = \mathcal{H}(p^{(\ell)}, q^{(\ell)}, t)$	$H \neq C^{ste}$	$\mathcal{M}es(\mathfrak{D}) = C^{ste}$	
$\not{H}$	$\not{H}$	$\mathcal{M}es(\mathfrak{D}) \neq C^{ste}$	systèmes non conser- vatifs ou "dissipatifs

Nous remarquerons pour terminer que le théorème de Liouville n'est rien d'autre que l'équation de continuité dans $\Gamma = \mathbb{R}^n$. Pour le vérifier, admettons qu'on sache définir, à l'instant initial, une densité d'états $\rho_o = \rho(X_o)$ en tout point $X_o \in \Gamma_o$. Le flot φ_t lui fait correspondre en $X_t \in \Gamma_t$ une densité d'états de la forme :

$$\rho_t = \rho(X_o) \, \mathscr{R}(X_t, t) \quad .$$

En effet, si $J_t = \dfrac{D[X_t]}{D[X_o]}$ est différent de zéro, on peut inverser $X_t = X(X_o, t)$, ce qui fournit $X_o = X^{-1}(X_t, t)$, d'où successivement :

$$dX_t = J_t \, dX_o = J(X_o, t) \, dX_o = J\left[X^{-1}(X_t, t), t\right] dX_o = \mathcal{J}(X_t, t) \, dX_o$$

Puisque les états intérieurs à dX_o se retrouvent dans dX_t, la densité se comporte comme l'inverse de l'élément d'hypervolume $dX_t = J_t \, dX_o$;en d'autres termes,

$$\rho_t = \frac{\rho_o}{J_t}$$

d'où :

$$\rho_t = \frac{\rho(X_o)}{\mathcal{J}(X_t,t)} = \rho(X_o) \; \mathfrak{R}(X_t,t) \quad .$$

Le théorème de Liouville ,

$$\frac{d}{dt} \operatorname{Log} J_t = \operatorname{div} F \quad ,$$

s'écrit donc également :

$$\frac{d}{dt} \operatorname{Log} \rho_t = - \operatorname{div} F$$

ou

$$\frac{d}{dt} \operatorname{Log} \mathfrak{R}(X_t,t) = - \operatorname{div} F(X_t,t) \; ,$$

c'est-à-dire :

$$\frac{\partial}{\partial t} \operatorname{Log} \mathfrak{R}(X_t,t) + \left[\operatorname{grad} \operatorname{Log} \mathfrak{R}(X_t,t)\right] . \frac{dX_t}{dt} + \operatorname{div} F(X_t, t) = 0$$

$$\frac{\partial}{\partial t} \mathfrak{R}(X_t,t) + \left[\operatorname{grad} \mathfrak{R}(X_t,t)\right] . \; F(X_t,t) + \mathfrak{R}(X_t,t) \operatorname{div} F(X_t,t) = 0 \quad .$$

En résumé,

$$\boxed{\frac{\partial \rho_t}{\partial t} + \operatorname{div} (\rho_t F) = 0} \quad , \text{ avec } F = \frac{dX_t}{dt}$$

On reconnaît la forme de l'équation de continuité, écrite en suivant le flot φ_t. On notera qu'il ne s'agit pas seulement ici de l'équation de continuité dans $\mathbb{R}^3$, qui est d'usage courant, mais de l'équation de continuité dans l'espace des états, $\Gamma = \mathbb{R}^n$, associé à tout système différentiel.

IV

Evolution et Stabilité

Si l'on consulte un ouvrage de physique ou de mécanique statistique, la probabilité est encore très grande aujourd'hui pour qu'on n'y trouve pas le théorème de Liouville énoncé et démontré comme au chapitre précédent. Le théorème de Liouville, pour la plupart des physiciens, c'est la conservation des volumes dans l'espace des phases de la Mécanique hamiltonienne. Autrement dit, c'est la cas particulier :

$$\operatorname{div} F \equiv 0 \quad , \quad J_t \equiv 1 \quad , \quad \mathcal{M}es(\mathcal{D}_t) \equiv \mathcal{M}es(\mathcal{D}_0) \text{ pour tout } \mathcal{D} .$$

Après avoir utilisé ce résultat pendant plusieurs années sans chercher à en savoir plus, il m'a semblé en 1964 que cette loi de conservation ne pouvait être qu'un cas particulier d'une loi d'évolution plus générale. La référence au mémoire original de Liouville [1] se trouvant chez Tolman[2] (qui ne l'utilise d'ailleurs pas explicitement), il m'a été facile de retrouver ce que j'ai alors appelé le théorème "vrai", c'est - à - dire la forme générale :

$$\frac{d}{dt} \operatorname{Log} J_t = \operatorname{div} F,$$

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[1] *J.LIOUVILLE . Journal de Math.pures et appliquées 3, 342(1838)*

[2] *R.C.TOLMAN . The principles of Statistical mechanics, Clarendon Press, Oxford (1938) [cf page 49]*

avec div F non identiquement nulle. Mais je continuais à ne pas comprendre pourquoi les auteurs ne faisaient jamais appel à cette forme originelle. Pourquoi tenait-on tellement au cas particulier, au point d'en oublier le cas général ? Car c'est bien ce dont il s'agissait : les physiciens, à force de travailler dans l'hypothèse conservative, avaient oublié l'énoncé général du théorème de Liouville. Pour s'en convaincre, il suffit de vérifier que ceux qui ont récemment utilisé le théorème "vrai", l'ont d'abord énoncé et démontré comme une extension du théorème de Liouville : la démonstration de S.Guiaşu (que je ne connaissais pas en 1965) date de 1962[1], celle de D.Kh.Morozov date de 1972[2]; V.P.Maslov en parle même comme d'un tout autre théorème, qu'il appelle le lemme de Sobolev[3]. Heureusement l'affaire est en cours de régularisation. V.I.Arnold , par exemple, énonce le théorème de Liouville sous son vrai nom et sous sa forme générale[4]. Le lecteur pensera peut-être que je donne trop d'importance à un point de terminologie : puisque le théorème existe, peu importe le nom qu'on lui octroie. J'acquiescerais s'il ne s'agissait que de cela. Mais, comme je l'ai déjà dit, c'est le théorème lui-même qui avait été oublié, et cet oubli cachait le fait suivant, qui est de la plus haute importance, et sur lequel nous nous étendrons dans tout ce livre : la physique orthodoxe contemporaine est une physique conservative ; tout modèle non conservatif, tout modèle dissipatif, est radicalement exclu des théories fondamentales. Pour le physicien orthodoxe, point n'est besoin de parler de la forme générale du théorème de Liouville, laquelle ne peut s'appliquer qu'à des modèles rejetés a priori. Là encore, les choses sont en train de changer (nous le montrerons plus loin) et les physiciens ne sont plus aussi intransigeants qu'il y a dix ans. Les termes que je viens d'employer ne sont donc plus rigoureusement exacts. Bien qu'ils soient trop catégoriques aujourd'hui, je les maintiendrai pour souligner l'impression d'étouffement que j'ai ressentie lorsqu'à partir de 1965 j'ai essayé de parler de modèles dissipatifs dans un milieu de Physique orthodoxe.

. L'idée était pourtant passionnante. L'une des formes élémentaires de l'Evolution n'est-elle pas la formation et la destruction d'agglomérats, et peut-on s'empêcher de penser à la genèse de toutes les structures matérielles ? Les noyaux se sont formés ; il a fallu pour cela que des nucléons s'agglutinent.

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[1] *S.GUIAŞU. C.R.Ac.Sciences de Roumanie 12, 1087 (1962)*

[2] *D.Kh.MOROZOV. Soviet physics JETP 35, 902(1972)*

[3] *V.P.MASLOV. Théorie des perturbations et méthodes asymptotiques. Dunod-Gauthier-Villars (1972) [voir page 214]*

[4] *V. ARNOLD. Equations différentielles ordinaires, Editions Mir, Moscou (1974) [voir page 196]*

Puis, lorsque les noyaux ont capturé des électrons périphériques, ce fut encore une forme d'agrégation. Ensuite, les molécules se sont formées par assemblage d'atomes, et pour parvenir aux organismes vivants, il a d'abord fallu que se constituent les macromolécules. A l'autre bout de la chaîne de l'univers, on retrouve le même fait : les planètes sont groupées, les étoiles aussi, les galaxies également. Or, comment imaginer que tous ces astres ont toujours été assemblés ainsi, de toute éternité ? Comment ne pas ressentir le besoin de comprendre le phénomène dynamique d'agglutinement, et son inverse, la désagrégation Ceci dit, je me garderai bien d'essayer de définir de façon plus philosophique ce que l'Homme entend par Evolution. En tant que physicien, je pense m'être déjà beaucoup avancé sur ce terrain incertain en introduisant, comme je viens de le faire, une notion générale d'évolution synonyme d'agglutinement et de désagrégation. Par la suite, j'essaierai au contraire de rapprocher ce concept trop vague des grandeurs précises qui sont familières aux physiciens.

Le lecteur aura déjà compris le rôle primordial que peut jouer le théorème de Liouville. Sous sa forme générale,

$$\frac{d}{dt} \operatorname{Log} \rho_t = - \operatorname{div} F ,$$

n'associe-t-il pas, en effet, un certain type d'agglutinement ou de désagrégation, que mesure la variation de la densité d'états dans $\Gamma = \mathbb{R}^n$, à un certain type de phénomènes physiques, à savoir les phénomènes non conservatifs ? Alors, comment refuser d'envisager l'hypothèse suivante qui vient immédiatement à l'esprit : l'Evolution est due aux phénomènes dissipatifs, et les modèles conservatifs ne peuvent décrire qu'une sorte de repos entre des périodes évolutives. Un point délicat doit être souligné dès maintenant. La densité ρ_t, dont la variation est une mesure de l'Evolution, est la densité dans l'espace des états, Γ, du système différentiel considéré. Si ce système résulte d'une description dynamique (qui est du second ordre différentiel), l'espace Γ ne sera pas l'espace de configuration $\mathbb{R}^L$ (dans lequel nous vivons si $L = 3$) mais l'espace des positions et des vitesses, $\mathbb{R}^{2L}$, et un agglutinement dans $\mathbb{R}^{2L}$ n'entraînera pas nécessairement un agglutinement dans $\mathbb{R}^L$. Passer de $\mathbb{R}^{2L}$ à $\mathbb{R}^L$ ne sera pas chose facile.

Pour la dynamique d'un système à une dimension ($L=1$), l'espace Γ est le le plan $\mathbb{R}^2$, et le théorème de Liouville donne une interprétation simple de quelques résultats établis depuis longtemps par les mathématiciens, l'avantage étant — et il n'est pas négligeable — de permettre au physicien de "sentir" la démonstration, de telle sorte que le résultat devienne pour lui quasi-évident. Considérons par exemple le système de deux équations

$$\begin{cases} \dfrac{dx^{(1)}}{dt} = f^{(1)}\left(x^{(1)}, x^{(2)}\right) \\[2ex] \dfrac{dx^{(2)}}{dt} = f^{(2)}\left(x^{(1)}, x^{(2)}\right) \end{cases}$$

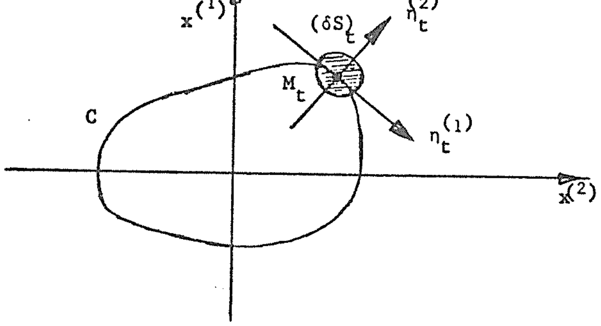
et plaçons-nous dans l'hypothèse où les fonctions $f^{(1)}$ et $f^{(2)}$ sont telles que le système admette une solution périodique, de période T,

$$\begin{cases} x^{(1)}_{t+T} = x^{(1)}_t \\[2ex] x^{(2)}_{t+T} = x^{(2)}_t \end{cases} \qquad \text{(pour tout t)}$$

la divergence étant négative, en moyenne, sur une période :

$$\frac{1}{T}\int_0^T (\operatorname{div} F)\, dt = \frac{1}{T}\int_0^T \left(\frac{\partial f^{(1)}}{\partial x^{(1)}} + \frac{\partial f^{(2)}}{\partial x^{(2)}} \right) dt < 0 \qquad .$$

Soit C la courbe fermée qui représente la solution périodique dans $\mathbb{R}^2$, et M_t le point courant de C. Introduisons alors le référentiel local formé de la tangente $M_t\ \eta_t^{(1)}$ et de la normale $M_t\ \eta_t^{(2)}$ à la trajectoire C, puis construisons une petite surface $(\delta S)_t$ qui contient M_t. Du fait de la périodicité, la dimension de cette petite surface suivant la tangente, $\delta\eta_t^{(1)}$, redevient périodiquement la même;



elle ne peut donc pas tendre vers zéro. Comme, par ailleurs, $(\delta S)_t$ tend vers zéro quand t tend vers l'infini (puisque la divergence est négative, en moyenne, le long de la trajectoire), c'est la dimension $\delta\eta_t^{(2)}$ de $(\delta S)_t$ qui tend vers zéro. Ainsi, avec le temps, la petite surface s'écrase le long de la trajectoire périodique C. En d'autres termes, toutes les trajectoires voisines de C tendent vers C. On dit que le système jouit de la stabilité orbitale asymptotique, et le fait que la condition

$$\frac{1}{T}\int_0^T \left(\frac{\partial f^{(1)}}{\partial x^{(1)}} + \frac{\partial f^{(2)}}{\partial x^{(2)}}\right) dt < 0$$

implique ce type de stabilité pour une trajectoire fermée de $\mathbb{R}^2$ constitue le critère de Poincaré. On trouvera facilement les démonstrations classiques chez J.Stoker et chez T.Vogel par exemple [1], et l'on verra que l'illustration qu'en donne le théorème de Liouville n'est pas inutile pour le physicien. La démonstration précédente présente aussi l'avantage de montrer simplement pourquoi l'on ne peut pas étendre le critère de Poincaré à un système différentiel dont l'espace des états, Γ, possède plus de deux dimensions. En effet, prenons par exemple le cas de $\Gamma = \mathbb{R}^3$. Soit un petit volume $(\delta V)_t$ qui accompagne M_t dans son mouvement périodique. La périodicité implique, comme plus haut, que la dimension $\delta\eta_t^{(1)}$ de $(\delta V)_t$ suivant la tangente ne tende pas vers zéro. Si la valeur moyenne de la divergence est négative, on en déduit, puisque $(\delta V)_t$ doit alors tendre vers zéro, que sa section par le plan normal à la trajectoire en M_t devient arbitrairement petite ; mais ceci ne signifie pas que les dimensions $\delta\eta_t^{(2)}$ et $\delta\eta_t^{(3)}$ de cette section tendent individuellement vers zéro. Les trajectoires voisines de C ne convergent donc pas nécessairement vers C.

Autre résultat classique qu'entraîne le théorème de Liouville, le critère négatif de Bendixson stipule que, dans tout domaine Δ de $\mathbb{R}^2$ où la divergence garde un signe constant, il ne peut exister de solution périodique [2]. En effet, soit dans $\Delta \subset \mathbb{R}^2$ une trajectoire fermée C_o. Elle est, par définition, sa propre transformée par le flot φ_t:

$$C_o \xrightarrow{\varphi_t} C_t \equiv C_o ,$$

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[1] *J.J.STOKER. Nonlinear vibrations in mechanical and electrical systems. Interscience publishers, New York (1950) [voir page 253]*
T.VOGEL Théorie des systèmes évolutifs. Gauthier-Villars (1965) [voir page 46]

[2] *S.LEFSCHETZ. Differential equations, geometric theory. Interscience publishers (1957) [voir page 227] ;*
T.VOGEL . Théorie des systèmes évolutifs Gauthier-Villars (1965) [voir page 42].

ce qui implique, pour l'aire de la surface qu'elle limite,

$$\mathcal{M}\text{es}\,(\mathcal{D}_t) \equiv \mathcal{M}\text{es}\,(\mathcal{D}_o)\ ;$$

or ceci est incompatible, d'après Liouville, avec une divergence de signe donné, laquelle impliquerait une variation de l'aire. Ainsi, si la divergence est de signe constant dans $\Delta \subset \mathbb{R}^2$, aucune courbe fermée de Δ ne peut prétendre être une trajectoire.

En 1965, lorsque je réfléchissais au théorème de Liouville et aux quelques applications que je viens de rappeler[1], ce qui m'amenait tout naturellement à sortir du cadre hamiltonien, quelques autres chercheurs isolés faisaient de même, dont je ne connaissais pas les travaux. Ils s'intéressaient évidemment tous à la Mécanique, et le titre très évocateur de l'ouvrage de T.Vogel[2] résume cette tendance. Cependant, deux voies apparaissaient déjà, nettement séparées. En effet, la Mécanique hamiltonienne est une mécanique différentielle à divergence nulle. A priori, deux possibilités se présentent donc à ceux qui cherchent à sortir de ce cadre. Ou bien l'on abandonne la formation différentielle, au profit, par exemple, d'une formulation intégro-différentielle, et c'est la Mécanique héréditaire que proposent T.Vogel[3] et F.Fer[4], ou bien l'on garde la formulation différentielle, mais avec une divergence qui n'est pas identiquement nulle, et c'est la Mécanique dissipative que S.Giuaşu[5] d'une part, et moi-même d'autre part, cherchons à introduire en physique théorique. Dans un livre récent, T.Vogel a de nouveau souligné l'intérêt de la Mécanique héréditaire. J'essaierai, dans les pages qui viennent, de montrer le rôle que peut jouer la Mécanique dissipative. Pour terminer ce chapitre, je me contenterai de souligner que la Mécanique dissipative, parce qu'elle est de forme purement différentielle, utilise une technique mathématique relativement simple, ce qui est un avantage non négligeable.

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[1] *J.FRONTEAU. CERN 65-38 (1965)*

[2] *T.VOGEL. Pour une théorie mécaniste renouvelée, Gauthier-Villars (1973)*

[3] *T.VOGEL. Théorie des systèmes évolutifs, Gauthier-Villars (1965)*

[4] *F.FER. CR. Acad. Sc. Paris 260, 3873 et 260, 4159 (1965)*

[5] *S.GUIAŞU. Atti dell' Acc. Naz. dei Lincei, Rome, 39, 447 (1965)*

V

L'entropie fine

On sait que Clausius[1], qui a introduit en physique le concept et le vocable d'entropie, a lui-même interprété la variation d'entropie comme une mesure de l'Evolution, et il est remarquable, par exemple, que Jean Perrin[2] ait intitulé "Evolution" le chapitre qu'il consacre à la thermodynamique. Puisque l'on vient de voir, en étudiant les systèmes différentiels, que la variation de la densité ρ_t dans l'espace des états, Γ, est également une certaine mesure de l'Evolution, le lecteur ne s'étonnera pas qu'on ait poursuivi le rapprochement et que l'auteur ait proposé[3] d'appeler "entropie fine" la quantité

$$\boxed{S_t^f = k \operatorname{Log} J_t = k \operatorname{Log} \frac{\rho_o}{\rho_t}}$$

où k est la constante de Boltzmann et J_t le jacobien de Liouville, l'indice supérieur f affecté à S_t rappelant l'épithète "fine". Entropie : on comprend cet emprunt à Clausius, au titre de l'Evolution ; mais pourquoi entropie "fine" alors que, depuis Boltzmann[4], l'entropie est une notion d'essence collective ? Tout simplement pour souligner qu'au contraire l'auteur conçoit l'Evolution comme un phénomène qui existe au plan <u>individuel</u> , c'est-à-dire pour chaque particule d'un système. Si même c'est la collectivité qui est responsable de l'évolution non conservative, cette évolution mérite d'être décrite pour <u>chaque</u> élément de l'ensemble. Techniquement, la grandeur Log J_t étant associée à tout

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[1] *R.CLAUSIUS. Théorie mécanique de la chaleur, Eugène Lacroix, Paris (1868)*

[2] *J.PERRIN. Les éléments de la physique. Albin Michel (1934)*

[3] *J.FRONTEAU. CERN, MPS/Int MU/EP 66-5 (1966)*

[4] *L.BOLTZMANN. Vorlesungen über Gastheorie, J.A.Barth, Leipzig (1896)*

point matériel dont la dynamique est régie par un système différentiel, elle permet de définir l'entropie de ce point, de même qu'on a su en définir analytiquement l'énergie et l'impulsion. En 1966, lorsque l'auteur a parlé pour la première fois d'entropie fine, la surprise a été grande : l'entropie est un concept essentiellement collectif ; l'entropie fine ne saurait donc avoir de sens. Louis de Broglie[1] avait pourtant introduit quelques années auparavant la notion d' "entropie de la particule isolée" mais, compte tenu de l'opposition existant entre Louis de Broglie et les théoriciens de l'Ecole de Copenhague à propos de la Mécanique quantique[2], ceci n'était pas fait pour amener les physiciens orthodoxes à accepter la notion d'entropie fine. Par contre, pour l'auteur, savoir que Louis de Broglie avait créé une Thermodynamique de la particule isolée était un encouragement à poursuivre dans sa propre voie et pourtant, à l'époque, rien ne permettait de saisir le lien analytique existant entre l'entropie fine et l'entropie de la particule isolée. Ce problème ne devait être abordé que beaucoup plus tard. [cf chapitre IX .]

Nous nous proposons de donner très vite quelques arguments physiques en faveur de la définition de l'entropie fine mais, auparavant, montrons qu'il est possible d'étendre la notion de moyenne de la Mécanique statistique au cas d'un flot non conservatif, et que cela conduit à des résultats cohérents. Revenons au système différentiel $\frac{dX}{dt} = F(X,t)$ à divergence non identiquement nulle, et considérons sa solution $X_t = X(X_o,t)$, le flot φ_t correspondant, et la densité ρ_t définie dans $\Gamma = \mathbb{R}^n$. Rappelons que :

$$\rho_t = \frac{\rho_o}{J_t} = \frac{\rho(X_o)}{J(X_o,t)} = \rho(X_o,t) \ ,$$

et qu'en inversant la relation $X_t = X(X_o,t)$ on obtient $X_o = X^{-1}(X_t,t)$, ce qui fournit :

$$\rho_t = \rho\left[X^{-1}(X_t,t),\ t\right] = \mathcal{J}(X_t,t).$$

En résumé, ρ_t peut s'exprimer de deux façon différentes, à savoir :

$$\rho_t = \rho(X_o,t) \qquad \text{et} \qquad \rho_t = \mathcal{J}(X_t,t).$$

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[1] *L. de BROGLIE . La thermodynamique de la particule isolée, Gauthier-Villars, Paris (1964)*

[2] *L. de BROGLIE . Une tentative d'interprétation causale et non linéaire de la Mécanique Ondulatoire , Gauthier-Villars (1956)*

Soit alors $g(X,t)$ une fonction donnée, qui est définie dans Γ et qui, pour cette raison, sera dite fonction d'état. Si le produit $g(X_t,t)\rho_t$ est sommable dans Γ_t, on introduit, par analogie avec la Mécanique Statistique classique, la moyenne :

$$<g>_{\Gamma_t} = \frac{1}{N}\int_{\Gamma_t} g(X_t,t)\ \rho_t\ dX_t = \frac{1}{N}\int_{\Gamma_t} g(X_t,t)\ \mathcal{P}(X_t,t)\ dX_t\ ,$$

où N est le nombre, constant, des états considérés .

Si la fonction $g(X_t,t)\rho_t$ n'est que localement sommable dans Γ_t, nous définirons la moyenne relative à tout domaine compact $\mathcal{D}_t \subset \Gamma_t$:

$$<g>_{\mathcal{D}_t} = \frac{1}{N}\int_{\mathcal{D}_t} g(X_t,t)\ \rho_t\ dX_t = \frac{1}{N}\int_{\mathcal{D}_t} g(X_t,t)\mathcal{P}(X_t,t)\ dX_t\ ,$$

Proposons-nous maintenant de calculer la dérivée $\frac{d}{dt} <g>$. (Formellement, c'est-à-dire aux difficultés de convergence près, le calcul qui suit est le même pour Γ_t et pour $\mathcal{D}_t$; c'est pourquoi nous ne le ferons que dans le cas Γ_t).

Effectuons donc le changement de variables défini par $X_t = X(X_o,t)$, t étant alors un paramètre. Il vient, compte tenu de ce que $J_t = J(X_o,t) = \frac{D(X_t)}{D(X_o)}$;

$$<g>_{\Gamma_t} = \frac{1}{N}\int_{\Gamma_t} g(X_t,t)\rho_t\ dX_t = \frac{1}{N}\int_{\Gamma_o} g\left[X(X_o,t),t\right]\rho(X_o,t)\ J(X_o,t)\ dX_o\ .$$

Du fait de la relation $\rho_t\ J_t = \rho_o = \rho(X_o)$, il reste :

$$<g>_{\Gamma_t} = \frac{1}{N}\int_{\Gamma_o} g\left[X(X_o,t),\ t\right]\ \rho(X_o)\ dX_o\ .$$

Le calcul de la dérivée en t est alors immédiat : puisque Γ_o ne dépend pas de t, on peut dériver sous le signe somme. On obtient ainsi :

$$\frac{d}{dt}<g>_{\Gamma_t} = \frac{1}{N}\int_{\Gamma_o}\left\{\text{grad } g\left[X(X_o,t),t\right]\ .\ \frac{dX}{dt}(X_o,t) + \frac{\partial g}{\partial t}\left[X(X_o,t),t\right]\right\}\rho(X_o)\ dX_o$$

d'où:

$$\frac{d}{dt} <g>_{\Gamma_t} = \frac{1}{N}\int_{\Gamma_o} \left\{ \text{grad } g \left[X(X_o,t),t\right] \cdot F\left[X(X_o,t),t\right] + \frac{\partial g}{\partial t}\left[X(X_o,t),t\right] \right\} \rho(X_o,t) \frac{D(X_t)}{D(X_o)} \, dX_o \; ,$$

c'est-à-dire, en revenant aux variables X_t,

$$\frac{d}{dt} <g>_{\Gamma_t} = \frac{1}{N}\int_{\Gamma_t} \left\{ \text{grad } g \,(X_t,t) . \, F(X_t,t) + \frac{\partial g}{\partial t}(X_t,t) \right\} \rho_t \, dX_t \quad .$$

En résumé :

$$\boxed{\frac{d}{dt} <g>_{\Gamma_t} = <\frac{dg}{dt}>_{\Gamma_t}} \quad .$$

On retrouve ainsi, dans le cas non conservatif, le résultat classique de la Mécanique Statistique conservative[1]. La trame de la démonstration donnée ci-dessus figure dans un rapport de 1966[2], mais à l'époque l'auteur n'en avait pas écrit le résultat général sous la forme précédente. Telle qu'elle est présentée aujourd'hui, la démonstration est beaucoup plus récente et résulte d'un échange épistolaire avec S.Guiaşu[3]. On remarquera encore que le résultat précédent n'est que l'extension à $\mathbb{R}^n$ d'un théorème[4] déjà démontré dans $\mathbb{R}^3$. En guise d'exercice (car le calcul direct est plus rapide), appliquons maintenant le théorème précédent au calcul de la dérivée de la mesure de $\mathcal{D}_t \subset \Gamma_t$ en admettant que ρ_t ne soit jamais nulle.

$$\mathcal{M}\text{es}(\mathcal{D}_t) = \int_{\mathcal{D}_t} dX_t \equiv \int_{\mathcal{D}_t} \frac{1}{\rho_t} \rho_t \, dX_t = N < \frac{1}{\rho_t} >_{\mathcal{D}_t}$$

$$\frac{d}{dt}\mathcal{M}\text{es}(\mathcal{D}_t) = N \frac{d}{dt} < \frac{1}{\rho_t} >_{\mathcal{D}_t} = N < \frac{d}{dt}\left(\frac{1}{\rho_t}\right) >_{\mathcal{D}_t} = N < -\frac{1}{\rho_t^2} \frac{d\rho_t}{dt} >_{\mathcal{D}_t}$$

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[1] *J.YVON. Les corrélations et l'entropie en Mécanique Statistique classique. Monographie Dunod (1966)* [*voir page 32*]

[2] *J.FRONTEAU. CERN MPS/Int MU/EP 66-5 (1966)* [*voir page 33*]

[3] *A.CHALJUB, J.FRONTEAU, S.GUIAŞU.Correspondance 1972-1974*

[4] *PHAM MAU QUAN. Sur une théorie relativiste des fluides thermodynamiques. Thèse, Paris(1955)* [*voir page 37*]

$$\frac{d}{dt}\mathcal{M}es\,(\mathcal{D}_t) = - N \left\langle \frac{1}{\rho_t}\,\frac{d}{dt}\,\mathrm{Log}\,\rho_t \right\rangle_{\mathcal{D}_t} = N \left\langle \frac{1}{\rho_t}\,\mathrm{div}\,F \right\rangle_{\mathcal{D}_t}$$

$$\boxed{\frac{d}{dt}\,\mathcal{M}es\,(\mathcal{D}_t) = \int_{\mathcal{D}_t} (\mathrm{div}\ F)\ dX_t} \quad .$$

C'est là une autre forme du théorème de Liouville [1]

Au vu du calcul et du résultat précédents, on comprend qu'il soit possible de mettre au point une mécanique statistique non conservative. C'est ce qu'a fait S.Guiaşu[2], sur les bases suivantes :

1) On détermine la distribution d'équilibre dans Γ_o en recherchant l'extremum de l'entropie de Boltzmann

$$- k \int_{\Gamma_o} \rho_o \ \mathrm{Log}\ \rho_o \ \ dX_o \quad ,$$

extremum lié par l'existence d'une énergie de valeur moyenne donnée. On sait qu'on trouve la distribution de Gibbs.

2) Cette distribution initiale est transformée par le flot φ_t en une nouvelle distribution, ρ_t.

3) On calcule la dérivée de la moyenne des fonctions d'état. (Le lecteur remarquera que les résultats de Guiaşu diffèrent des nôtres).

4) On étend au cas non conservatif le théorème de Birkhoff relatif à l'égalité des moyennes temporelles et des moyennes prises sur Γ_o pour un système en équilibre.

Nous n'en dirons pas plus sur la mécanique statistique non conservative, puisque divers ouvrages de S.Guiaşu y sont consacrés. Le lecteur pourra également prendre connaissance d'un intéressant article de P.Caldirola[3].

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[1] *J.FRONTEAU, CERN 65-38 (1965) [voir page 5]*
V.ARNOLD, Equations différentielles ordinaires, Editions Mir, Moscou(1974) [voir page 196]

[2] *S.GUIAŞU. Atti dell'Accademia Nazionale dei Lincei, Rome,39, 447 (1965) ;*
S.GUIAŞU. Revue roumaine de math.pures et appliquées,11, 541 (1966) ;
S.GUIAŞU. Aplicaţii ale teoriei informaţiei.Sisteme dinamice, Sisteme cibernetice. Editions de l'Académie de Bucarest (1968)
O.ONICESCU, S.GUIAŞU. Mécanique statistique. International Centre for mechanical Sciences, Udine (1971) Springer Verlag

[3] *P.CALDIROLA. Nuovo Cimento 46 B, 172 (1966)*

Revenons enfin à l'entropie fine et présentons deux résultats curieux dont, pour l'auteur, la coexistence a toujours été plus qu'un hasard heureux. Dès qu'on accepte la notion d'entropie fine,

$$S_t^f = k \text{ Log } J_t = k \text{ Log } \frac{\rho_o}{\rho_t} \quad ,$$

on peut calculer l'entropie moyenne,

$$< S_t^f >_{\Gamma_t} = \frac{1}{N} \int_{\Gamma_t} k \left(\text{Log } \frac{\rho_o}{\rho_t} \right) \rho_t \, dX_t \quad ,$$

c'est-à-dire :

$$< S_t^f >_{\Gamma_t} = - \frac{k}{N} \int_{\Gamma_t} \rho_t \text{ Log } \rho_t \, dX_t + \frac{k}{N} \int_{\Gamma_t} (\text{Log } \rho_o) \, \rho_t \, dX_t .$$

On sait que ρ_t peut s'écrire $\mathcal{P}(X_t,t)$; en appliquant le changement de variables $X_t = X(X_o,t)$ à la seconde intégrale, il vient donc :

$$< S_t^f >_{\Gamma_t} = - \frac{k}{N} \int_{\Gamma_t} \mathcal{P}(X_t,t) \text{ Log } \mathcal{P}(X_t,t) \, dX_t + \frac{k}{N} \int_{\Gamma_o} \rho(X_o) \text{ Log } \rho(X_o) \, dX_o .$$

On reconnaît la forme de la fonction H^B de Boltzmann,

$$H^B = \int_{\Gamma} \rho \text{Log } \rho dX \ ,$$

et le résultat précédent s'écrit :

$$\boxed{- k H_t^B = N<S_t^f> - k H_o^B} \quad .$$

A la constante $k H_o^B$ près, l'entropie de Boltzmann, $- k H_t^B$, apparaît donc bien comme l'entropie totale du système, puisque c'est N fois l'entropie moyenne des N états considérés. Ceci est en soi une première justification de la définition de S_t^f et du vocable d'entropie fine, mais considérons une autre conséquence de cette définition.

Soit la dynamique dissipative la plus simple possible, à savoir :

$$m_o \frac{d^2\vec{Y}}{dt^2} = A \frac{d\vec{Y}}{dt} \qquad \left[\begin{array}{l} \vec{Y} \in \mathbb{R}^3 \ , \ \vec{Y} = (y^{(1)}, y^{(2)}, y^{(3)}) \\ t \in \mathbb{R} \ , \ m_o = \text{constante réelle positive,} \\ A = \text{constante réelle (positive ou négative).} \end{array}\right.$$

Introduisons le système du premier ordre équivalent :

$$\left\{\begin{array}{l} \dfrac{d\vec{Y}}{dt} = \vec{V} \\ \dfrac{d\vec{V}}{dt} = \dfrac{A}{m_o} \vec{V} \end{array}\right.$$

c'est-à-dire, en projection,

$$\left\{\begin{array}{l} \dfrac{dy^{(\ell)}}{dt} = v^{(\ell)} \\ \dfrac{dv^{(\ell)}}{dt} = \dfrac{A}{m_o} v^{(\ell)} \end{array}\right. \qquad \ell = 1, 2, 3 \ .$$

Calculons alors la divergence de ce système, les $y^{(\ell)}$ et $v^{(\ell)}$ étant indépendants :

$$\operatorname{div} F = \sum_{\ell=1}^{3} \left\{ \frac{\partial v^{(\ell)}}{\partial y^{(\ell)}} + \frac{\partial}{\partial v^{(\ell)}} \left[\frac{A}{m_o} v^{(\ell)} \right] \right\} = 3 \frac{A}{m_o} \ .$$

On en déduit, compte tenu du théorème de Liouville et de la définition de l'entropie fine,

$$\frac{dS_t^f}{dt} = k \frac{d}{dt} \operatorname{Log} J_t = k \operatorname{div} F = 3k \frac{A}{m_o} \ .$$

Si maintenant l'on utilise l'expression de la dérivée de l'énergie cinétique,

$$\frac{dE_{cin}}{dt} = m_o \vec{V} . \frac{d\vec{V}}{dt} = m_o \vec{V} . \frac{A}{m_o} \vec{V} = AV^2 = 2 \frac{A}{m_o} E_{cin} \ ,$$

il vient :

$$\frac{dE_{cin}/dt}{E_{cin}} = 2\,\frac{A}{m_o}$$

d'où :

$$\frac{d\,S_t^f}{dt} = \frac{3}{2}\,k\,\frac{dE_{cin}/dt}{E_{cin}} \quad .$$

En introduisant T^f et dQ^f, définies par les relations

$$E'_{cin} = \frac{3}{2}\,k\,T^f$$

$$\text{et} \quad dQ^f = dE_{cin} \,,$$

le résultat précédent s'écrit sous une forme qu'on reconnaît immédiatement :

$$\boxed{dS^f = \frac{dQ^f}{T^f}} \quad .$$

Ainsi, si l'on imagine de décrire un apport de chaleur (positif ou négatif) par un modèle dynamique non conservatif —— le modèle précédent, beaucoup trop élémentaire, sera étendu par la suite (chapitre VI)—— la notion d'entropie fine réalise la synthèse des deux définitions classiques de l'entropie. D'une part, par sa moyenne statistique, S_t^f conduit à la fonction H_t^B de Boltzmann ; d'autre part, appliquée à une dynamique dissipative, elle conduit à la forme de Clausius $dS = \frac{dQ}{T}$. Que ce fût là coïncidence fortuite, l'auteur n'a jamais pu le croire. C'était pour lui, au contraire, les prémices d'une thermodynamique fine.

En 1966, la Physique ne pouvait accepter cette idée. Fondement de la Mécanique Statistique et de la Mécanique Quantique , le formalisme hamiltonien était inattaquable. Les modèles dissipatifs ne pouvaient être que des palliatifs macroscopiques. Il était impensable de les introduire au niveau de compréhension le plus profond. Je l'ai bien senti lorsque j'ai publié ces quelques pages intitulées "L'entropie et la physique moderne"[1]. Les réactions furent pour le moins réservées. Je reçus quelques lettres en réponse à mon rapport, mais les encouragements furent extrêmement rares. Je profiterai donc de l'occasion pour remercier aujourd'hui ceux qui, très tôt dans le courant de 1966, m'ont

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[1] *J. FRONTEAU CERN MPS/Int MU/EP 66-5 (1966)*

apporté un élément d'espoir. Je pense à ce professeur de l'Université de Genève, à ce grand physicien britannique et à ces quelques compatriotes que je ne nommerai d'ailleurs pas, par souci d'anonymat, de même que je ne nommerai pas ceux que je n'ai pas su intéresser. Je ne citerai qu'une phrase extraite d'une lettre que je n'ai jamais oubliée, et qui m'a beaucoup aidé à poursuivre mon travail : "Ce que j'approuve entièrement chez vous est que vous sortiez carrément des idées courantes et des chemins battus. Je crois en effet que c'est la seule chance de sortir de la crise actuelle de la théorie. Je vous félicite, et je vous assure de toute ma sympathie pour votre effort".

Cependant, le comportement moyen des physiciens m'avait quelque peu désespéré. L'incompréhension était profonde ; en effet, à l'époque, la mécanique dissipative ne constituait pas une discipline ; c'était un domaine fou ; j'y travaillais seul (je ne connaissais pas les travaux de Guiaşu, et réciproquement d'ailleurs), et je comprenais d'autant moins les réactions de la majorité que mon comportement scientifique me paraissait très normal. Spécialiste d'optique corpusculaire, je n'avais ni le temps ni les compétences pour développer seul l'étude des modèles dissipatifs, pas plus en Thermodynamique fine qu'en Mécanique quantique, où cependant je pressentais déjà qu'on pourrait trouver des applications. Je venais donc demander de l'aide aux physiciens compétents. En réponse je ne trouvais guère que scepticisme et froideur. Jeune encore, prompt à la révolte, j'avais de la peine à admettre cette fin de non-recevoir, car j'avais l'impression que ce n'était pas à moi qu'on s'en prenait, mais à toute une forme de pensée qui me semblait possible, et qu'on refusait a priori. Profondément déçu, je résolus néanmoins de continuer à étudier les modèles dissipatifs pendant les quelques années que je m'apprêtais à passer loin de l'Europe, dans un poste d'enseignement que j'avais accepté à l'Université de Tananarive.

C. R. Acad. Sc. Paris, t. 280 (26 mai 1975) Série A — 1405

PHYSIQUE MATHÉMATIQUE. — *Une dynamique associée à l'équation cinétique Frey-Salmon.* Note (*) de M. **Jean Fronteau**, présentée par M. André Lichnerowicz.

On propose d'associer une dynamique continue à l'équation cinétique du fluide isotherme en théorie Frey-Salmon.

Soit un fluide isotherme à un seul composant; t étant le temps, et m, $\vec{x}$, $\vec{w}$ la masse, la position et la vitesse d'une molécule, $T = T(t)$ sera la température du fluide, et $\vec{v} = \vec{v}(\vec{x}, t)$ la vitesse moyenne de l'écoulement dans un champ de forces $\vec{X} = \vec{X}(\vec{x}, t)$. Les hypothèses de J. Frey et J. Salmon (^{6}) conduisent à une équation cinétique du type Fokker-Planck :

$$\boxed{\frac{\partial f}{\partial t} + \vec{w} \cdot \overrightarrow{\text{grad}}_x f + \frac{\vec{X}}{m} \cdot \overrightarrow{\text{grad}}_w f = \alpha \frac{kT}{m}\left[3f + (\vec{w} - \vec{v}) \cdot \overrightarrow{\text{grad}}_w f + \frac{kT}{m} \Delta_w f\right]}, \tag{1}$$

où k est la constante de Boltzmann, $f(\vec{x}, \vec{w}, t)$ la fonction de distribution simple, et $\alpha = \alpha(\vec{x}, t)$ un coefficient positif caractérisant le fluide à la température T. Ceci étant admis, nous suggérons de prendre en considération l'équation suivante, qui pourrait décrire le mouvement de toute molécule du fluide soumise à son proche environnement (le fluide voisin) et au champ de forces $\vec{X}(\vec{x}, t)$:

$$\boxed{m \frac{d\vec{w}}{dt} = \vec{X} - \alpha k T (\vec{w} - \vec{v}) - \frac{\alpha}{m} (kT)^2 \, \overrightarrow{\text{grad}}_w \log f}. \tag{2}$$

Nous allons montrer que — sous certaines hypothèses — (2) implique (1); (2) sera donc un modèle dynamique possible.

Formulation eulérienne de la démonstration. — Soit $\Gamma_{x, w} = \mathbb{R}^6$ l'espace des phases des particules du fluide; $\vec{x}$ et $\vec{w}$ repèrent un point fixe de $\Gamma_{x, w}$. Faisons les hypothèses suivantes :

(A_1) La densité du fluide de phases est une fonction $f(\vec{x}, \vec{w}, t)$.

(A_2) La vitesse d'écoulement dans $\Gamma_{x, w}$, vecteur de $\mathbb{R}^6$, est une fonction $V(\vec{x}, \vec{w}, t)$.

(A_3) Le fluide de phases se conserve : $(\partial f/\partial t) + \text{div}_{x, w}(f V) = 0$.

(A_4) Le fluide réel, lui, s'écoule dans $\Gamma_x = \mathbb{R}^3$ à la vitesse moyenne $\vec{v}(\vec{x}, t)$; il est soumis à un champ de forces $\vec{X}(\vec{x}, t)$ et sa température est uniforme, $T = T(t)$; un coefficient scalaire $\alpha = \alpha(\vec{x}, t)$ complète la description.

(A_5) Le vecteur $V(\vec{x}, \vec{w}, t)$ est de la forme suivante, qui exprime (2) en coordonnées d'Euler :

$$V = \begin{pmatrix} \vec{w} \\ \dfrac{1}{m}\left[\vec{X} - \alpha k T (\vec{w} - \vec{v}) - \dfrac{\alpha}{m} (kT)^2 \, \overrightarrow{\text{grad}}_w \, \text{Log} f\right] \end{pmatrix} \in \mathbb{R}^6;$$

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il vient alors :

$$\frac{\partial f}{\partial t} + \mathrm{V}.\mathrm{grad}_{x,\,w} f = -f\,\mathrm{div}_{x,\,w}\mathrm{V} \qquad [\mathit{cf.}\,(\mathrm{A}_3)],$$

$$\frac{\partial f}{\partial t} + \vec{w}.\overrightarrow{\mathrm{grad}}_x f + \frac{1}{m}\left[\vec{\mathrm{X}} - \alpha k\mathrm{T}(\vec{w}-\vec{v}) - \frac{\alpha}{m}(k\mathrm{T})^2\,\overrightarrow{\mathrm{grad}}_w \mathrm{Log} f\right].\overrightarrow{\mathrm{grad}}_w f$$

$$= -f\left\{\mathrm{div}_x\vec{w} + \frac{1}{m}\mathrm{div}_w\left[\vec{\mathrm{X}} - \alpha k\mathrm{T}(\vec{w}-\vec{v}) - \frac{\alpha}{m}(k\mathrm{T})^2\,\overrightarrow{\mathrm{grad}}_w \mathrm{Log} f\right]\right\} \qquad [\mathit{cf.}\,(\mathrm{A}_5)].$$

Tous calculs faits, avec l'hypothèse (A_4), on trouve (1) puisque $\mathrm{div}_x\,\vec{w} \equiv 0$. On remarquera que le calcul précédent n'est qu'une extension à $\mathbb{R}^6$ de la méthode (³) qui permet d'établir l'équation de diffusion dans $\mathbb{R}^3$, $(\partial\rho/\partial t) = \mathrm{D}\,\Delta_x\,\rho$, à partir de l'équation de continuité $(\partial\rho/\partial t) + \mathrm{div}_x(\rho\,\vec{v}) = 0$ et de la relation $\vec{v} = -\mathrm{D}\,\overrightarrow{\mathrm{grad}}_x\,\mathrm{Log}\,\rho$.

FORMULATION LAGRANGIENNE. — Soit l'espace des phases à l'instant t_0, $\Gamma_{x_0,\,w_0}$, et à tout instant t, $\Gamma_{x_t,\,w_t}$. $\mathscr{D}_0$ étant un domaine de $\Gamma_{x_0,\,w_0}$, nous admettrons les hypothèses suivantes :

(B_1) La densité dans $\mathscr{D}_0$ est uniforme, $f_0 \equiv 1$.

(B_2) il existe un flot φ_t toujours inversible

$$\left|\begin{array}{l}\vec{x}_t = \vec{x}(\vec{x}_0, \vec{w}_0, t)\\ \vec{w}_t = \vec{w}(\vec{x}_0, \vec{w}_0, t)\end{array}\right. \qquad \text{avec} \quad \mathrm{J}_t = \frac{\mathrm{D}(\vec{x}, \vec{w})}{\mathrm{D}(\vec{x}_0, \vec{w}_0)} \neq 0, \qquad (\forall t).$$

On a donc aussi :

$$\left|\begin{array}{l}\vec{x}_0 = \vec{\chi}(\vec{x}_t, \vec{w}_t, t),\\ \vec{w}_0 = \vec{\psi}(\vec{x}_t, \vec{w}_t, t)\end{array}\right.$$

et l'on en déduit que $[d\vec{x}_t/dt, d\vec{w}_t/dt]$ est un vecteur de $\mathbb{R}^6$ qui s'exprime sous la forme $\mathrm{V}(\vec{x}_t, \vec{w}_t, t)$.

(B_3) Le fluide de phases est conservé par le flot φ_t, ce qui peut s'écrire $f_t = f_0/\mathrm{J}_t = 1/\mathrm{J}_t$. En effet, J_t commande l'évolution temporelle des volumes; il commande donc la variation de l'inverse de la densité f. On en déduit que

$$f_t = \frac{1}{\mathrm{J}_t} = \frac{1}{\mathrm{J}(\vec{x}_0, \vec{w}_0, t)}$$

s'écrit aussi, en utilisant $\vec{\chi}$ et $\vec{\psi}$, $f_t = f(\vec{x}_t, \vec{w}_t, t)$.

Enfin le théorème de Liouville [(¹), (⁵), (⁷)], appliqué au flot φ_t, s'énonce :

$$\frac{d\mathrm{J}_t}{dt} = \mathrm{J}_t\,\mathrm{div}_{x_t,\,w_t}\mathrm{V}, \tag{3}$$

ou encore, puisque $f_0 \equiv 1$, $df/dt = -f\,\mathrm{div}_{x_t,\,w_t}\mathrm{V}$.

(B_4) Le fluide réel s'écoule dans R^3 à la vitesse moyenne $\vec{v}\,(\vec{x}_t, t)$; il est soumis à chaque instant au champ de forces $\vec{\mathrm{X}}\,(\vec{x}_t, t)$ et sa température est uniforme, $\mathrm{T} = \mathrm{T}(t)$; le coefficient scalaire $\alpha = \alpha(\vec{x}_t, t)$ complète la description.

$$(4)\quad (\mathrm{B}_5)\quad \left\{\begin{aligned} \frac{d\vec{x}_t}{dt} &= \vec{w}_t,\\ \frac{d\vec{w}_t}{dt} &= \frac{1}{m}\left[\vec{\mathrm{X}} - \alpha k\mathrm{T}(\vec{w}_t - \vec{v}) - \frac{\alpha}{m}(k\mathrm{T})^2\,\overrightarrow{\mathrm{grad}}_{w_t}\mathrm{Log} f\right]\end{aligned}\right. \qquad [\text{dynamique (2)}].$$

A partir de (3) et (4), même calcul que dans le cas de la formulation eulérienne; on retrouve l'équation (1), écrite en suivant le flot φ_t :

$$\frac{\partial f}{\partial t} + \vec{w}_t\cdot\overrightarrow{\mathrm{grad}}_{x_t} f + \frac{\vec{\mathrm{X}}}{m}\cdot\overrightarrow{\mathrm{grad}}_{w_t} f = \alpha\frac{k\mathrm{T}}{m}\left[3f + (\vec{w}_t - \vec{v})\cdot\overrightarrow{\mathrm{grad}}_{w_t} f + \frac{k\mathrm{T}}{m}\Delta_{w_t} f\right].$$

Remarques. — (*a*) l'équation (2) est l'équation de Langevin, dans laquelle le terme de diffusion aléatoire a été remplacé par un terme de diffusion continue exprimé à l'aide de la fonction de distribution $f(\vec{x}, \vec{w}, t)$.

(*b*) La dynamique (2)-(4) n'est pas hamiltonienne. Cependant, elle devient conservative quand les deux termes en $k\,\mathrm{T}$ et en $(k\,\mathrm{T})^2$ se compensent identiquement, c'est-à-dire lorsque :

$$-\ \alpha k\,\mathrm{T}(\vec{w}_t - \vec{v}) - (\alpha/m)(k\,\mathrm{T})^2\,\overrightarrow{\mathrm{grad}}_{w_t}\mathrm{Log} f = 0, \text{ ce qui équivaut à :}$$

$$f = g(\vec{x}_t, t)\exp\left\{-\frac{m[\vec{w}_t - \vec{v}(\vec{x}_t, t)]^2}{2k\mathrm{T}(t)}\right\},$$

g étant une fonction indépendante de $\vec{w}_t$.

(*c*) Le terme de diffusion peut s'écrire de façon plus condensée à l'aide de la fonction :

$$(5)\qquad \boxed{\mathrm{S}_t^f = \mathrm{Log}\,\mathrm{J}_t}$$

que nous avons introduite en 1966 sous le nom d'entropie fine (⁷) et qui, avec les hypothèses (B_1) et (B_3), devient $\mathrm{S}_t^f = -\mathrm{Log} f_t$.

La dynamique (2)-(4) pend alors la forme :

$$(6)\qquad \boxed{m\frac{d\vec{w}_t}{dt} = \vec{\mathrm{X}} - \alpha k\mathrm{T}(\vec{w}_t - \vec{v}) + \frac{\alpha}{m}(k\mathrm{T})^2\,\overrightarrow{\mathrm{grad}}_{w_t}\mathrm{S}^f}$$

et la diffusion est ainsi reliée à la croissance de l'entropie dès le niveau microscopique.

Signalons enfin que le concept d'entropie fine qui vient d'être utilisé est très proche de la notion d'entropie de la particule isolée au sens de M. Louis de Broglie (²) [la comparaison a été abordée récemment (⁷)], et qu'il a vraisemblablement des points communs — quoique aucune comparaison n'ait encore été publiée — avec le concept d'entropie microscopique introduit par l'école de Bruxelles (⁴).

(*) Séance du 21 avril 1975.

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Université d'Orléans,
U. E. R. de Sciences fondamentales et appliquées,
45045 Orléans Cedex.

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MÉCANIQUE STATISTIQUE. — *Une nouvelle hypothèse d'irréversibilité.*

Note (*) de M. **Jean Salmon**, présentée par M. André Lichnerowicz.

Une mécanique statistique irréversible est obtenue en modifiant la loi du mouvement de deux particules en interaction centrale. Le second principe de la thermodynamique est conséquence de cette loi et la nécessité d'un postulat d'irréversibilité du genre chaos moléculaire disparait.

1. Introduction. — Le système d'équations de B. B. G. K. Y représente la forme évoluée et rigoureuse de la mécanique statistique classique. Pour un gaz de particules de masse m soumises à une force d'interaction centrale X_{ij} dérivant d'un potentiel φ, l'équation d'évolution de la fonction de distribution double f_{12} s'écrit en désignant par f_{123} la fonction de distribution triple, par t le temps, par x et w les vecteurs position et vitesse,

$$(1)\qquad \frac{\partial f_{12}}{\partial t}+w_1\frac{\partial f_{12}}{\partial x_1}+w_2\frac{\partial f_{12}}{\partial x_2}+\frac{X_{12}}{m}\frac{\partial f_{12}}{\partial w_1}+\frac{X_{21}}{m}\frac{\partial f_{12}}{\partial w_2}+\iint\left[\frac{X_{13}}{m}\frac{\partial f_{123}}{\partial w_1}+\frac{X_{23}}{m}\frac{\partial f_{123}}{\partial w_2}\right]dx_3\,dw_3=0.$$

La loi du mouvement est

$$(2)\qquad m\frac{dw_i}{dt}=X_{ij}=-\frac{\partial\varphi}{\partial x_i}.$$

Le caractère réversible de l'équation (2) à la suite de l'équation (1) la rend incompatible avec le second principe de la Thermodynamique. L'équation (2) contient en outre la fonction inconnue f_{123}. Il est donc indispensable d'introduire un postulat qui ferme le système B. B. G. K. Y en le rendant irréversible. Pour un gaz dilué, deux postulats ont été proposés. Le premier est celui du chaos moléculaire de Boltzmann $f_{12}=f_1 f_2$ en dehors de la zone d'interaction. Il fut très vivement critiqué à une certaine époque parce qu'au début d'une collision il impose que les particules oublient les corrélations de vitesse passées mais il permet d'obtenir une équation cinétique efficace, conduisant à des résultats bien vérifiés par l'expérience, tandis que la perte d'information liée au chaos moléculaire apporte l'accroissement d'entropie conforme au second principe de la thermodynamique. En revanche, l'équation de Boltzmann n'est pas adaptée au cas des gaz denses.

Le second postulat est celui de la relaxation linéaire de J. Frey et J. Salmon [(¹), (²), (³)]. Les fonctions ψ désignant les fonctions de corrélation de position de l'équilibre local, il s'écrit :

$$(3)\qquad \left\{\begin{aligned}&\chi_{12}=f_{12}-f_1 f_2\psi_{12},\qquad \chi_{123}=f_{123}-f_1 f_2 f_3\psi_{123},\\&\iint\left[\frac{X_{13}}{m}\frac{\partial}{\partial w_1}+\frac{X_{23}}{m}\frac{\partial}{\partial w_2}\right]\chi_{123}\,dx_3\,dw_3=\frac{\chi_{12}}{\tau}.\end{aligned}\right.$$

τ désignant la valeur moyenne du temps de passage dans la partie répulsive du potentiel d'interaction lors d'une collision et f la fonction de distribution simple. Ce postulat conduit à l'équation cinétique Frey-Salmon dans laquelle n_1 est la densité particulaire, v_1 le vecteur vitesse moyenne, T la température et K la constante de Boltzmann :

$$(4)\qquad \frac{\partial f_1}{\partial t}+w_1\frac{\partial f_1}{\partial x_1}=\frac{n_1\,KT}{2m}\,\tau\,B\left[3f_1+(w_1-v_1)\frac{\partial f_1}{\partial w_1}+\frac{KT}{m}\Delta_w f_1\right],$$

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avec

$$B = -\frac{8\pi}{3\,KT}\int_0^{\infty}\frac{d\varphi}{dx}\,\frac{d\psi}{dx}\,x^2\,dx = \frac{8\pi}{3\,K^2T^2}\int_0^{\infty}\left(\frac{d\varphi}{dx}\right)^2 e^{-\varphi/KT}\,x^2\,dx. \tag{5}$$

Il en résulte que

$$S_1 = -K\int f_1 \operatorname{Log} f_1\,dx_1\,dw_1, \qquad \frac{\partial S_1}{\partial t} \geqq 0. \tag{6}$$

L'entropie simple S_1 ne peut décroître tandis que la formule du coefficient de viscosité $\mu = m(\tau\,B)^{-1}$ est bien vérifiée par l'expérience (⁴). En outre la présence des fonctions ψ élimine les divergences en gaz denses. Le postulat de la relaxation linéaire peut comme celui du chaos moléculaire sembler absurde, mais si l'on s'interdit tout postulat l'équation (1) devient, en négligeant f_{123} en milieu dilué :

$$\frac{\partial f_{12}}{\partial t} + w_1\frac{\partial f_{12}}{\partial x_1} + w_2\frac{\partial f_{12}}{\partial x_2} + \frac{X_{12}}{m}\,\frac{\partial f_{12}}{\partial w_1} + \frac{X_{21}}{m}\,\frac{\partial f_{12}}{\partial w_2} = 0, \tag{7}$$

d'où pour l'entropie double S_2 un résultat physiquement inacceptable.

$$S_2 = -K\int f_{12} \operatorname{Log} f_{12}\,dx_1\,dw_1\,dx_2\,dw_2, \qquad \frac{\partial S_2}{\partial t} = 0, \tag{8}$$

S_2 est une entropie statistique, alors que S_1 à la suite du postulat d'irréversibilité est une entropie thermique (⁵).

2. UNE NOUVELLE LOI DE LA DYNAMIQUE. — Le caractère réversible de l'équation du mouvement entraîne l'obligation de casser la réversibilité du système B. B. G. K. Y au moyen d'un postulat. Pour éviter cette contrainte, nous proposons de modifier la loi du mouvement, en écrivant :

$$m\,\frac{dw_1}{dt} = -\frac{\partial\varphi}{\partial x_1} + \tau\,\Delta\varphi\left[(w_2 - w_1) + \frac{KT}{m}\left(\frac{\partial}{\partial w_2} - \frac{\partial}{\partial w_1}\right)\operatorname{Log} f_{12}\right] \tag{9}$$

Au terme habituel en $-\nabla\varphi$ se superpose un terme donnant à cette équation un caractère irréversible. Il contient le temps de relaxation τ et l'entropie fine $\log f_{12}$, notion introduite par J. Fronteau (⁶). τ et $\log f_{12}$ traduisent des effets collectifs. Le laplacien $\Delta\varphi$ de φ est en facteur. Par suite ce terme irréversible s'annule pour un potentiel en $1/r$. Bien que l'interaction entre deux molécules soit d'origine coulombienne le potentiel φ est par suite d'effets quantiques du type Lennard Jones ou Sutherland, son laplacien n'est pas nul et le terme irréversible intervient. Dans cette perspective, l'irréversibilité est d'origine quantique.

L'équation de Liouville déduite de cette nouvelle loi du mouvement est

$$\begin{aligned} &\frac{\partial f_{12}}{\partial t} + w_1\frac{\partial f_{12}}{\partial x_1} + w_2\frac{\partial f_{12}}{\partial x_2} - \frac{1}{m}\,\frac{\partial\varphi}{\partial x_1}\,\frac{\partial f_{12}}{\partial w_1} - \frac{1}{m}\,\frac{\partial\varphi}{\partial x_2}\,\frac{\partial f_{12}}{\partial w_2} \\ &= \frac{\tau\,\Delta\varphi}{m}\left[\left[\frac{\partial}{\partial w_1}\left[(w_1 - w_2)f_{12} + \frac{KT}{m}\left(\frac{\partial f_{12}}{\partial w_1} - \frac{\partial f_{12}}{\partial w_2}\right)\right]\right] + [1 \leftrightarrow 2]\right]. \end{aligned} \tag{10}$$

A l'équilibre maxwellien, le terme irréversible s'annule.

Effectuons maintenant dans le second membre de (10), l'approximation

$$f_{12} = f_1 f_2 e^{-\varphi\ KT}. \tag{11}$$

Cette approximation est valable si dans le développement de f_{12} en fonction de f_1, f_2 et de leurs dérivées, le terme (11) est dominant. Ce fait a été établi dans les travaux qui ont conduit à l'équation cinétique Frey-Salmon. Admettons en outre que les fonctions f_1 et f_2 varient très peu en position à l'intérieur de la sphère d'interaction. Nous allons obtenir deux résultats. D'une part en multipliant par $\mathbf{dx}_{12}\ \mathbf{dw}_2$ ($\mathbf{x}_{12} = \mathbf{x}_2 - \mathbf{x}_1$), en intégrant et en tenant compte de

$$a^2 = \int_0^\infty \Delta\varphi\, e^{-\varphi/KT} x^2\, dx = \int_0^\infty \frac{1}{KT}\left(\frac{d\varphi}{dx}\right)^2 e^{-\varphi/KT}\ x^2\, dx, \tag{12}$$

nous retrouvons l'équation cinétique Frey-Salmon avec $\partial S_1/\partial t \geqq 0$. D'autre part en posant $f = f^M\ h$, f^M désignant la distribution maxwellienne, il vient :

$$\frac{\partial S_2}{\partial t} = \frac{4\pi a^2 K^2 \tau T}{m^2} \int f_1^M f_2^M \left[\frac{h_2}{h_1}\left(\frac{\partial h_1}{\partial \mathbf{w}_1}\right)^2 + \frac{h_1}{h_2}\left(\frac{\partial h_2}{\partial \mathbf{w}_2}\right)^2\right] \mathbf{dx}_1\, \mathbf{dw}_1\, \mathbf{dw}_2 \geqq 0. \tag{13}$$

Les entropies simple et double S_1 et S_2 ne peuvent décroître. Cette nouvelle loi du mouvement assure la cohérence entre la dynamique et la thermodynamique.

3. CONCLUSION. — Nous avons modifié la loi de la dynamique dans un champ de forces de telle manière qu'elle entraîne sous cette nouvelle forme le second principe de la thermodynamique, alors que sous sa forme usuelle, elle ne pouvait en rendre compte. Le prix à payer a été lourd, car il a fallu introduire des effets collectifs. Ainsi l'interaction entre deux particules n'est plus totalement indépendante du comportement de la population des particules.

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Conservatoire national des Arts et Métiers,
292, rue Saint-Martin,
75141 Paris Cedex 03.

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On Functional Relations between Reduced Distribution Functions and Entropy Production by Non-Hamiltonian Perturbations

R. Dobbertin

Université Paris VII, Laboratoire de Physique Théorique et Mathématique, Paris, France

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Abstract

On functional relations between reduced distribution functions and entropy production by non-hamiltonian perturbations. R. Dobbertin (Université Paris VII, Laboratoire de Physique Théorique et Mathématique, Paris, France). *Physica Scripta (Sweden) 14*, 85–88, 1976.

Functional relations are derived which link the reduced distribution functions of a classical N-particle system through the entropy production due to microscopic deviations from hamiltonian dynamics. These relations have been used in an earlier paper for the closure of the BBGKY-hierarchy and may be useful for the establishment of collective particle models in particular and the understanding of irreversibility in general.

1. Introduction

In a recent paper [1], we established relations between reduced distribution functions and non-hamiltonian perturbations of a system of N classical particles. These relations allow to close the BBGKY-hierarchy in a new way and to reproduce certain well known approximation schemes. The non-hamiltonian perturbation was introduced in a rather formal way as a relaxation term in the Liouville equation.

In this paper, we are not concerned with the technical aspects of the closure problem, but we ask and try to answer the question whether such concise relations have a more fundamental significance in statistical mechanics. For this purpose, we derive them under less formal although quite general conditions.

As long as an N-particle system can be described by a hamiltonian, Gibbs' statistics is founded on the well-known Liouville equation. In this case, the statistics can be based on the distribution of conserved quantities, in particular energy. If a hamiltonian is not sufficient to describe the system (e.g. open systems in contact with reservoirs, random perturbations, collective models etc.), the only conserved quantity may be the extension in phase. The concept of Gibbs' ensemble still holds; as the evolution of the probability density is naturally described by a continuity equation, the only possible generalization of the Liouville equation is to allow that the particles of the system may move according to other equations of motion than the hamiltonian ones (the addition of an inhomogeneous term to the Liouville equation in form of a collision integral implies in fact the same extension).

In spite of the great success of Hamilton's dynamics, there are some fundamental reasons to assume that real processes follow only approximately the hamiltonian laws of evolution. As Ruelle [2] pointed out, the time evolution of large systems of particles as considered in statistical mechanics is probably characterized by a sensitive dependence on initial conditions. On the one hand, a real physical system is never totally isolated and even very weak random perturbations will be amplified and shall affect significantly the evolution of the system. On the other hand, very small systematic deviations from the hamiltonian interparticle forces, in particular collective contributions, will in general modify considerably the microscopic time evolution. Recently, Ingarden and Kossakowski [3] claimed the need of generalized dynamics for a sound foundation of quantum statistical mechanics. Assuming the particle dynamics to be described by semi-group rather than group transformations (and that leads immediately to non-hamiltonian dynamics), they got, differently from the more or less subjective manipulations like coarse-graining, perturbation approaches etc., true (non cyclic) irreversibility without using the thermodynamic limit with its serious restriction of generality.

The persistent inability to prove the ergodic hypothesis in order to justify the microcanonical ensemble could express the possibility that real physical systems are not ergodic [2]. This conjecture and the various attempts to understand elementary particles as collective phenomena are sufficient motivations for exploring the concept of statistical mechanics of non-hamiltonian systems.

We generalize thus Gibbs' statistical mechanics according to an approved heuristic principle by attenuation of its fundamental assumptions; the general admission of non-hamiltonian dynamics would not correspond to observations; but we suppose the microscopic evolution to be determined by perturbed Hamilton equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} + X_i(x_1, \ldots, x_N, t) \tag{1}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} + Y_i(x_1, \ldots, x_N, t) \tag{2}$$

such that in the macroscopic limit, the ensemble averages of total momentum and energy

$$P = \sum_i \int p_i D_N \, \mathrm{d}\Gamma_N \tag{3}$$

$$E = \int H D_N \, \mathrm{d}\Gamma_N \tag{4}$$

be conserved in absence of external forces.

The hamiltonian expresses that part of reality that can be described in invariant space and time (characterized by the corresponding conservation laws) and the perturbations X and Y reflect the (random or systematic) deviations of real systems from the idealized hamiltonian world.

For the sake of simplicity, we assume the system to be isolated (zero-boundary-conditions for the distribution functions), but the system is nevertheless open in the sense that the particles (the

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hamiltonian degrees of freedom) interact with something else inside the volume of the system.

The probability density D_N is described in the phase space spanned by the $x_i = (p_i, q_i)$, $i = 1, 2, \ldots, N$ and its temporal evolution obeys the generalized Liouville equation [4]:

$$\frac{\partial D_N}{\partial t} + \sum_i \left(\frac{\partial H}{\partial p_i}\frac{\partial D_N}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial D_N}{\partial p_i}\right) + \sum_i \left[\frac{\partial}{\partial p_i}(X_i D_N) + \frac{\partial}{\partial q_i}(Y_i D_N)\right] = 0 \tag{5}$$

$$\int D_N \mathrm{d}\Gamma_N = 1; \quad \mathrm{d}\Gamma_N = \mathrm{d}x_1 \ldots dx_N \tag{6}$$

The "divergence" of the non-hamiltonian "forces" must not be identically zero, otherwise they could be brought into a hamiltonian form:

$$\alpha_i \equiv \frac{\partial \dot{p}_i}{\partial p_i} + \frac{\partial \dot{q}_i}{\partial q_i} = \frac{\partial X_i}{\partial p_i} + \frac{\partial Y_i}{\partial q_i} \not\equiv 0 \tag{7}$$

The Gibbs entropy (which gives in the asymptotic limit the correct expression for the thermodynamic equilibrium) is

$$S_N = S_{N0} - \int D_N \ln D_N \mathrm{d}\Gamma_N$$

and its time derivative becomes after substitution of (5)

$$\dot{S}_N = -\int \frac{\partial D_N}{\partial t}(A + \ln D_N)\,\mathrm{d}\Gamma_N$$
$$= \sum_i \int D_N \left(\frac{\partial X_i}{\partial p_i} + \frac{\partial Y_i}{\partial q_i}\right) \mathrm{d}\Gamma_N = \sum_i \int \alpha_i D_N \mathrm{d}\Gamma_N \tag{8}$$

The α_i can thus be considered as microscopic entropy production rates. Micro-irreversibility in a general sense means $\dot{S}_N > 0$, unless the equilibrium state is reached. A sufficient, but probably not necessary condition for $\dot{S}_N > 0$ is the assumption $\alpha_i > 0$, which selects among all admissible dynamical models a particular class that we call strongly micro-irreversible. In the following paper, we will give a particular model for a non-hamiltonian system for which the Gibbs entropy is not conserved.

The question of measurability is not really important for our purpose; we mention only that the microscopic entropy production rate is in general not directly measurable in one macroscopic experiment. According to Jaynes [5], the Gibbs entropy is the minimum value of the measured entropy and the microscopic entropy production rate is therefore the minimum growth rate of measured entropy. We add the remark, that we limit ourselves to classical systems, the problems being the same in quantal systems (excepted the terminology).

2. Functional derivatives of the reduced distribution functions

$D_N = 1$ is no longer a solution of the generalized Liouville equation and the concept of equal a priori probabilities is no longer justified. It is possible to take this fact into consideration in setting up the initial distribution. But we prefer not to prepare particular initial states; therefore we make the mentioned property of the generalized Liouville system explicit in the definitions of the reduced distribution functions. We introduce a set of conveniently gentle functions χ_a which attribute certain weights to the solutions of the generalized Liouville equation and define the reduced distribution functions now as follows:

$$F_a(x_A, t) = \frac{V}{Q_N} \int \exp\left[-\sum_{a,i} \chi_a(x_i)\right] D_N \mathrm{d}x_2 \ldots \mathrm{d}x_N \tag{9}$$

$$F_{ab}(x_1, x_2, t) = \frac{V^2}{Q_N} \int \exp\left[-\sum_{a,i} \chi_a(x_i)\right] D_N \mathrm{d}x_3 \ldots \mathrm{d}x_N \tag{10}$$

with

$$Q_N = \int \exp\left[-\sum_{a,i} \chi_a(x_i)\right] D_N \mathrm{d}\Gamma_N. \tag{11}$$

If the initial condition or the final asymptotic state allow it, we can put $\chi = 0$ and recover the Liouville statistics.

Latin indices indicate particle species and serve frequently as shorthands for the phase space variables. N_a is the number of particles of species a and $n_a = N_a/V$. We use now for the six generalized forces the notations $K_i = (X_i, Y_i)$.

Let Λ_N be the hamiltonian Liouville operator; we write then the generalized Liouville equation as

$$\frac{\partial D_N}{\partial t} + \Lambda_N D_N + \sum_i K_i \frac{\partial D_N}{\partial x_i} + \alpha_N D_N = 0 \tag{12}$$

with

$$\alpha_N = \sum_{i=1}^{N} \alpha_i.$$

Q_N, F_a, F_{ab} etc. are functionals of the α_i and we are going now to calculate their functional derivatives with respect to the α_i. As (12) contains

$$\alpha_i \equiv \frac{\partial K_i}{\partial x_i} \equiv K_{i,i} \tag{13}$$

as well as K_i, we write for instance the functional Q_N in the form

$$Q_N(K_i + \varepsilon\varphi_i, K_{i,i} + \varepsilon\varphi_{i,i})$$
$$= \int e^{-\chi_N}\left\{D_N(|K_i, K_{i,i}) + \varepsilon\left[\sum_i \varphi_i \frac{\partial D_N}{\partial K_i} + \sum_i \varphi_{i,i}\frac{\partial D_N}{\partial K_{i,i}}\right] + \ldots\right\} \mathrm{d}\Gamma_N. \tag{14}$$

Using the definition of the first functional derivative

$$\left.\frac{\mathrm{d}Q_N}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = \int \frac{\delta Q_N}{\delta K(x_1)} \varphi(x_1)\,\mathrm{d}x_1,$$

we get by partial integration

$$\left.\frac{\mathrm{d}Q_N}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = \sum_i \int \varphi_i \left[e^{-\chi_N}\frac{\partial D_N}{\partial K_i} - \frac{\partial}{\partial x_i}\left(e^{-\chi_N}\frac{\partial D_N}{\partial K_{i,i}}\right)\right] \mathrm{d}\Gamma_N$$

and finally

$$\frac{\delta Q_N}{\delta K_a(x_1)} = N_a \int \left[e^{-\chi_N}\frac{\partial D_N}{\partial K_1} - \frac{\partial}{\partial x_1}\left(e^{-\chi_N}\frac{\partial D_N}{\partial \alpha_1}\right)\right] \mathrm{d}x_2 \ldots \mathrm{d}x_N \tag{15}$$

and proceeding in the same way, we obtain

$$\frac{\delta}{\delta K_b(y)} \int e^{-\chi_N} D_N \mathrm{d}x_2 \ldots \mathrm{d}x_N$$
$$= \int e^{-\chi_N}\left(\delta(x_1 - y)\frac{\partial D_N}{\partial K_a} + \frac{\partial \delta(x_1 - y)}{\partial x_1}\frac{\partial D_N}{\partial K_{a,1}}\right) \mathrm{d}x_2 \ldots \mathrm{d}x_N$$
$$+ (N_b - \delta_{ab}) \int \left[e^{-\chi_N}\frac{\partial D_N}{\partial K_b} - \frac{\partial}{\partial x_2}\left(e^{-\chi_N}\frac{\partial D_N}{\partial K_{b,2}}\right)\right]$$
$$\times\, \delta(x_2 - y)\,\mathrm{d}x_2 \ldots \mathrm{d}x_N. \tag{16}$$

The δ-functions come in because $\int D_N \mathrm{d}x_2 \dots \mathrm{d}x_N$ is not only a functional but also a function of α.

In order to calculate (15) and (16), we need now the partial derivatives of D_N with regard to K and α. To get them, we derive (12) with respect to α and K:

$$\left(\frac{\partial}{\partial t} + \Lambda_N + \sum_i K_i \frac{\partial}{\partial x_i} + \alpha_N\right) \frac{\partial D_N}{\partial \alpha_1} = -D_N \tag{17}$$

$$\left(\frac{\partial}{\partial t} + \Lambda_N + \sum K_i \frac{\partial}{\partial x_i} + \alpha_N\right) \frac{\partial D_N}{\partial K_1} = -\frac{\partial D_N}{\partial x_1}. \tag{18}$$

The solutions of the equations of motion (1) and (2) are the characteristics of the first order partial differential equations (12), (17) and (18).

In order to make our initial conditions maximally noncommital, we switch on the perturbing forces in a sufficiently smooth manner at $t = t_0$. Using shorthands like $\alpha(\tau) \equiv \alpha(x(\tau), \tau)$, we can now easily write down the solutions of (12), (17) and (18):

$$D_N(t) = \exp\left(-\int_{t_0}^{t} \alpha_N(\sigma)\,\mathrm{d}\sigma\right) D_N(t_0) \tag{19}$$

$$\frac{\partial D_N(t)}{\partial \alpha_1} = -(t-t_0)\, D_N(t) \tag{20}$$

$$\frac{\partial D_N(t)}{\partial K_1} = -\int_{t_0}^{t} \frac{\partial D_N(\tau)}{\partial x_1(\tau)} \exp\left(-\int_{\tau}^{t} \alpha_N(\sigma)\,\mathrm{d}\sigma\right) \mathrm{d}\tau. \tag{21}$$

The substitution of (20) and (21) into (15) yields

$$\begin{aligned}\frac{\delta \ln Q_N}{\delta K_1} = \frac{N_a}{Q_N} \int \Big\{ & \frac{\partial}{\partial x_1}((t-t_0)\, e^{-\chi_N} D_N(t)) \\ & - e^{-\chi_N} \int_{t_0}^{t} \frac{\partial D_N(\tau)}{\partial x_1(\tau)} \exp\left(-\int_{\tau}^{t} \alpha_N(\sigma)\,\mathrm{d}\sigma\right) \mathrm{d}\tau \Big\} \mathrm{d}x_2 \dots \mathrm{d}x_N\end{aligned} \tag{22}$$

With the aid of the rule

$$\frac{\delta Q_N}{\delta \alpha(x)} = \int \frac{\delta K(x_1)}{\delta \alpha(x)} \frac{\delta Q_N}{\delta K(x_1)} \mathrm{d}x_1 \tag{23}$$

and the relation

$$\frac{\partial}{\partial x_1} \frac{\delta K(x_1)}{\delta \alpha(x)} = \delta(x - x_1) \tag{24}$$

derived by functional differentiation of (13), we calculate now the functional derivatives with respect to the α_a:

$$\frac{\delta \ln Q_N}{\delta \alpha_a(x)} = -n_a(t-t_0)[F_a(x, t\,|\,\alpha) + R_N(x, t\,|\,\alpha)] \tag{25}$$

$$\begin{aligned}R_N(x, t\,|\,\alpha) = -V \int \frac{\delta K(x_1)}{\delta \alpha(x)} e^{-\chi_N} \frac{1}{t-t_0} \int_{t_0}^{t} \frac{\partial D_N(\tau)}{\partial x_1(\tau)} \\ \times \exp\left(-\int_{\tau}^{t} \alpha_N(\sigma)\,\mathrm{d}\sigma\right) \mathrm{d}\tau\, \mathrm{d}\Gamma_N.\end{aligned} \tag{26}$$

If the system is strongly micro-irreversible,

$$R_N(x, t\,|\,\alpha) \underset{t-t_0 \to \infty}{\Rightarrow} 0.$$

Otherwise, we write $\alpha = \int \alpha D_N \mathrm{d}\Gamma_N + \Delta\alpha = \eta + \Delta\alpha$, where $\eta > 0$ according to the assumption of micro-irreversibility and we get at least

$$R_N(x, t\,|\,\eta) \underset{t-t_0 \to \infty}{\Rightarrow} 0.$$

In the limit $t_0 \to -\infty$, we have thus

$$F_a(x, t\,|\,\eta) = -\frac{1}{n_a(t-t_0)} \left.\frac{\delta \ln Q_N}{\delta \alpha_a(x, t)}\right|_{\alpha \to \eta}. \tag{27}$$

The substitution of (20) and (21) into (16) and the use of the rule (23) yield

$$\begin{aligned}&\frac{1}{Q_N} \frac{\delta}{\delta \alpha_b(y)} \int e^{-\chi_N} D_N \,\mathrm{d}x_2 \dots \mathrm{d}x_N \\ &\quad = -n_b(t-t_0)\, F_{ab}(x_1, y, t) - \delta(x_1 - y)\delta_{ab} F_a \\ &\qquad - V \iint_{t_0}^{t} e^{-\chi_N} \exp\left(-\int_{\tau}^{t} \alpha_N(\sigma)\,\mathrm{d}\sigma\right) \\ &\qquad \times \left[\frac{\delta K(x_1)}{\delta \alpha_b(y)} \frac{\partial D_N(\tau)}{\partial x_1(\tau)} + (N_b - \delta_{ab}) \frac{\delta K(x_2)}{\delta \alpha_b(y)} \frac{\partial D_N(\tau)}{\partial x_2(\tau)}\right] \mathrm{d}\tau\, \mathrm{d}x_2 \dots \mathrm{d}x_N\end{aligned} \tag{28}$$

The last integral in (28) disappears again in the asymptotic limit $\alpha \to \eta$, $t - t_0 \to \infty$. We find thus, in the asymptotic limit, the functional derivative of F_a with respect to α_b:

$$\begin{aligned}\frac{\delta F_a}{\delta \alpha_b} &= -\frac{\delta \ln Q_N}{\delta \alpha_b} F_a + \frac{1}{Q_N} \frac{\delta}{\delta \alpha_b} \int e^{-\chi_N} D_N \,\mathrm{d}x_2 \dots \mathrm{d}x_N \\ &= n_b(t-t_0) \left[F_a F_b - F_{ab} - \frac{\delta_{ab}}{n_b} F_a\right]\end{aligned} \tag{29}$$

or

$$F_{ab} = F_a F_b - \frac{1}{n_b(t-t_0)} \frac{\delta F_a}{\delta \alpha_b} - \frac{\delta_{ab}}{n_b} F_a. \tag{30}$$

In a similar way, we get

$$F_{abc} = F_{ab} F_c - \frac{1}{n_c(t-t_0)} \frac{\delta F_{ab}}{\delta \alpha_c} - \frac{\delta_{ac} + \delta_{bc}}{n_c} F_{ab} \tag{31}$$

and so on for the higher distribution functions.

We see that the eventual weighting of the Liouville distribution does not affect these relations. It is easy to verify, that a functional differentiation with respect to the weights χ_a would give the same relations (30), (31) etc. In that case, one recovers Bogoljubov's generating functional for the BBGKY-hierarchy. In another paper, we will study the possibility to interprete the weights as the kernels of integral transforms relating different ranks of randomness in the sense of Tchen's repeated cascades in turbulence theory [6].

3. Conclusions

We have derived with a minimum of assumptions the expected functional relations that link two reduced distribution functions through the microscopic entropy production.

As the tendency to overcome the fundamental problems of statistical mechanics by attenuation of the hamiltonian dynamics is rather new and certainly not yet generally admitted, we have spent some place for arguments in favour of this procedure, but it was not the purpose of this paper to study the various problems raised by this generalized approach. Nevertheless, the established relation between correlation and entropy production is thought to be a significant, although tiny contribution to the general problem and it may be useful as well for the study of collective elementary particle models.

As we mentioned, there are other ways to get these functional relations much easier and the closure techniques developed in [1] are independent of the specific meaning of α and do thus not hinge upon the interpretation given in this paper.

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Université Paris VII
Laboratoire de Physique Théorique et Mathématique
Tour 33/43, 1er ét.
F 75221 Paris Cedex 05

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Thermodynamic Properties of Non-Equilibrium States Subject to Fokker-Planck Equations

Hiroshi HASEGAWA

Department of Physics, Kyoto University, Kyoto 606

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We investigate the relationship between fluctuation theory and thermodynamic theory of non-equilibrium states assuming the Fokker-Planck equation for the evolution law, and deduce two formulas corresponding to the entropy and entropy-production balance equations in thermodynamics

$$\text{I.}\qquad \frac{\partial}{\partial t}\left(-\log\frac{\psi}{\psi_0}\right)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi=V_\mu X_\mu\psi\geq 0\,,$$

$$\text{II.}\qquad \frac{\partial}{\partial t}(V_\mu X_\mu)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\leq 0\,.$$

(ψ and ψ_0 are time-dependent and steady-state solutions of the F-P equation. They are also contained in J_λ, V_μ, X_μ and $T_{\mu\nu}$). The inequality in I represents the second law of thermodynamics (ensured automatically by the F-P equation) while that in II the evolution criterion for stability (not automatically ensured) reflecting the Glansdorff-Prigogine theory, and are considered to realize the thermodynamic proposition without recourse to the local-equilibrium assumption. We discuss briefly the laser instability as an example.

§ 1. Introduction

Fokker-Planck equations have been a useful tool in studies of fluctuation phenomena since the physical investigation of the Brownian motion was advanced in early days.[1,2] It was attempted also with the equations to provide a statistical mechanical framework for the theory of non-equilibrium states so that the pertinent physical law may be formulated; for example, the entropy increase and Onsager's principle.[*]

Thus it would be natural to imagine that an intimate relationship might exist between the statistical theory of fluctuations with Fokker-Planck equations and the thermodynamic theory of non-equilibrium states due to Glansdorff and Prigogine.[5,6] To date, however, little has been analyzed about the relationship. The present paper (together with a forthcoming one) aims to fill this gap: We intend to show that several important concepts in thermodynamics can be incorporated

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[*] The first important investigation along this direction which we wish to cite is the paper by M. S. Green[3] who showed the H-theorem and a derivation of the Onsager's reciprocal relations in the framework of Fokker-Planck equations, and the paper by N. Hashitsume[4] who showed the Onsager's principle (according to his nomination) of variation in some limited case of the equations. (For this see a recent paper by the author.[15])

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into the statistical mechanical framework by means of the Fokker-Planck equations. The concepts of interests are; entropy flow, entropy production, balance equations, stability-instability, and also several types of variational principles. In this paper we discuss these matters except the variational principles for which a more comprehensive treatment is necessary and is deferred to our later paper.[10] Sections 2∼4 are devoted to establishing the two formulas of entropy and entropy-production balance equation. Their thermodynamic significance is discussed in § 5, which is shown to be connected closely with the evolution criterion of Glansdorff and Prigogine[7] and is useful in studies of instability.

In spite of the thermodynamic feature so announced, we must remark here on a difference between the starting point assumed by the ordinary thermodynamics and that by our Fokker-Planck framework. That is, the former requires the so-called "local equilibrium assumption" on the basis of which the entropy concept is introduced similarly to that in thermal equilibrium, whereas in the latter it is discarded and replaced by the explicit use of "ensemble" the probability density of which is made subject to the Fokker-Planck equation. However, this change will make the applicability of thermodynamics unifying. A good example is laser, for which a qualitative discussion is included in § 6.

§ 2. Balance equations

Let us denote a probability density function of the set of n state variables $\{x_\mu\}$ (in the Cartesian coordinate system) by ψ. Then, the Fokker-Planck equation for ψ which we treat throughout this study will be chosen in the form

$$\frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial x_\mu}(v_\mu \psi) + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial \psi}{\partial x_\nu}\right), \tag{2·1}$$

where $D_{\mu\nu}$, a symmetric and positive tensor satisfying

$$D_{\nu\mu} = D_{\mu\nu}\,,\ D_{\mu\nu}\xi_\mu \xi_\nu \geq 0 \text{ for any real vector } \xi_\mu\,, \tag{2·2}$$

will be designated as the *diffusion tensor*, and v_μ as the *total drift vector*. (In presenting such equations as in the above, we use the usual summation convention such that a doubly repeated index implies the summation with respect to that index.) These are in general functions of $\{x_\mu\}$ and t. It is known[8] that Eq. (1) is a truncation up to second order of a series with derivatives to infinite order, i.e.,

$$\frac{\partial \psi}{\partial t} = \sum_{s=1}^{\infty} \frac{(-1)^s}{s!} \frac{\partial^s}{\partial x_{\mu_1} \cdots \partial x_{\mu_s}} (K_{\mu_1 \cdots \mu_s} \psi) \tag{2·3}$$

so that the drift vector and the diffusion tensor are expressed as

$$v_\mu = K_\mu - \frac{1}{2}\frac{\partial K_{\mu\nu}}{\partial x_\nu} \tag{2·4}$$

and

$$D_{\mu\nu}=\frac{1}{2}K_{\mu\nu}\,. \tag{2·5}$$

As is known from the theory of stochastic processes,[9] the coefficients K's are related to the conditional expectation of the Wiener process as follows:

$$K_\mu(x)=\lim_{\Delta t\downarrow 0}\left\langle\frac{x_\mu(t+\Delta t)-x_\mu(t)}{\Delta t};\ x_\lambda(t)=x_\lambda\right\rangle, \tag{2·6}$$

$$K_{\mu\nu}(x)=\lim_{\Delta t\downarrow 0}\left\langle\frac{(x_\mu(t+\Delta t)-x_\mu(t))\,(x_\nu(t+\Delta t)-x_\nu(t))}{\Delta t};\ x_\lambda(t)=x_\lambda\right\rangle. \tag{2·7}$$

It is notable that the mean forward derivative $K_\mu(x)$ which arises in the corresponding Langevin equation for a Brownian motion $\boldsymbol{B}(x(t))$ in

$$dx_\mu=K_\mu(x)\,dt+dB_\mu \tag{2·8}$$

as its mean velocity is generally unequal to the total drift $v_\mu(x)$, but is related to the latter as Eq. (2·4). The writing of a Fokker-Planck equation in the form (2·1) (which retains the diffusion part as self-adjoint) is not just for the purpose of convenience but for the physical significance of the total drift v_μ in many respects.[*] Note that the adjoint manipulation associated with the spatial differential operations on ψ is possible only under the satisfaction of the boundary condition for ψ: That is, the probability density function $\psi(x\ t)$ must be rapidly decreasing for $|x|\to\infty$ (the *natural boundary condition* according to Graham[8]) which we assume throughout.

Let us rewrite the Fokker-Planck equation (2·1) in the form of equation of continuity, and consider its effect on any quantity M represented as a function of the space-time variables:

$$\frac{\partial\psi}{\partial t}+\frac{\partial}{\partial x_\mu}(J_\mu\psi)=0\,. \tag{2·9}$$

We may write an equation involving $M\psi$, by virtue of Eq. (2·9), as

$$\frac{\partial}{\partial t}(M\psi)+\frac{\partial}{\partial x_\mu}(J_\mu M\psi)=\left(\frac{\partial M}{\partial t}+J_\mu\frac{\partial M}{\partial x_\mu}\right)\psi\,. \tag{2·10}$$

Here, the current vector J_μ which continues ψ may be obtained from Eq. (2·1) as

$$J_\mu=v_\mu-D_{\mu\nu}\frac{\partial}{\partial x_\nu}\log\psi\,, \tag{2·11}$$

showing that the current vector is linearly dependent on $\log\psi$; a fact which is specific to the Fokker-Planck equations. Equation (2·10) represents the local time variation of the density associated with M which consists of two origins;

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[*] This conforms to a description by R. Graham in a recent article,[8] where he changed the notation of the total drift (the present v_μ) to K_μ.

viz., the divergence term $-(\partial/\partial x_\mu)(J_\mu M\psi)$ and the source term $((\partial M/\partial t)+J_\mu \times(\partial M/\partial x_\mu))\psi$. Thus, it corresponds to the *balance equation* associated with the quantity M in thermodynamic theory of irreversible processes.[6] (Here, the probability density ψ replaces the mass density of a constituent substance, and the space of the state variables (i.e., the phase space) by which the F-P equation is written replaces the real space.) It is more clearly demonstrated as follows:

$$\frac{d}{dt}\int_\Omega M\psi dx = \int_{\partial\Omega} M\psi J_\mu d\sigma_\mu(x) + \int_\Omega \left(\frac{\partial M}{\partial t} + J_\mu \frac{\partial M}{\partial x_\mu}\right)\psi dx\,, \qquad (2\cdot 12)$$

where the two kinds of the integration are specified by the volume element dx and the μ-th normal component of the surface element $d\sigma_\mu(x)$ of a region Ω whose boundary, $\partial\Omega$, is a smooth surface of Ω. On the right-hand side of (2·12) the first surface integral represents the contribution to M in Ω flowing from outside and the second volume integral that produces within Ω itself. The natural boundary condition on ψ ensures that the integral on the whole space (denoted by R^n) makes the flow contribution to vanish, so that

$$\frac{d}{dt}\int_{R^n} M\psi dx = \int_{R^n} \left(\frac{\partial M}{\partial t} + J_\mu \frac{\partial M}{\partial x_\mu}\right)\psi dx\,. \qquad (2\cdot 13)$$

§ 3. Entropy and entropy production

The notion "entropy production" is a basic one in thermodynamics of irreversible processes, which we wish to formulate from the present standpoint. Here we assume that the diffusion process described by the Fokker-Planck equation (2·1) is *stationary* by requiring the coefficient functions v_μ and $D_{\mu\nu}$ to be all time-independent. We also assume the existence of a steady-state distribution ψ_0 which satisfies

$$0 = -\frac{\partial}{\partial x_\mu}(v_\mu \psi_0) + \frac{\partial}{\partial x_\mu}\left(D_{\mu\nu}\frac{\partial \psi_0}{\partial x_\nu}\right) \qquad (3\cdot 1)$$

under the natural boundary condition. This may impose some further restrictions on the nature of the total drift v_μ and the diffusion coefficients $D_{\mu\nu}$, which we will discuss later to an extent of the stability consideration.

Entropy is a curious quantity since Boltzmann, Gibbs, Ehrenfest and Shannon.[*] Concerning the Fokker-Planck equations (2·1) and (3·1), the natural definition of the entropy functional of the distribution ψ relative to ψ_0 is the following integral:

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[*] We will not go into the historical problem of how to define the entropy in non-equilibrium states.[10] Our standpoint is, however, that as far as concerning Fokker-Planck equations the adoption of the Gibbs entropy functional could provide a far-reaching understanding of thermodynamics. Note that De Groot and Mazur[6] used the same Gibbs functional to discuss the entropy balance equation set up in the coordinate space. The present formulation extends their treatment to the whole phase space.

$$S\{\psi,\psi_0\}=-\int\left(\log\frac{\psi}{\psi_0}\right)\psi dx\,. \tag{3·2}$$

This is under the normalization condition

$$\int\psi dx=\int\psi_0 dx=1\,, \tag{3·3}$$

which are ensured by the respective Fokker-Planck equations. This suggests to introduce the *entropy* for the present purpose as a space-time function $M(x\ t)$ whose balance equation is to be sought:

$$M=-\log\frac{\psi}{\psi_0}\,. \tag{3·4}$$

Our first theorem, then, is expressed by the formula which corresponds to the *entropy balance* in thermodynamics as follows:

$$\frac{\partial}{\partial t}\left(-\log\frac{\psi}{\psi_0}\right)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi=V_\mu X_\mu\psi\,, \tag{3·5}$$

where

$$X_\mu\equiv\frac{\partial}{\partial x_\mu}\left(-\log\frac{\psi}{\psi_0}\right), \tag{3·5a}$$

$$V_\mu\equiv D_{\mu\nu}X_\nu=D_{\mu\nu}\frac{\partial}{\partial x_\nu}\left(-\log\frac{\psi}{\psi_0}\right), \tag{3·5b}$$

and regarding the current vector introduced in (2·16)

$$J_\mu=v_\mu-v_\mu{}^0+V_\mu\,,\quad v_\mu{}^0\equiv D_{\mu\nu}\frac{\partial}{\partial x_\nu}\log\psi_0\,. \tag{3·5c}$$

We have arranged this formula together with several defining equalities so that it may preserve a formal analogy to the usual thermodynamic version of the entropy balance. That is, the divergence-characteristic term of the entropy flow $J_\lambda(-\log(\psi/\psi_0))\psi$ plus the extra one $-V_\lambda\psi$ on the left-hand side and a term bilinear in regards to the two vectors X_μ and V_μ defined in Eqs. (3·5a) and (3·5b), respectively, on the right-hand side of Eq. (3·5). Evidently, the vector X_μ corresponds to the (generalized) *force* and V_μ to the *flux*, although in the present version these quantities contain the instantaneous distribution $\psi(x\ t)$; a basically different feature from what the ordinary thermodynamics indicates. The point of implication of formula (3·4) is that the removal of the local equilibrium assumption in the ordinary theory still enables one to maintain its essence of the assertion of entropy balance written in the phase space in the present Fokker-Planck framework, provided the entropy density is so defined as to conform to the Gibbs functional.

Thus, in view of the right-hand expression of Eq. (3·5), we designate the quantity $V_\mu X_\mu$ as the *entropy production* in the present framework. It is then interesting to inquire the balance equation associated with this quantity in connection with the work of Glansdorff and Prigogine.[5] Our second theorem is to answer to this inquiry, and is expressed as follows:

$$\frac{\partial}{\partial t}(V_\mu X_\mu)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$

$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi, \tag{3·6}$$

where the tensor $T_{\mu\nu}$, *designated as the stress tensor, is given by*

$$T_{\mu\nu}=-\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda{}^0)+D^{-1}_{\mu\lambda}\frac{\partial}{\partial x_\nu}(v_\lambda-v_\lambda{}^0)+\frac{1}{2}J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda} \tag{3·6a}$$

in which D^{-1} *is the inverse tensor of* $D(D^{-1}_{\mu\lambda}D_{\lambda\nu}=\delta_{\mu\nu})$ *and* $v_\lambda{}^0$ *is defined in Eq.* (3·5c). We will show the derivation of the two formulas (3·5) and (3·6) and discuss their physical significance separately in the following sections. Here we note a simplification of the expression (3·6a) under the satisfaction of the *potential condition.*[8),11)]

If there exists a set of symmetry relations among the n components of the vector $(D^{-1}v)_\mu=D^{-1}_{\mu\lambda}v_\lambda$

$$\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda)=\frac{\partial}{\partial x_\mu}(D^{-1}_{\nu\lambda}v_\lambda), \tag{3·7}$$

then the differential form $-D^{-1}_{\mu\lambda}v_\lambda dx_\mu$ is the total differential of a scalar function denoted by ϕ so that

$$d\phi=-D^{-1}_{\mu\lambda}v_\lambda dx_\mu\,. \tag{3·8}$$

It satisfies

$$D_{\mu\nu}\frac{\partial\phi}{\partial x_\nu}=-v_\mu$$

and, by setting $-(\partial\phi/\partial x_\mu)=(1/\psi_0)(\partial\psi_0/\partial x_\mu)$, is equivalent to

$$-v_\mu\psi_0+D_{\mu\nu}\frac{\partial\psi_0}{\partial x_\nu}=0\,,$$

reducing to the Fokker-Planck equation for the steady-state (3·1). This is the simplest case of the potential condition[11)] for which the steady-state distribution ψ_0 is given by

$$\psi_0=e^{-\phi} \tag{3·9}$$

$$=\exp\left(\int^x D^{-1}_{\mu\nu}v_\nu dx_\mu+\text{const}\right). \tag{3·9a}$$

Under this circumstance

$$v_\lambda{}^0 = v_\lambda\,, \quad J_\lambda = V_\lambda = D_{\lambda\mu} X_\mu\,, \tag{3·10}$$

and the stress tensor $T_{\mu\nu}$ becomes symmetric and is simplified to

$$T_{\mu\nu}(=T_{\nu\mu}) = \frac{\partial^2\phi}{\partial x_\mu \partial x_\nu} + \frac{1}{2} V_\lambda \frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda}\,, \tag{3·6a$'$}$$

indicating that the principal part of the stress tensor comes from the second-order derivative tensor of the potential ϕ. Such an exposition of the tensor $T_{\mu\nu}$ is, however, always possible (even in the absence of the simplest potential condition as above), if the steady-state distribution ψ_0 is represented in terms of the potential as in (3·9) (thereby (3·9a) may not hold), so that

$$T_{\mu\nu} = \frac{\partial^2\phi}{\partial x_\mu \partial x_\nu} + \frac{1}{2} J_\lambda \frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda} + D^{-1}_{\mu\lambda} \frac{\partial}{\partial x_\nu}(v_\lambda - v_\lambda{}^0)\,. \tag{3·6a$''$}$$

(Under general circumstances the tensor $T_{\mu\nu}$ given by (3·6a″) may not be symmetric, the asymmetric part coming from the third term on the right. Note that the antisymmetric part of $T_{\mu\nu}$ is irrelevant to the balance equation (3·6).)

§ 4. Detailed derivation of the two balance equations

***Derivation of the entropy balance equation* (3·5)**

Let us put $M = \log(\psi/\psi_0)$, where ψ and ψ_0 are time-dependent and a steady-state solution of the Fokker-Planck equation, respectively, and obtain the right-hand side of the balance equation for M. For this purpose it is convenient to rewrite the respective Fokker-Planck equations in the form

$$\frac{\partial}{\partial t}\log\psi + (v_\lambda - v_\lambda{}^0 + V_\lambda)\frac{\partial}{\partial x_\lambda}\log\psi + \frac{\partial}{\partial x_\lambda}(v_\lambda - v_\lambda{}^0 + V_\lambda) = 0\,, \tag{4·1}$$

$$(v_\lambda - v_\lambda{}^0)\frac{\partial}{\partial x_\lambda}\log\psi_0 + \frac{\partial}{\partial x_\lambda}(v_\lambda - v_\lambda{}^0) = 0\,, \tag{4·2}$$

i.e., the evolution equations pertaining to the *logarithm* of the probability densities. The two velocity-vectors V_λ and $v_\lambda{}^0$ are the same as defined before, i.e.,

$$V_\lambda = D_{\lambda\nu}\frac{\partial}{\partial x_\nu}\Big(-\log\frac{\psi}{\psi_0}\Big), \quad v_\lambda{}^0 = D_{\lambda\nu}\frac{\partial}{\partial x_\nu}\log\psi_0\,. \tag{4·3}$$

A subtraction of Eq. (4·2) from (4·1) on both sides yields

$$\frac{\partial}{\partial t}\log\frac{\psi}{\psi_0} + J_\lambda\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0} = -V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0 - \frac{\partial}{\partial x_\lambda}V_\lambda\,. \tag{4·4}$$

By multiplying both sides of Eq. (4·4) by ψ, we get

$$\Big(\frac{\partial}{\partial t}\log\frac{\psi}{\psi_0} + J_\lambda\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0}\Big)\psi = \Big(-\frac{\partial}{\partial x_\lambda}V_\lambda\Big)\psi - \Big(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\Big)\psi$$

$$= -\frac{\partial}{\partial x_\lambda}(V_\lambda \psi) + V_\lambda \frac{\partial \psi}{\partial x_\lambda} - \left(V_\lambda \frac{\partial}{\partial x_\lambda} \log \psi_0\right)\psi$$

$$= -\frac{\partial}{\partial x_\lambda}(V_\lambda \psi) + V_\lambda \left(\frac{\partial}{\partial x_\lambda} \log \frac{\psi}{\psi_0}\right)\psi . \qquad (4\cdot5)$$

This last expression is inserted into the right-hand side of the balance equation, leading us to write Eq. (2·15) for $M=\log(\psi/\psi_0)$ as

$$\frac{\partial}{\partial t}\left(\log \frac{\psi}{\psi_0}\right)\psi + \frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(\log \frac{\psi}{\psi_0}\right)\psi\right) = -\frac{\partial}{\partial x_\lambda}(V_\lambda \psi) + V_\lambda\left(\frac{\partial}{\partial x_\lambda} \log \frac{\psi}{\psi_0}\right)\psi .$$

The first term on the right-hand side may be transferred to the left and incorporated into the divergence term. Consequently, introducing the "force"

$$X_\mu = \frac{\partial}{\partial x_\mu}\left(-\log \frac{\psi}{\psi_0}\right) \text{(so that } V_\mu = D_{\mu\nu} X_\nu\text{)}, \qquad (4\cdot6)$$

and making a sign-reverse, we obtain the result

$$\frac{\partial}{\partial t}\left(-\log \frac{\psi}{\psi_0}\right)\psi + \frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log \frac{\psi}{\psi_0}\right) - V_\lambda\right)\psi = V_\mu X_\mu \psi . \qquad (4\cdot7)$$

Derivation of the entropy-production balance equation (3·6)

We put $M=V_\mu X_\mu$ as before, where X_μ and V_μ are defined in (3·5a) and (3·5b) (also in (4·6) and (4·3)). Then, to deduce the right-hand side of the balance equation (3·6), we begin with the following manipulation:

$$\frac{\partial}{\partial t}(V_\mu X_\mu) + J_\lambda \frac{\partial}{\partial x_\lambda}(V_\mu X_\mu)$$

$$= V_\mu\left(\frac{\partial X_\mu}{\partial t} + J_\lambda \frac{\partial X_\mu}{\partial x_\lambda}\right) + \left(\frac{\partial V_\mu}{\partial t} + J_\lambda \frac{\partial V_\mu}{\partial x_\lambda}\right) X_\mu$$

$$= D_{\mu\nu} X_\nu \left(\frac{\partial X_\mu}{\partial t} + J_\lambda \frac{\partial X_\mu}{\partial x_\lambda}\right) + D_{\mu\nu}\left(\frac{\partial X_\nu}{\partial t} + J_\lambda \frac{\partial X_\nu}{\partial x_\lambda}\right) X_\mu$$

$$+ J_\lambda \frac{\partial D_{\mu\nu}}{\partial x_\lambda} X_\mu X_\nu$$

$$= 2V_\nu\left(\frac{\partial X_\nu}{\partial t} + J_\lambda \frac{\partial X_\nu}{\partial x_\lambda}\right) + J_\lambda \frac{\partial D_{\mu\nu}}{\partial x_\lambda} D^{-1}_{\mu\mu'} D^{-1}_{\nu\nu'} V_{\mu'} V_{\nu'} .$$

In the last expression we may use the relation

$$\frac{\partial D_{\mu\nu}}{\partial x_\lambda} D^{-1}_{\mu\mu'} D^{-1}_{\nu\nu'} = -\frac{\partial D^{-1}_{\mu'\nu'}}{\partial x_\lambda} \qquad (4\cdot8)$$

as a consequence of the derivation of the identity $D_{\mu\nu} D^{-1}_{\nu\nu'} = \delta_{\mu\nu'}$, so that we have

$$\frac{\partial}{\partial t}(V_\mu X_\mu) + J_\lambda \frac{\partial}{\partial x_\lambda}(V_\mu X_\mu)$$

$$=2V_\nu\left(\frac{\partial X_\nu}{\partial t}+J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}\right)-J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda}V_\mu V_\nu\,. \tag{4·9}$$

Thus the problem reduces to reexpressing $(\partial X_\nu/\partial t)+J_\lambda(\partial X_\nu/\partial x_\lambda)$ in terms of V_μ, $\partial V_\mu/\partial x_\nu$ etc., for which our previous result may be aided.

Let us recall Eq. (4·4), i.e.,

$$\frac{\partial}{\partial t}\log\frac{\psi}{\psi_0}+J_\lambda\frac{\partial}{\partial x_\lambda}\log\frac{\psi}{\psi_0}=-V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0-\frac{\partial}{\partial x_\lambda}V_\lambda\,, \tag{4·10}$$

where

$$J_\lambda=v_\lambda-v_\lambda^0+V_\lambda\,. \tag{4·10a}$$

We apply the differential operation $-(\partial/\partial x_\nu)$ on both sides of Eq. (4·10), writing

$$\frac{\partial}{\partial t}\frac{\partial}{\partial x_\nu}\left(-\log\frac{\psi}{\psi_0}\right)+J_\lambda\frac{\partial^2}{\partial x_\lambda\partial x_\nu}\left(-\log\frac{\psi}{\psi_0}\right)+\frac{\partial J_\lambda}{\partial x_\nu}\frac{\partial}{\partial x_\lambda}\left(-\log\frac{\psi}{\psi_0}\right)$$

$$=\frac{\partial}{\partial x_\nu}\left(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\right)+\frac{\partial^2 V_\lambda}{\partial x_\lambda\partial x_\nu}\,. \tag{4·11}$$

The last term on the left-hand side of Eq. (4·11) may be transferred to the right, and by virtue of the definition of the "force" in (4·6), Eq. (4·11) is rewritten as

$$\begin{aligned}\frac{\partial X_\nu}{\partial t}+J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}&=\frac{\partial}{\partial x_\nu}\left(V_\lambda\frac{\partial}{\partial x_\lambda}\log\psi_0\right)-\frac{\partial J_\lambda}{\partial x_\nu}X_\lambda+\frac{\partial^2 X_\lambda}{\partial x_\lambda\partial x_\nu}\\
&=\frac{\partial}{\partial x_\nu}\left(V_\mu\frac{\partial}{\partial x_\mu}\log\psi_0\right)-\frac{\partial V_\lambda}{\partial x_\nu}X_\lambda\\
&\qquad\qquad-\frac{\partial(v_\lambda-v_\lambda^0)}{\partial x_\nu}X_\lambda+\frac{\partial^2 V_\lambda}{\partial x_\lambda\partial x_\nu}\\
&=\frac{\partial}{\partial x_\nu}\left(V_\mu\frac{\partial}{\partial x_\mu}\log\psi_0\right)-\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\log\psi_0\\
&\qquad\qquad-D^{-1}_{\mu\lambda}\frac{\partial(v_\lambda-v_\lambda^0)}{\partial x_\nu}V_\mu\\
&\quad+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\log\psi+\frac{\partial^2 V_\mu}{\partial x_\mu\partial x_\nu}\,.\end{aligned} \tag{4·12}$$

(A use of Eqs. (4·10a), (4·6) and a change of running index have been made.) This last expression is readily simplified, by regrouping the 1st and 2nd and also 4th and 5th terms on the right-hand side of (4·12), so that

$$\begin{aligned}\frac{\partial X_\nu}{\partial t}+J_\lambda\frac{\partial X_\nu}{\partial x_\lambda}&=\left(\frac{\partial}{\partial x_\nu}(D^{-1}_{\mu\lambda}v_\lambda^0)-D^{-1}_{\mu\lambda}\frac{\partial(v_\lambda-v_\lambda^0)}{\partial x_\nu}\right)V_\mu\\
&\quad+\frac{1}{\psi}\frac{\partial}{\partial x_\mu}\left(\psi\frac{\partial V_\mu}{\partial x_\nu}\right)\end{aligned} \tag{4·13}$$

which can be inserted into Eq. (4·9). The result is

$$\frac{\partial}{\partial t}(V_\mu X_\mu)+J_\lambda\frac{\partial}{\partial x_\lambda}(V_\mu X_\mu)$$

$$=-2T_{\mu\nu}V_\mu V_\nu+\frac{2}{\psi}V_\nu\frac{\partial}{\partial x_\mu}\left(\psi\frac{\partial V_\mu}{\partial x_\nu}\right), \tag{4·14}$$

where

$$T_{\mu\nu}=-\frac{\partial}{\partial x_\nu}(D_{\mu\lambda}^{-1}v_\lambda{}^0)+D_{\mu\lambda}^{-1}\frac{\partial}{\partial x_\nu}(v_\lambda-v_\lambda{}^0)+\frac{1}{2}J_\lambda\frac{\partial D_{\mu\nu}^{-1}}{\partial x_\lambda}\,. \tag{4·14a}$$

Finally, in terms of this stress tensor $T_{\mu\nu}$ the entropy-production balance equation is obtained through a procedure just the same as before (from (4·4) to (4·7)) in the form

$$\frac{\partial}{\partial t}(V_\mu X_\mu\psi)+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$

$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\,. \tag{4·15}$$

§ 5. The second law of thermodynamics and the stability problem

Consider first the entropy balance equation (3·5):

I. $$\frac{\partial}{\partial t}\left(-\log\frac{\psi}{\psi_0}\right)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi=V_\mu X_\mu\psi\,.$$

The right-hand side of this formula may be designated as the entropy production density in accordance with the argument in § 3, for which by virtue of (2·2) and (3·5b)

$$V_\mu X_\mu\psi=D_{\mu\nu}X_\mu X_\nu\psi\geq 0\,, \tag{5·1}$$

indicating that the entropy production is always positive. Formula I with the inequality (5·1) is a local representation of the second law of thermodynamics. For, an integration over the whole space of both sides of I yields the well-known H-theorem[3, 12]

$$\frac{d}{dt}\int_{R^n}\left(-\log\frac{\psi}{\psi_0}\right)\psi dx=\int_{R^n}D_{\mu\nu}\left(\frac{\partial}{\partial x_\mu}\log\frac{\psi}{\psi_0}\right)\left(\frac{\partial}{\partial x_\nu}\log\frac{\psi}{\psi_0}\right)\psi dx\,.$$

$$\geq 0\,. \tag{5·2}$$

As to a restricted region Ω, the integration shows that the entropy change comes from two origins:

$$\frac{d}{dt}\int_\Omega\left(-\log\frac{\psi}{\psi_0}\right)\psi dx=\int_{\partial\Omega}\left(J_\lambda\left(-\log\frac{\psi}{\psi_0}\right)-V_\lambda\right)\psi d\sigma_\lambda(x)$$

$$+\int_{\Omega} D_{\mu\nu}\Big(\frac{\partial}{\partial x_\mu}\log\frac{\psi}{\psi_0}\Big)\Big(\frac{\partial}{\partial x_\nu}\log\frac{\psi}{\psi_0}\Big)\psi dx\,, \qquad (5\cdot 3)$$

viz., the production contribution inside of the region (≥ 0) and the flow contribution through the boundary $\partial\Omega$, the latter sign being not definite. Consequently, the left-hand side of Eq. (5·3) may be of negative sign, if the flow contribution exceeds negatively the internal production. Such is the case, as we will discuss in § 6, if an instability takes place.

Next, we discuss the entropy-production balance equation (3·6):

$$\text{II.}\qquad \frac{\partial}{\partial t}(V_\mu X_\mu \psi)+\frac{\partial}{\partial x_\lambda}\Big(J_\lambda V_\mu X_\mu - 2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\Big)\psi$$

$$=-2\Big(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\Big)\psi\,.$$

The thermodynamic theory of the Glansdorff-Prigogine states that the time derivative of the entropy production should be of negative sign for a stable evolution of the system. This is based on the consideration that the increase of entropy by the second law must be more gradual when the system approaches the equilibrium position (linked with the principle of minimum entropy production), which has been proved near-equilibrium situation and extended to far from equilibrium.[7],[*] This criterion of evolution suggests that in the present Fokker-Planck framework one puts a negative sign on the right-hand side of formula II, so that

$$\Big(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\Big)\psi\geq 0\,. \qquad (5\cdot 4)$$

Unlike the second law inequality (5·1), this inequality is not verifiable from the Fokker-Planck equation (2·1) in itself: One has always

$$\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\geq 0\,, \qquad (5\cdot 5)$$

but $T_{\mu\nu}$ is not necessarily a positive tensor.

As we have discussed in the end of § 3, the stress tensor $T_{\mu\nu}$ is expressed in terms of the potential $\phi=-\log\psi_0$ as

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[*] The statement may be interpreted in the present notation by

$$\int V_\mu\frac{\partial X_\mu}{\partial t}\psi dx\leq 0 \qquad (\text{A})$$

but not in the form expressed as the total time-derivative as in formula II. In view of this, we examine the validity of this inequality in the present framework. A mainipulation similar to § 4 gives

$$\int V_\mu\frac{\partial X_\mu}{\partial t}\psi dx=-\int(v_\lambda-v_\lambda^0)X_\lambda\frac{\partial(V_\mu\psi)}{\partial x_\mu}dx-\int\Big(\frac{\partial}{\partial x_\mu}(V_\mu\psi)\Big)^2\frac{1}{\psi}dx\,. \qquad (\text{B})$$

This shows that the potential condition (3·7) and hence (3·10) ensures the inequality $\int V_\mu(\partial X_\mu/\partial t)\cdot\psi dx\leq 0$, but otherwise (A) is generally not true.

$$T_{\mu\nu}=\frac{\partial^2\phi}{\partial x_\mu \partial x_\nu}+\frac{1}{2}J_\lambda\frac{\partial D^{-1}_{\mu\nu}}{\partial x_\lambda}+D^{-1}_{\mu\nu}\frac{\partial}{\partial x_\nu}(v_\lambda-v_\lambda{}^0). \tag{5·6}$$

Generally, the second-order derivative tensor $(\partial^2/\partial x_\mu \partial x_\nu)\phi$ dominates over the other terms (which is true at least under the potential condition and the constant diffusion tensor), and

$$\frac{\partial^2\phi}{\partial x_\mu \partial x_\nu}\xi_\mu \xi_\nu \geq 0 \text{ for } |x|\to\infty \tag{5·7}$$

because of the assumption that the steady-state distribution ψ_0 exists satisfying the natural boundary condition. Thus inequality (5·4) holds provided the deterministic motion by the potential ϕ is stable. It is an instability of the motion that the evolution criterion (5·4) becomes critical, where the left-hand side consists of the two competing quantities; one negative due to the unstable motion and the other positive which represents the effect of fluctuations relaxing the former. The Fokker-Planck equation therefore establishes a representation of the Glansdorff-Prigogine criterion of evolution in the form of competition between the organization and the randomness and the prediction of the latter to overcome the former for the over all stability.

Remark The inequality of stability evolution criterion in II is a proposition which has not been established with a general proof, as mentioned above. It is interesting, therefore, to discover its condition of validity. One conjectures that the existence of the solutions ψ and ψ_0 is sufficient for it. It is highly desirable to ascertain whether it is true or not.

§ 6. Application to laser instability

The best example to which the foregoing formulation may apply is the single-mode laser action which has been studied extensively by using a Fokker-Planck equation.[13] We reconsider the problem qualitatively from the present thermodynamic point of view.*) The laser Fokker-Planck equation may be written (after the elimination of an atomic freedom) as

$$\frac{\partial\psi}{\partial t}=-\left(\frac{\partial}{\partial x}v_x\psi+\frac{\partial}{\partial y}v_y\psi\right)+D\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right), \tag{6·1}$$

$$D=\text{const}, \tag{6·1a}$$

$$v_x(x,y)=D(a-a_2r^2)x\ ,\ v_y(x,y)=D(a-a_2r^2)y \tag{6·1b}$$

which satisfies the potential condition, so that

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*) A unification of the laser theory in a macroscopic standpoint and the Glansdorff-Prigogine theory has been discussed by R. Graham,[14] who pointed out some difficulty in associating the concepts of both entropy and entropy production with quantities to be derived from the single potential function ϕ, proposing a counter consideration. Our formulation should answer to his questioning, which will be discussed elsewhere together with a full numerical analysis. (Note added in proof)

$$\phi(x,y) = -\frac{a}{2}r^2 + \frac{a_2}{4}r^4, \quad r = \sqrt{x^2+y^2}, \tag{6·2}$$

$$v_x = -D\frac{\partial\phi}{\partial x}, \quad v_y = -D\frac{\partial\phi}{\partial y} \tag{6·3}$$

and

$$\psi_0(x,y)\,(\equiv\psi_0(r)) = Ne^{-\phi(x,y)}. \tag{6·4}$$

The natural boundary condition requires that the constant a_2 must be positive while the other one a, the pumping parameter, may vary from $-\infty$ to $+\infty$, but the situation

$$a \gg \sqrt{a_2} \tag{6·5}$$

is of particular interest which corresponds to far above threshold.

In the situation of (6·5), the potential ϕ is of the form such that its minimum points encircles the origin of the x-y plane, i.e., the complex plane of the active mode amplitude. These minima yield the stable equilibrium of the deterministic motion

$$\dot{x} = v_x, \quad \dot{y} = v_y, \tag{6·6}$$

and corresponds to the state of steady photon generation, while the origin, the 0-photon state, yields the unique unstable equilibrium. It is the most interesting feature of a transient laser action that the initial distribution peaked at the 0-photon state undergoes flattening, not to reach a completely broadened distribution, but to reach the steady-state distribution ψ_0 peaked at around the minimum circle of ϕ, the appearance of this peak being considered as a kind of the "dissipative structure" formation.[14]

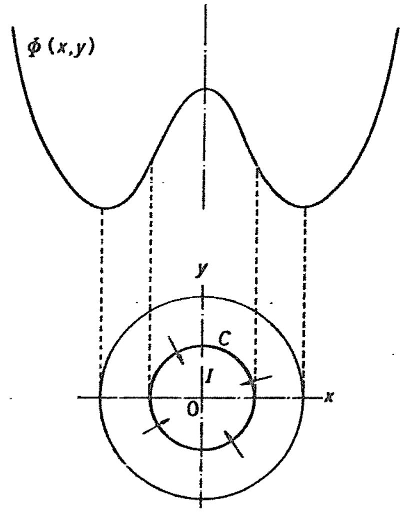

Fig. 1. The instability region (denoted by I) which is surrounded by the instability circle (denoted by C) in the complex plane of the active mode amplitude in the laser action. The arrows indicate a systematic entropy flow to cause the "grow" of the steady state distribution.

The disappearance of the 0-photon peak at the initial stage may be considered as a consequence of the entropy production accompanied by the dissipative time-evolution of the states. Actually, it is not a mere dissipation, the instability of the motion (6·6) enhancing the "fall". The effect of this enhancement can be seen from the entropy production balance equation II as follows:

$$\frac{\partial}{\partial t}(V_\mu X_\mu)\psi+\frac{\partial}{\partial x_\lambda}\left(J_\lambda V_\mu X_\mu-2\frac{\partial V_\lambda}{\partial x_\mu}V_\mu\right)\psi$$
$$=-2\left(T_{\mu\nu}V_\mu V_\nu+\frac{\partial V_\mu}{\partial x_\nu}\frac{\partial V_\nu}{\partial x_\mu}\right)\psi\,,\quad \lambda,\mu,\nu=x \text{ and } y$$

where

$$T_{\mu\nu}=\frac{\partial^2\phi}{\partial x_\mu\partial x_\nu} \tag{6·7}$$

by virtue of the potential condition and of the constancy of the diffusion coefficient. Let us call the region where $T_{\mu\nu}\xi_\mu\xi_\nu\leq 0$ the *instability region.* For the function ϕ given in (6·2) it is the inside of a circle C specified by

$$C:\ \frac{d^2\phi}{dr^2}=0 \text{ inside of which } \frac{d^2\phi}{dr^2}<0\,, \tag{6·8}$$

which is located inside the minimum circle. (Fig. 1) Thus, on the right-hand side of the formula II the two terms $T_{\mu\nu}V_\mu V_\nu$ and $(\partial V_\mu/\partial x_\nu)(\partial V_\nu/\partial x_\mu)$ are competing each other, implying that the increase of entropy by the second law is hardly suppressed in the instability region. In this sense, the instability of the deterministic motion is *against* the evolution criterion (as it should). The second term $(\partial V_\mu/\partial x_\nu)(\partial V_\nu/\partial x_\mu)$ which arises due to fluctuations moderates the negative value of the first term $(\partial^2\phi/\partial x_\mu\partial x_\nu)V_\mu V_\nu$ to recover the evolution criterion generally. (This is a feature of the present formulation to remedy the inadequacy[14)] of the theory which identifies $-\phi(x)=\log\psi_0(x)$ with the entropy to be applied to the Glansdorff-Prigogine theory.)

The enhancement of the entropy increase at around the instability region should be linked with a "grow" of the distribution ψ outside of the instability region, producing ψ_0. This is because a systematic entropy flow is needed through the instability circle C from outside to inside of the instability region, so that the flow contributes additively to the internal entropy production there:

$$\frac{d}{dt}\int_I\left(-\log\frac{\psi}{\psi_0}\right)\psi da=\frac{dS_e}{dt}+\frac{dS_i}{dt}\,,$$
$$\frac{dS_e}{dt}\equiv\int_C\left(-\log\frac{\psi}{\psi_0}\right)\psi V dl>0\,,$$
$$\frac{dS_i}{dt}\equiv\int_I\left(\left(\frac{\partial}{\partial x}\log\frac{\psi}{\psi_0}\right)^2+\left(\frac{\partial}{\partial y}\log\frac{\psi}{\psi_0}\right)^2\right)\psi da>0\,. \tag{6·9}$$

The grow of the peak at around the minimum circle of ϕ is a consequence of the flow which results in

$$\frac{d}{dt}\int_O\left(-\log\frac{\psi}{\psi_0}\right)\psi da<0\,. \tag{6·10}$$

(I and O denote the inside and outside of the instability region.)
We examine these predictions by computing explicitly time-dependent solutions of the laser Fokker-Planck equation (6·1). Details will be reported in the near future. (See Note added in proof.)

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Note added in proof: The numerical analyses of the laser instability from the present standpoint by using the variational method[16] have been successfully carried out by S. Sawada, which will be presented at the 4th Rochester Conference on Coherence and Quantum Optics (1977).

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From deterministic dynamics to probabilistic descriptions

(Markov semigroups/Bernoulli systems/$\mathcal{H}$-theorem/internal time and entropy operator)

B. MISRA, I. PRIGOGINE[†], AND M. COURBAGE

Faculté des Sciences Université Libre de Bruxelles, Campus Plaine, Boulevard du Triomphe, 1050 Bruxelles, Belgium

Contributed by I. Prigogine, April 9, 1979

ABSTRACT The present work is devoted to the following question: What is the relationship between the deterministic laws of dynamics and probabilistic description of physical processes? It is generally accepted that probabilistic processes can arise from deterministic dynamics only through a process of "coarse graining" or "contraction of description" that inevitably involves a loss of information. In this work we present an alternative point of view toward the relationship between deterministic dynamics and probabilistic descriptions. Speaking in general terms, we demonstrate the possibility of obtaining (stochastic) Markov processes from deterministic dynamics simply through a "change of representation" that involves no loss of information provided the dynamical system under consideration has a suitably high degree of instability of motion. The fundamental implications of this finding for statistical mechanics and other areas of physics are discussed. From a mathematical point of view, the theory we present is a theory of invertible, positivity-preserving, and necessarily nonunitary similarity transformations that convert the unitary groups associated with deterministic dynamics to contraction semigroups associated with stochastic Markov processes. We explicitly construct such similarity transformations for the so-called Bernoulli systems. This construction illustrates also the construction of the so-called Lyapounov variables and the operator of "internal time," which play an important role in our approach to the problem of irreversibility. The theory we present can also be viewed as a theory of entropy-increasing evolutions and their relationship to deterministic dynamics.

1. Introduction

According to both classical and quantum mechanics, the time-evolution of states obeys deterministic laws that are symmetric with respect to inversion of time. Irreversibility of physical processes, on the other hand, is expressed by the second law of thermodynamics. For isolated systems, it affirms the existence of a physical quantity, the entropy, that increases monotonically with time until it reaches its maximum at equilibrium. To elucidate the connection between the dynamical description with its reversible and deterministic laws and the thermodynamical description with its law of monotonic increase of entropy is a fundamental problem of statistical mechanics.

This problem is closely related to the question of the possible relations that might exist between the deterministic and probabilistic descriptions of physical processes. Indeed, the stochastic Markov processes provide the best possible models to represent irreversible evolution obeying the law of increasing of entropy. As is well known, the usual expression for entropy

$$\int_\Gamma \rho_t \ln \rho_t \, d\mu \qquad [1.1]$$

(and, in fact, any convex function of the distribution functions ρ on the phase space Γ) is a Lyapounov functional ("$\mathcal{H}$-function") for such processes (1). One would thus achieve a dynamical interpretation of the second law if one could establish a satisfactory link between deterministic dynamical evolutions and probabilistic Markov processes.

The interest of the problem of the possible connections between probabilistic and deterministic descriptions is, however, not confined to the domain of statistical mechanics. It concerns the problem of the meaning of probability in natural science.

It is generally believed that probabilistic processes can arise from deterministic dynamics only as a result of some form of "coarse-graining" or approximations. The main purpose of this paper is to develop an alternative viewpoint toward the relation between deterministic and probabilistic descriptions. More specifically, we develop a theory of "equivalence," mediated by nonunitary similarity transformations, between deterministic evolution and stochastic (Markov) processes.

The viewpoint toward the relation between deterministic evolution and stochastic Markov processes developed here is closely related to the theory of irreversibility developed by Prigogine *et al.* (2). The main feature of this theory is that the problem of reconciling dynamical evolution and irreversible (thermodynamical) evolution is viewed in terms of establishing an "equivalence" between them via a nonunitary similarity transformation. In essence, the approach thus consists in the determination of a suitable nonunitary transformation Λ acting on the distribution function ρ so that the original deterministic Liouville equation

$$i\frac{\partial \rho_t}{\partial t} = L\rho_t \qquad [1.2]$$

is transformed by it to a dissipative evolution equation describing the irreversible approach of the system to equilibrium. The transformation $\rho_t \rightarrow \bar{\rho}_t = \Lambda\rho_t$ converts the Liouville equation into the equation

$$i\frac{\partial \bar{\rho}_t}{\partial t} = \Phi\bar{\rho}_t,\ \Phi = \Lambda L\Lambda^{-1}. \qquad [1.3]$$

The above-mentioned requirement on Λ is thus the requirement that the functional

$$\Omega = \int_\Gamma |\bar{\rho}_t|^2 \, d\mu \qquad [1.4]$$

is a Lyapounov functional ($\mathcal{H}$-function) for the evolution obeying Eq. 1.3. This is the main condition on Λ. Naturally, there are other physically motivated conditions to be fulfilled by Λ. But we need not discuss them here because they are treated in refs. 2 and 3. For our purpose, the main point to retain is the important notion of "equivalence," via a nonunitary Λ, between the dynamical and thermodynamical descriptions. In conformity with this idea, we seek to determine the conditions on dynamics so that it becomes equivalent, via a similarity transformation Λ, to a stochastic Markov process.

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[†] Also at the Center for Statistical Mechanics at the University of Texas, Austin, TX.

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It is easy to show that the existence of such a transformation connecting the dynamical evolution to a stochastic Markov process entails the existence of an operator M (acting on the distribution function) with the property that

$$\langle \rho_t, M \rho_t \rangle \qquad [1.5]$$

decreases monotonically with t as ρ_t evolves according to the Liouville equation. Here we have used the inner product notation $\langle \rho,\varphi \rangle$ to denote the integral

$$\int_\Gamma \rho^* \varphi \, d\mu. \qquad [1.6]$$

The monotonic decrease of the expression 1.5 can be succinctly expressed by the commutation relation

$$i[L,M] \equiv D \leq 0 \qquad [1.7]$$

with $\langle \rho,D\rho \rangle = 0$ only for the equilibrium ensemble.

In this way, the possibility of relating the dynamical evolution to a stochastic Markov process turns out to be closely linked with the possibility of introducing a new dynamical variable M satisfying 1.7. These operators, called Lyapounov variables, have been studied by Misra to display the intrinsic irreversibility of appropriate classes of dynamical systems (4).

If one could introduce a new observable representing nonequilibrium entropy, it would be given by such a Lyapounov variable M with a change of sign. In this sense, then, the existence of M expresses the intrinsic irreversibility of the dynamical evolution.

Naturally, one does not expect M to exist for all dynamical systems. Moreover, one expects that (even if it exists) it can be defined only in an extended frame of dynamics. In fact, an important observation of Poincaré (5) shows that the operator M cannot correspond to multiplication by a phase function. It can be defined only as acting on the distribution functions and not on individual phase points. One thus expects the existence of M to be associated with some physical mechanism that renders the description of dynamical evolution in terms of phase space trajectories an unobservable idealization, thus forcing the use density functions.

Recent developments in classical mechanics show that such a mechanism is the phenomenon of instability of dynamical motion. Many forms of instability have been discovered, and they are found to be more common than originally believed (6). The common feature of dynamical systems having a suitably high degree of instability is that each finite region of phase space, no matter how small, contains phase points that move along rapidly diverging or qualitatively distinct types of trajectories. Obviously, in this situation, the concept of deterministic evolution along phase space trajectories cannot be defined operationally and, hence, constitutes a physically unrealizable idealization. Therefore, in dealing with dynamically unstable systems, classical mechanics seems to have reached the limit of the applicability of some of its own concepts. This limitation on the applicability of the classical concept of phase space trajectories is—it seems to us—of a fundamental character. It forces upon us the necessity of a new approach to the theory of dynamical evolution of such systems that involves the use of distribution functions in an essential manner.

It is shown in ref. 4 that the mixing property is necessary and the condition of K-flow is sufficient for the existence of a Lyapounov variable M. As is well known, mixing flows and (*a fortiori*) K-flows are unstable to a high degree: arbitrarily close phase points move along widely diverging trajectories.

It is also found in ref. 4 that for K-flows there exists an operator time T satisfying the commutation relation

$$i[L,T] = I. \qquad [1.8]$$

The existence of an operator of time or "age" satisfying 1.8 seems to express in a compact manner the inherent (but hidden) stochastic and nondeterministic character of the evolution.

Once T has been constructed, it is easy to proceed further. Lyapounov variables M can be constructed as monotonically decreasing positive operator functions of T

$$M = M(T). \qquad [1.9]$$

and the nonunitary Λ connecting the given dynamical evolution with a dissipative irreversible evolution can be constructed as a square root of M:

$$\Lambda = M^{1/2}. \qquad [1.10]$$

In this way, we see that, at least for a class of abstract dynamical systems, the K-flows, the dynamical evolution is equivalent to a dissipative irreversible evolution.

However, let us keep in view that it might be possible to establish the desired "equivalence" with a Markov process, *for a suitably restricted class of initial conditions*, even for systems that are not mixing, but present other types of instabilities (such as Poincare's catastrophe). This would correspond to allowing M and Λ to be more singular objects than those we have considered in this paper (7). Although this situation could be of considerable interest in statistical mechanics, we do not consider it further in this paper.

Obviously, the central question of our approach is: What form of instability ensures the existence of an equivalence between the dynamical evolution and a stochastic Markov process? As explained before, for K-flows, both M and Λ can be constructed by a "canonical" procedure as functions of an operator time T. It is tempting to conjecture that in this case the transformation not only converts the dynamical evolution of the K-flow to a dissipative process but also converts it to a stochastic Markov process. At present, we are not able to decide this conjecture in its full generality. However, we show (and this is the main purpose of the rest of the paper) that this conjecture is true for an important subclass of K-systems—the so-called Bernouilli systems (8, 9).

It seems to us that the significance of this result extends far beyond its immediate application in statistical physics. It proves, of course, the Boltzmann's $\mathcal{H}$-theorem for the Bernouilli systems without invoking the questionable "molecular chaos" hypothesis or any form of "coarse-graining." But more importantly, it confirms our view of how probabilities could arise in physics other than as a result of approximation.

From a mathematical point of view, the theory we present is a theory of positivity preserving similarity transformations that connect unitary groups describing deterministic dynamical evolution with dissipative semigroups associated with Markov processes. This theory is, evidently, in its infancy. In fact, the very possibility of such a connection between deterministic and probabilistic descriptions (which is established here in the specific case of Bernouilli systems) is rather an unexpected result that puts the entire problem of the role of probability in physics in a new perspective.

To keep the article brief, we shall omit most of the details of proofs in the following. A more complete version of this paper will appear in a forthcoming publication (10).

2. Notion of "equivalence" between deterministic dynamics and probabilistic processes

We now proceed to formulate and discuss in greater detail the notion of "equivalence" between deterministic evolution and probabilistic Markov processes. Let Γ denote the state space (a constant energy surface of the phase space) of the system.

Deterministic evolution of the system is described by a one-parameter group T_t of one-one transformations that map Γ onto itself:

$$T_tT_s = T_{t+s}. \qquad [2.1]$$

In the case of Hamiltonian systems, T_t will be a group of canonical transformations generated by the Hamiltonian.

We shall suppose that there is a measure μ (defined on a σ-algebra $\mathcal{B}$ of subsets of Γ) that is invariant under the dynamical group T_t. For Hamiltonian systems, the existence of such an invariant measure is guaranteed by Liouville's theorem. Furthermore, the invariant measure will be supposed to be a finite and, for convenience, normalized measure.

To define a probabilistic process (within the same state space Γ), one needs to specify the transition probabilities $P(t,\omega,\Delta)$ that the system starting initially from the state ω will reach the subset Δ of Γ in time t. It is evident that the function P should satisfy the following conditions:

(*i*) $P(t,\omega,\Delta) \geq 0$
(*ii*) $P(t,\omega,\Gamma) = 1$
(*iii*) For t, ω fixed the function $P(t,\omega,\Delta)$ defines a probability measure on Γ. [Moreover, one imposes the technical condition that for fixed t and Δ, $P(t,\omega,\Delta)$ is a measurable function of ω.] The probabilistic process defined by the transition probabilities is called a Markov process if P satisfies the Chapman–Kolmogorov equation:

$$P(t+s,\omega,\Delta) = \int P(t,\omega,d\omega')P(S,\omega',\Delta). \qquad [2.2]$$

As explained in many textbooks, this important condition expresses the important property of Markov process that the future statistical behavior of the system depends solely on the initial condition *independently* of the past history.

A measure μ on Γ is said to be an invariant measure for the process [with transition probabilities $P(t,\omega,\Delta)$] if

$$\int_\Gamma P(t,\omega,\Delta)d\mu = \mu(\Delta) \qquad [2.3]$$

for all $t \geq 0$ and $\Delta \in \mathcal{B}$.

To formulate the notion of equivalence between deterministic evolutions and stochastic Markov processes, it is necessary to consider how the distribution functions on Γ transform under respective evolutions. In the case of deterministic evolution, it is easy to see that the initial distribution ρ transforms in time t to the distribution ρ_t defined by

$$\rho_t(\omega) = \rho(T_{-t}\omega). \qquad [2.4]$$

The transformations U_t mapping ρ to ρ_t are unitary operators of L^2_μ (= the Hilbert space of square integrable functions with respect to μ):

$$(U_t\rho)(\omega) = \rho(T_{-t}\omega). \qquad [2.4']$$

The group property of T_t passes on to U_t. The generator of this unitary group is the Liouvillian operator L:

$$U_t = e^{-iLt}. \qquad [2.5]$$

For Hamiltonian systems L is given by

$$L\rho = i[H,\rho]_{PB}. \qquad [2.6]$$

in which $[,]_{PB}$ denotes the familiar Poisson bracket.

Let us now consider the transformation of distribution functions under the stochastic evolutions corresponding to Markov processes. To this end, let us first note that with every Markov process [with transition probabilities $P(t,\omega,\Delta)$] having an invariant measure μ, one can associate a family W_t of operators defined by

$$W_tf(\omega) = \int_\Gamma f(\omega')P(t,\omega,d\omega') \qquad [2.7]$$

for $f \in L^2_\mu$.

The Chapman-Kolmogorov equation for $P(t,\omega,\Delta)$ then implies the semigroup property for W_t:

$$W_tW_s = W_{t+s} \text{ (for } t,s \geq 0). \qquad [2.8]$$

Moreover, the previously stated properties (*i–iii*) of the transition probabilities entail the following properties of W_t:

(*a*) The operation W_t preserves positivity. This means that, if $f(\omega) \geq 0$ for almost all (a.a.) $\omega \in \Gamma$, then $W_tf(\omega) \geq 0$ for a.a. ω too.
(*b*) $W_t\,\rho_{\mathrm{equ}} = \rho_{\mathrm{equ}}$, in which ρ_{equ} is the uniform distribution $\rho_{\mathrm{equ}} = 1$.

By putting $f = \varphi_\Delta$, the characteristic function of the set $\Delta \subset \Gamma$ in 2.7, one finds

$$P(t,\omega,\Delta) = (W_t\varphi_\Delta)(\omega). \qquad [2.9]$$

By using the above relation between W_t and $P(t,\omega,\Delta)$, the invariance of the measure μ for the process (relation 2.3) is easily seen to be equivalent to the condition:

(*c*) $W^*_t\,\rho_{\mathrm{equ}} = \rho_{\mathrm{equ}}$.

To sum up, every Markov process with an invariant measure defines through formula 2.7 a semigroup W_t of operators acting on L^2_μ and having properties *a* through *c*. The converse of this statement is also true: every semigroup W_t of operators on L^2_μ with properties *a* through *c* defines a Markov process (having μ as invariant measure) whose transition probabilities $P(t,\omega,\Delta)$ are obtained from W_t by formula 2.9 [by a slight variation of theorem 2-1 given by Dynkin (11)].

It is easy to see that if $\tilde{\rho}$ denotes the distribution function describing the initial state of the system, the state $\tilde{\rho}_t$ to which it evolves in time t under the Markov process is given by

$$\tilde{\rho}_t = W^*_t\,\tilde{\rho}. \qquad [2.10]$$

It seems natural now to consider the deterministic evolution described by the unitary group U_t (induced from T_t) as "equivalent" to the stochastic evolution associated with the semigroup W_t (see relation 2.7 and 2.9) if there exists a bounded transformation Λ on L^2_μ such that

(*i*) $\Lambda U_t\rho = W^*_t\Lambda\rho$ (for $t \geq 0$),
(*ii*) Λ preserves positivity,
(*iii*) $\int\rho d\mu = \int\Lambda\rho d\mu$,
(*iv*) Λ has a densely defined inverse, Λ^{-1}, and
(*v*) $\Lambda\rho_{\mathrm{equ}} = \rho_{\mathrm{equ}}$.

Condition *i* simply says that the "change of representation" $\rho \rightarrow \Lambda\rho$ converts the deterministic evolution corresponding to U_t to the stochastic evolution associated with W_t. Conditions *ii* through *v* are necessary requirements (from a physical point of view) in order that Λ may be interpreted as a "change of representation." In fact, conditions *ii* and *iii* simply express the requirement that Λ maps "states" into "states"; *v* says that the contemplated change of representation leaves the equilibrium state unchanged; and condition *iv* expresses the important requirement that the passage from deterministic to probabilistic description brought about by Λ involves "*no loss of information.*" Condition *i* can be rewritten in the form

$$W^*_t = \Lambda U_t\Lambda^{-1} \quad \text{(for } t \geq 0). \qquad [2.11]$$

The problem for us now is to determine the class of dynamical groups U_t similar to semigroups W_t that satisfy (*in addition to conditions* a *through* c) the following requirement:

$$\|W^*_t(\rho - \rho_{\mathrm{equ}})\|^2 = \|W^*_t\rho - \rho_{\mathrm{equ}}\|^2 \rightarrow 0 \qquad [2.12]$$

monotonically with t as $t \rightarrow \infty$.

Semigroups satisfying conditions *a* through *c* and 2.12 will be referred to as *strong Markov semigroups*. They are associated (through formulas 2.7 and 2.9) with truly stochastic Markov processes that display the irreversibility expressed in the second law. In fact, condition 2.12 just says that ρ_{equ} is an "attractor" for the process in question and the approach to ρ_{equ} proceeds "monotonically." Now not only expression 2.12, but also the usual expression [1.1] for negative entropy (as indeed any convex functions of ρ) decreases monotonically for such processes provided $\rho \neq \rho_{\text{equ}}$.

The existence of a similarity transformation Λ connecting (through 2.11) the dynamical group U_t to a strong Markov semigroup W_t^* seems to express the *inherent* stochastic and irreversible character of the original dynamical evolution. One thus expects such a transformation to exist (if at all) only for systems with a suitably high degree of instability of motion. This intuitive idea is confirmed by the following:

PROPOSITION. *In order that the dynamical group* U_t *be similar to a strong Markov semigroup* W_t^* *(for* $t \geq 0$*), it is necessary that the dynamical evolution be* mixing *in the sense of ergodic theory.*

The proof of this statement follows from noting that, if $\Lambda U_t \Lambda^{-1} = W_t^*$ is a (strong) Markov semigroup (for $t \geq 0$), then $\Lambda^* \Lambda = M$ is a Lyapounov variable for the evolution U_t. As shown in ref. 4, the existence of Lyapounov variables implies that the Liouvillian (restricted to $K_o^{\perp}$ = the subspace orthogonal to ρ_{equ}) has absolutely continuous spectrum, which in its turn implies that the system is mixing.

3. Time and entropy operators for Bernoulli systems

This and the following section are devoted to carrying out this program of *Section 2* for the class of the so-called *Bernoulli systems* (8, 9). For the sake of simplicity of exposition, however, we shall limit our consideration to the simplest of the Bernoulli systems, the *baker's transformation*. But we emphasize that all the results found in this and the next section generalize to arbitrary Bernoulli systems.

Let us start with a brief description of the baker's transformation. The phase space Γ is now the unit square in the plane, and the measure μ is the usual Lebesgue measure of the square. The baker's transformation B sends a point $\omega = (p,q)$ of the phase space to the point $B\omega$ with

$$B\omega = (2p, q/2) \quad \text{if } 0 \leq p < \tfrac{1}{2} \quad \text{and}$$

$$B\omega = (2p - 1, q/2 + \tfrac{1}{2}) \quad \text{if } \tfrac{1}{2} \leq p \leq 1.$$

The discrete group B^n, $(n = 0, \pm 1, \pm 2, \ldots)$ that replaces the continuous parameter group T_t of the preceding section may be thought as describing a discrete deterministic process taking place at regular (unit) intervals of time.

A striking, and indeed the characteristic, property of the baker's transformation B is that the partition $P = \{\Delta_0, \Delta_0^c\}$ of the unit square into the right and left halves is "*independent*" and "generating" with respect to B. (For the definitions of these two concepts, see refs. 8 and 9.) It is the existence of an independent and generating partition that characterizes a general Bernoulli system. The baker's transformation corresponds to the special case that the independent and generating partition can be chosen to consist of exactly *two* sets Δ_0, Δ_0^c with $\mu(\Delta_0) = \mu(\Delta_0^c) = \tfrac{1}{2}$.

Returning to the baker's transformation, the discrete group B^n now induces a discrete unitary group U^n on L_μ^2: (cf. Eq. 2.4). By a Lyapounov variable (or negative entropy operator) of the baker's transformation, we mean a bounded operation M on L_μ^2 such that

(*i*) $M \geq 0$; i.e., $\langle \rho, M\rho \rangle \geq 0$ for all $\rho \in L_\mu^2$;
(*ii*) $M\rho_{\text{equ}} = \rho_{\text{equ}}$, and
(*iii*) $\langle U^n f, MU^n f \rangle \to 0$ *monotonically* as $n \to \infty$ for all f in $K_o^{\perp}$, the orthogonal complement of ρ_{equ}.

To construct the Lyapounov variables M for the discrete group U^n, we follow the general scheme described in ref. 4 and construct first the operator T representing "internal-time" or "age" of the system. In the case of continuous parameter group $U_t = e^{-iLt}$, the operator T is, by definition, a self-adjoint operator that satisfies the canonical commutation relation 1.8 on a suitable dense set of vectors of $K_o^{\perp}$. Expressed in terms of the unitary group e^{-iLt}, this relation becomes

$$e^{iLt} T e^{-iLt} = T + tI. \qquad [3.1]$$

Thus the operator of "age" for the baker's system is, by definition, a self-adjoint operator T that satisfies

$$U^{-n} T U^n = T + nI \qquad [3.2]$$

on $K_o^{\perp}$.

Let E_n denote the eigen projection of T corresponding to the eigen value n:

$$T = \sum_{n=-\infty}^{\infty} nE_n. \qquad [3.3]$$

The E_ns being eigen projections of a self-adjoint operator satisfy

$$E_n E_m = \delta_{nm} E_n$$

and

$$\sum_{n=-\infty}^{+\infty} E_n = I. \qquad [3.4]$$

Condition 3.2 is now equivalent to the condition

$$U^{-1} E_m U = E_{m-1}. \qquad [3.5]$$

Thus the problem before us is to construct a family E_n (n integers from $-\infty$ to $+\infty$) satisfying 3.4 and 3.5. To this end, we make use of a special basis of $K_o^{\perp}$ constructed below.

Let $P = \{\Delta_0, \Delta_0^c \equiv \Delta_1\}$ be the partition of the unit square into left and right halves. Define

$$\chi_o = 1 - 2\varphi_{\Delta_o} \quad \text{and}$$

$$\chi_n = U^n \chi_o \quad (n = \pm 1, \pm 2, \ldots). \qquad [3.6]$$

For any finite set $S = (n_1, n_2, \ldots n_r)$ of (positive or negative) integers, put

$$\chi_S = \chi_{n_1} \chi_{n_2} \cdot \ldots \cdot \chi_{n_r}. \qquad [3.7]$$

Making use of the independence of the partition P, one can verify that the collection of functions $\{\chi_S\}$, with S finite subsets of integers, is an orthonormal set and the generating property of P entails the *completeness* of the set (in $K_o^{\perp}$). Moreover, from the definitions of χ_n and χ_S, it follows that the unitary operator U induced from the baker's transformation B acts as a shift on the orthonormal basis:

$$U\chi_S = \chi_{S+1}. \qquad [3.8]$$

Here $S + 1$ denotes the subset $(n_1 + 1, n_2 + 1, \ldots, n_r + 1)$ if S stands for $(n_1, \ldots n_r)$. In view of 3.8, the eigen projection $E_n (n = 0, \pm 1, \pm 2, \ldots)$ of the operator time T can now be defined as the projection onto the subspace spanned by all χ_S corresponding to subsets S such that $n \in S$ and all other integers in S are less than n. The property 3.4 of the E_ns thus defined follows from the fact that $\{\chi_S\}$ is a complete orthonormal basis in $K_o^{\perp}$ and condition 3.5 is a consequence of 3.8.

The construction of Lyapounov variables M now follows directly. They are monotonically decreasing operator functions of T. Corresponding to every (two-sided) sequence λ_n^2 of nonnegative numbers bounded by 1 and decreasing *monotonically* to 0 as $n \to +\infty$ the operator

$$M = \sum_{-\infty}^{+\infty} \lambda_n^2 E_n + P_0 \qquad [3.9]$$

(with E_n eigen projections of T and P_0 the projection onto ρ_{equ}) is easily verified to be a Lyapounov variable for the discrete group U^n.

To conclude this section, let us mention how the operator time T allows us to associate an "age" or "internal time" with well-defined distribution functions ρ, or rather with the excess distribution functions $\bar{\rho} \equiv \rho - \rho_{equ}$. If $\bar{\rho}$ is an eigen function of T, the corresponding eigen value is the "age" associated with the distribution function ρ. For instance, the excess function for the distribution function $(1 - \chi_n)$ is χ_n, which is an eigen vector of T for eigen value n. Condition 3.5 or 3.8 makes this association a "consistent" one in the sense that it ensures that the change in "internal time" or "age" of the system brought about by the dynamical evolution matches with the progress of external (or observer's) time that serves to label the dynamical group. Existence of a consistent "internal time" operator T in this sense is, of course, not allowed for all dynamical systems.

If the excess distribution function $\bar{\rho}$ is not an eigen function of T but a combination of eigen functions corresponding to two or more distinct eigen values, then one cannot associate a well-defined age to ρ. But one can still associate an "average age" $T(\rho)$ to ρ by the formula

$$T(\rho) = \frac{1}{\|\bar{\rho}\|^2} \langle \bar{\rho}, T\bar{\rho} \rangle, \qquad [3.10]$$

just as in quantum mechanics.

4. "Equivalence" of Bernoulli systems with stochastic Markov processes

Let $0 < \lambda_n < 1$ $(n = 0, \pm 1, \ldots)$ be any sequence of positive numbers decreasing *monotonically* as n increases. If

$$\Lambda = \sum_{n=-\infty}^{+\infty} \lambda_n E_n + P_0, \qquad [4.1]$$

in which E_ns are the eigen projections of the operator time T.

It can be shown (10) that this transformation preserves the positivity and the normality. However, Λ^{-1} is not positivity preserving. Therefore, to make $\Lambda U^n \Lambda^{-1}$ positivity preserving we require that λ_n be such that the sequence $r_n = \lambda_{n+1}/\lambda_n$ also decreases monotonically as n increases [for instance, take $\lambda_n = (1 + e^n)^{-1}$]. With this requirement, it can be shown that $\Lambda U^n \Lambda^{-1}$ is a semigroup of Markov process and that Λ has all the properties listed in *Section 2*, for $n \geq 0$. The transformed group $\Lambda U^n \Lambda^{-1}$ is of course defined for both positive and negative n. But it is important to note that it is only for $n \geq 0$ that $\Lambda U^n \Lambda^{-1}$ preserves positivity. We may of course define another transformation $\tilde{\Lambda}$ such that $\tilde{\Lambda} U^n \tilde{\Lambda}^{-1}$ preserves positivity for $n \leq 0$. The important point is that the same transformed group $\Lambda U^n \Lambda^{-1}$ cannot correspond to probabilistic process for both positive and negative time n. This breaks the symmetry between the positive and negative direction of time and causes the physical evolution to be described by a semigroup rather than a group.

5. Concluding remarks

The most striking conclusion to emerge from our discussion is that the deterministic and probabilistic descriptions are not as radically different as it has been thought in the past and "coarse-graining" or "contraction" is not the only way of relating them. We have demonstrated the possibility of linking probabilistic descriptions and deterministic descriptions by simply a "change of representation" that involves "*no loss of information*."

Looked at from a slightly different point of view, the present work could be considered as a part of a theory of *entropy-increasing evolutions* and their relations to deterministic dynamics. Historically, Boltzmann's kinetic equation represents the first example of an entropy-increasing evolution. To arrive at this equation, Boltzmann had to introduce probability into dynamics from outside. In this work we have demonstrated that entropy-increasing evolutions can arise from deterministic dynamics simply as a result of "change of representation" brought about by invertible (nonunitary) similarity transformations Λ. This finding is in conformity with, and concretely illustrates, the point of view towards the problem of irreversibility developed in ref. 2.

A specially attractive feature of the theory of irreversibility emerging from the considerations of refs. 2 and 4 and the present work is the close links it establishes between *instability* (expressed in terms of mixing and other ergodic properties), the *inherent irreversibility* (expressed in terms of the existence of Lyapounov variables M), and the *intrinsic randomness* (expressed in terms of the existence of an "equivalence" with a stochastic Markov process) of dynamical motion. We have shown that the class of systems exhibiting instability contains the class featuring inherent irreversibility (for instance, the K-systems), which in its turn contains the class (e.g., Bernoulli systems) displaying intrinsic randomness of motion. The precise boundary between these classes is, however, at present not known. It will be an interesting problem to determine the precise extent of these classes. Let us also note that the notion of intrinsic randomness of dynamical systems formulated here differs from—and seems to refer to a more intrinsic form of the randomness of dynamical evolution than—that expressed by strict positivity of Kolmogorov "entropy."

The concepts of instability, inherent irreversibility, and intrinsic randomness are formulated and studied here in the frame of classical mechanics. It obviously will be interesting and important to extend and study these concepts for quantum systems as well as for gravitational systems requiring general relativity for their description. We plan to come back to this question in subsequent communications.

Let us note that for an arbitrary system, the average $\langle T \rangle$ of the internal time operator in a state ρ given by 3.10 can be easily shown to be equal to the change in the ordinary time dt. The internal time operator (when it exists) contains, however, additional information about the physical system that concerns the fluctuation or dispersion of the "internal age" around the average value. In both classical and quantum dynamics, time appears simply as an external parameter to label the dynamical group. In contrast, the internal time operators considered here are new physical observables associated with the irreversible evolution of the system. From this point of view the concept of internal time operator is closer to the concepts of thermodynamic and biological time and may serve as the "microscopic" counterpart of the latter phenomenological concepts.

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GENERALIZED LIOUVILLE EQUATION, ENTROPY, AND DYNAMIC SYSTEMS CONTAINING LIMIT CYCLES

WILLI-HANS STEEB

Universität Paderborn, Arbeitsgruppe Theoretische Physik, D-4790 Paderborn, West Germany

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The relation between the generalized Liouville equation, entropy production rates and autonomous systems of differential equations containing limit cycles is investigated. Moreover, the connection between the generalized Liouville equation and the Lie derivative of a differential form with respect to a vector field is discussed.

1. Introduction

As long as a classical N-particle system can be described by a hamiltonian function $H(p, q)$, the Liouville equation takes the form

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^{N} \left(\frac{\partial H}{\partial p_i} \cdot \frac{\partial f_N}{\partial q_i} - \frac{\partial H}{\partial q_i} \cdot \frac{\partial f_N}{\partial p_i} \right) = 0, \tag{1}$$

where $f_N(p, q)$ is the probability density. Now there are many dynamic systems where a hamiltonian is not sufficient to describe the system (for example: dynamic systems possessing limit cycles or chaotic behaviour, open systems in contact with reservoirs, random perturbation, collective models and so on). Hence, it is necessary to extend the Liouville equation in order to involve such cases. For example, given a dynamic system $\dot{x} = X(x, t)$, where $\dot{x} = \mathrm{d}x/\mathrm{d}t$ and X is a smooth function of x and t, let us consider the Liouville equation for this case. The Liouville equation which includes the above eq. (1) for a dynamic system $\dot{x} = X(x, t)$ has been derived by Gerlich[1]) and has been used by Dobbertin[2,3]) to study functional relations between reduced distribution functions and entropy production by non-hamiltonian perturbations. The equation has the following form:

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^{N} X_i \frac{\partial f_N}{\partial x_i} + f_N \sum_{i=1}^{N} \frac{\partial X_i}{\partial x_i} = 0. \tag{2}$$

The second and third terms on the right-hand side can be written as $\sum_{i=1}^{N} \partial(X_i f_N)/\partial x_i$ and therefore eq. (2) is in analogy with the mass-conservation equation of three-dimensional hydrodynamics $\partial\rho/\partial t + \mathrm{div}(\rho v) = 0$.

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The purpose of the present paper is twofold. First, we study the generalized Liouville equation from a new point of view utilizing the Lie derivative of a differential form w.r.t. a vector field (what in physics is called an infinitesimal generator). In contrast to the derivation of Gerlich[1]), the present derivation is mathematically more rigorous and from the physical point of view the derivation becomes clearer. Moreover, to find solutions of the generalized Liouville we also apply the concept of Lie derivative. Second, we investigate the connection between the generalized Liouville equation, entropy-production rate, and autonomous systems of differential equations containing limit cycles.

Recently, in a series of papers, the author[4–8]) studied a connection between Lie's theory of one-parameter groups and autonomous non-linear systems of differential equations containing periodic orbits. In particular, such systems have been considered where the periodic orbits are limit cycles. For a given system of linear differential equations $\dot{x} = X(x) = Ax$ (A an $n \times n$ matrix with constant coefficients) with periodic solutions a non-linear system $\dot{x} = Y(x)$ is constructed via the relation $[X, Y] = gY$ or, in a modern form, $L_X\alpha = h\alpha$: $[\,,]$ denotes the commutator of the C^∞-vector fields X and Y; X and Y are written (in local coordinates) as $X = X_1\partial/\partial x_1 + \cdots + X_n\partial/\partial x_n$ and $Y = Y_1\partial/\partial x_1 + \cdots + Y_n\partial/\partial x_n$. Furthermore, $L_X\alpha$ stands for the Lie derivative of the differential form α with respect to X, where α is given by the inner product $\alpha = Y \lrcorner\, \omega$: $\omega(\omega = dx_1 \wedge \cdots \wedge dx_n)$ is the standard volume in $\mathbf{R}^n$. The connection between both conditions of invariance[7]) is given by the relation $L_X(Y \lrcorner\, \omega) = (g + \operatorname{div} X)(Y \lrcorner\, \omega)$, where we have used $[X, Y] = gY$. The aim of the present paper is to discuss some aspects concerning the vector fields X and Y and the Liouville equation and to calculate the entropy-production rate of Y using Gibbs statistics.

Our mathematical tool will be the Lie derivative[9]) of a differential form (or a vector field) with respect to a vector field. Hence in section 2 a brief review concerning this mathematical tool is given and the generalized Liouville equation is derived applying the Lie derivative. Moreover, we investigate the generalized Liouville equation itself with the concept of Lie derivative. Section 3 is devoted to finding the connection between the vector fields X and Y, and the generalized Liouville equation. Furthermore we calculate the entropy-production rate. Section 4 is devoted to a widely discussed example. In the final section we summarize the results obtained.

2. The Lie derivative and the generalized Liouville equation

The concept of the Lie derivative of a differential form (or a vector field) with respect to a vector field plays an important role in many domains in physics. Applications have been made to classical mechanics, hydrodynamics, optics, quantum mechanics, supergravity, and statistical mechanics. Moreover partial differential equations, which play an important role in physics, can be treated within this so-called geometric approach (Steeb[9]) and refs. herein).

Let M be a n-dimensional C^∞-differentiable manifold with local coordinates x_i. Real valued C^∞-vector fields (denoted by X, Y) and real valued C^∞-differential forms (denoted by Greek letters) on M can be considered. The components of the vector field X are denoted by $X_i\partial/\partial x_i$, this means $X = X_1\partial/\partial x_1 + \cdots + X_n\partial/\partial x_n$ (in local coordinates). Moreover, we have the space of the real valued C^∞-functions $f\colon M \to \mathbb{R}$. We assume throughout that all mathematical objects are smooth.

Now the concept of the Lie derivative of a form w.r.t. a vector field can be introduced. The Lie derivative of a form α w.r.t. X is defined by the derivative of α along the integral curve $t \to \Phi_t$ of X, i.e.,

$$L_X\alpha = \lim_{t\to 0} \frac{\Phi_t^*\alpha - \alpha}{t}. \tag{3}$$

The definition of the Lie derivative is not useful for practical calculations, because the integral curve $t \to \Phi_t$ of X is not known in general. Rather, we use the important identity

$$L_X\alpha = \mathrm{d}(X \lrcorner\, \alpha) + X \lrcorner\, (\mathrm{d}\alpha), \tag{4}$$

where $\mathrm{d}\alpha$ denotes the exterior derivative of the form α and $X \lrcorner\, \alpha$ is the contraction of α by X (also called inner product). For a form α, the Lie derivative L_X may be viewed as the propagator of the form α, down the trajectories of the vector field X. To sum up: The vector field X (infinitesimal generator) gives rise (under suitable assumptions such as compact support or restriction to local considerations) to a one-parameter family of diffeomorphisms Φ_t (local flows, local one-parameter transformation group) of the manifold M (or a subset thereof) into itself. Each diffeomorphism gives rise to a bundle map $\Phi_t\colon E \to E$ for each (covariant) tensor bundle E defined over M. To every local cross section α of E there corresponds a cross section $\alpha(t)$ of E for each diffeomorphism Φ_t. The Lie derivative of α is then defined by eq. (3).

For vector fields the Lie bracket can also be considered as a Lie derivative. This means $(L_X Y)f = [X, Y]f = X(Yf) - Y(Xf)$. The rules of manipulation can be found in Steeb[7]).

Now we wish to derive the extended Liouville equation using the Lie derivative of a form with respect to a vector field. To this end, consider the autonomous system of differential equation $\dot{x} = X(x)$. We assume that the right-hand side of this equation does not depend explicitly on t. We require that the vector field X is complete. X is complete iff each integral curve can be extended so that its domain becomes $(-\infty, \infty)$. Let X be a linear vector field and $M = \mathbb{R}^n$. Then X is complete. For example, the damped harmonic oscillator governed by the equation $\ddot{x} + \dot{x} + x = 0$ $(\dot{x} = y, \dot{y} = -x - y)$ leads to the complete vector field $X = y\partial/\partial x + (-x - y)\partial/\partial y$.

Now we consider the vector field $Y = T + X$ on space time where $T = \partial/\partial t$. We have the following theorem:

Theorem. Let Y be the vector field given above. Let $f(x, t)$ be an arbitrary C^∞-function and $\omega = \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_n$. If $L_Y f\omega = 0$ (this means the form $f\omega$ is invariant w.r.t. Y and therefore does not change as it propagated down the trajectories of Y), then f satisfies the generalized Liouville equation, viz.

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{n} X_i \frac{\partial f}{\partial x_i} + f \operatorname{div} X = 0. \tag{5}$$

Proof. Applying the rules for the Lie derivative of a differential form (Steeb[9]), we obtain

$$0 = L_Y f\omega = (Yf)\omega + f(L_Y\omega) = (Yf)\omega + f(L_T\omega) + f(L_X\omega)$$

$$= (Yf)\omega + f(L_X\omega) = (Yf)\omega + f(\operatorname{div} X)\omega = ((Yf) + f \operatorname{div} X)\omega.$$

Since ω is a basic element, the theorem has been proved. If $\operatorname{div} X = 0$, then the last term on the right hand side vanishes and we obtain the usual Liouville equation.

An additional comment is in order. If we consider time-dependent vector fields, i.e. $Y = \Sigma_{i=1}^{n} X_i(x, t)\partial/\partial x_i + \partial/\partial t$, then the condition $L_Y f\omega = 0$ leads to an additional requirement, namely $\partial X_i/\partial t = 0$ $(i = 1, \ldots, n)$. This means, the flow must be steady. However, if we consider the space-time volume element $\Omega = \omega \wedge \mathrm{d}t$, then such a condition does not appear.

Let us discuss how the generalized Liouville equation can be studied within the described approach. To this end, we cast the partial differential equation in an equivalent set of differential forms. In the present case we obtain the $(n + 1)$-form

$$\alpha = \mathrm{d}f \wedge \omega + \mathrm{d}t \wedge \left(\sum_{i=1}^{n} (-1)^{i+1} X_i \, \mathrm{d}f \wedge \mathrm{d}x_1 \wedge \cdots \wedge \widehat{\mathrm{d}x_i} \wedge \cdots \wedge \mathrm{d}x_n\right)$$
$$+ f(\operatorname{div} X)\, \mathrm{d}t \wedge \omega. \tag{6}$$

The circumflex indicates omission and we have put $\omega = \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_n$. By straightforward calculation we find that $\mathrm{d}\alpha = 0$. To see that the form α is equivalent with the generalized Liouville equation we consider the sectioned form $\tilde{\alpha}$ (we distinguish between independent variables $x_1, \ldots, x_n, t$ and the that the vector field X is complete. X is complete iff each integral curve can be extended so that its domain becomes $(-\infty, \infty)$. Let X be a linear vector field and $M = R^n$. Then X is complete. For example, the damped harmonic oscillator governed by the equation $\ddot{x} + \dot{x} + x = 0$ ($\dot{x} = y$, $\dot{y} = -x - y$) leads to the complete vector field $X = y\partial/\partial x + (-x - y)\partial/\partial y$.

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Let us discuss how the generalized Liouville equation can be studied within the described approach. To this end, we cast the partial differential equation in an equivalent set of differential forms. In the present case we obtain the $(n + 1)$-form

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$$+ f(\operatorname{div} X)\, \mathrm{d}t \wedge \omega. \tag{6}$$

The circumflex indicates omission and we have put $\omega = \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_n$. By straightforward calculation we find that $\mathrm{d}\alpha = 0$. To see that the form α is equivalent with the generalized Liouville equation we consider the sectioned form $\underset{\sim}{\alpha}$ (we distinguish between independent variables $x_1, \ldots, x_n, t$ and the dependent variable f). Because of

$$\mathrm{d}f = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \mathrm{d}x_i + \frac{\partial f}{\partial t} \mathrm{d}t, \tag{7}$$

$\mathrm{d}t \wedge \mathrm{d}t = 0$, and $\mathrm{d}x_i \wedge \mathrm{d}x_i = 0$ we arrive at

$$\tilde{\alpha} = \left[\frac{\partial f}{\partial t} + \sum_{i=1}^{n} X_i \frac{\partial f}{\partial x_i} + f(\mathrm{div}\, X)\right] \mathrm{d}t \wedge \omega. \tag{8}$$

If we put $\tilde{\alpha} = 0$, then we obtain the generalized Liouville equation.

Now let us study the form α. This means we seek vector fields, say $Z_1, \ldots, Z_n$, such that $L_{Z_i}\alpha = h\alpha$ with the arbitrary function $h(x_1, \ldots, x_n, t, f)$. We consider the extended concept of invariance (Harrison and Estabrook[10])) for the treatment of partial differential equations. Since we are investigating the autonomous system $\dot{x} = X(x)$, we find that $L_T\alpha = 0$ where $T = \partial/\partial t$. This means that the generalized Liouville equation is invariant under time translation. The vector field T is associated with the differential equation $\mathrm{d}t/\mathrm{d}\tau = 1$, which has the solution $t = t_0 + \tau$.

Now let us consider the vector field $f\partial/\partial f$. A straightforward calculation yields $L_{f\partial/\partial f}\alpha = \alpha$. Hence, we have found a further invariant of α. The vector field $f\partial/\partial f$ is associated with the ordinary differential equation $\dot{f} = f(\dot{f} = \mathrm{d}f/\mathrm{d}\tau)$ with the solution $f = f_0 \exp \tau$ (one parameter transformation group). Consequently the generalized Liouville equation is invariant under this transformation group. The Lie derivative of α with respect to $\partial/\partial f$ yields $L_{\partial/\partial f}\alpha = (\mathrm{div}\, X)\, \mathrm{d}t \wedge \omega$. Consequently, α is invariant under the vector field iff $\mathrm{div}\, X = 0$. This is the case for hamiltonian systems.

It is obvious that the form α is invariant under the vector field X. To find further vector fields such that $L_Z\alpha = h\alpha$ holds, we must solve the resulting partial differential equation. In general, this is an impossible task. However, if $X(x) = Ax$, where A is an $n \times n$ matrix with constant coefficients, then we can easily find further vector fields. Any non-linear autonomous system can be cast into an infinite linear system (Carleman linearization) (Carleman[11])). The linearized system can be treated in an approximate manner (Montroll and Helleman[12])).

3. Limit cycles and entropy production rate

First of all we wish to derive an expression for the entropy production rate. In order to see the connection with classical mechanics we assume that $N = 2n$ (n natural number) so that the equation of motion $\dot{x} = Y(x)$ can be written as

$$\begin{aligned} \dot{p}_i &= -\frac{\partial H}{\partial q_i} + A_i(p, q), \\ \dot{q}_i &= \frac{\partial H}{\partial p_i} + B_i(p, q). \end{aligned} \tag{9}$$

This means that a part of the equations of motion can be expressed by a hamiltonian function. Consequently, we require that the divergence of the non-hamiltonian forces is not equal to zero, i.e.

$$\frac{\partial A_i}{\partial p_i} + \frac{\partial B_i}{\partial q_i} \neq 0, \tag{10}$$

because, if so, they could be cast into a hamiltonian form. Obviously, if we consider dynamic systems containing limit cycles, then A_i and B_i exist so that condition (10) is satisfied.

The Gibbs entropy S yielding in the asymptotic limit the correct expression for the thermodynamic equilibrium, is given by

$$S = S_0 - \int f_n \ln f_n \, \mathrm{d}p \, \mathrm{d}q, \tag{11}$$

where $\mathrm{d}p = \mathrm{d}p_1 \ldots \mathrm{d}p_n$ and $\mathrm{d}q = \mathrm{d}q_1 \ldots \mathrm{d}q_n$. By differentiating S with respect to time we obtain

$$\dot{S} = -\int (1 - \ln f_n) \frac{\partial f_n}{\partial t} \, \mathrm{d}p \, \mathrm{d}q. \tag{12}$$

For a purely hamiltonian system we find that $\dot{S} = 0$ and therefore $S = \text{const.}$ The concept of Gibbs' ensemble still holds when we consider the generalized Liouville equation. On substituting the generalized Liouville equation [using the equations of motion given by eq. (9)] and integrating by parts it follows that

$$\dot{S} = \sum_{i=1}^{n} \int f_n \left(\frac{\partial A_i}{\partial p_i} + \frac{\partial B_i}{\partial q_i} \right) \mathrm{d}p \, \mathrm{d}q. \tag{13}$$

Hence, one interprets the quantities $\dot{s}_i$ defined by

$$\dot{s}_i = \frac{\partial A_i}{\partial p_i} + \frac{\partial B_i}{\partial q_i}, \tag{14}$$

as the microscopic entropy production rates^{2}). The condition $\dot{S} > 0$ is fulfilled if $\dot{s}_i > 0$ for all i. A crucial point is that the condition is not necessary.

Now let us discuss the connection of the described approach and a certain class of autonomous systems of differential equations containing limit cycles.

Let

$$Q_{ij} = x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i} \tag{15}$$

$\{Q_{ij}: i, j = 1, \ldots, n\}$ represents a basis of the Lie algebra so(n). Now we assume that the vector field X is a linear combination of the basis $\{Q_{ij}: i, j = 1, \ldots, n\}$. The vector field X is complete on the manifold $M = \mathrm{R}^n$. Let $\omega = \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_n$, the standard volume in R^n. We find that $L_{Q_{ij}}\omega = 0$. The reason is that the divergence of the vector field Q_{ij} vanishes. At once it follows that for every linear combination of the Q_{ij}'s the Lie derivative of ω vanishes. The vector field X is associated with an autonomous linear system of differential equations with constant coefficients $\dot{x} = X(x) = Ax$. The matrix A is skew symmetric. We assume that n is even and that none of the eigenvalues of A is equal to zero. Then all eigenvalues are purely imaginary. Consequently there is no damping in the system and it possesses periodic solutions. For such a vector field X we wish to find the most general (non-linear) vector field Y such that $[X, Y] = 0$. The way to find it has been suggested by the author[4–8]. In the two-dimensional case[8] (where $X = x\partial/\partial y - y\partial/\partial x$) the resulting vector field Y may be viewed as the "prototype" of a vector field possessing limit cycles. Now the vector field can be written as $Y = f_1 Z^1 + f_2 Z^2 + \cdots + f_n Z^n$, where we assume that the argument of the functions f_i is given by the invariants (first integrals) of X (this means $Xf_i = 0$) and $[X, Z^i] = 0$. Two vector fields, say Z^1 and Z^2, can be given at once. First, we have $[X, X] = 0$. Second, we find that $[X, I] = 0$ where

$$I = \sum_{i=1}^{n} x_i \frac{\partial}{\partial x_i}. \tag{16}$$

Note that the divergence of I is given by div $I = n$. Moreover, an invariant of X can be given, namely the invariant of the Lie algebra so(n). The only invariant of the Lie algebra so(n) is $(x_1^2 + x_2^2 + \cdots + x_n^2 - c)$. We notice that the other invariants of X are polynomial, too. There are $(n - 1)$ invariants. The further invariants can easily be found solving the subsidiary equations associated with X. In the next section we discuss a concrete example.

4. An example

As a concrete example, let us study the system

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 & -1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}. \tag{17}$$

with the associated vector field $X = Q_{12} + Q_{14} + Q_{23} + Q_{34}$ where Q_{ij} is given by eq. (15). An appropriate hamiltonian function is given by

$$H = x_1^2/2 + x_2^2/2 - x_3^2/2 - x_4^2/2 - x_1x_3 + x_2x_4, \tag{18}$$

with the equations of motion $\dot{x}_1 = -\partial H/\partial x_2$, $\dot{x}_2 = \partial H/\partial x_1$, $\dot{x}_3 = \partial H/\partial x_4$, and $\dot{x}_4 = -\partial H/\partial x_3$. The only critical point of X is $x = 0$. In other words the only time-independent solution of eq. (17) (or steady state solution) is $x = 0$. The eigenvalues of the matrix on the right-hand side of equation (17) are given by $\lambda_{1,2} = \mathrm{i}\sqrt{2}$ and $\lambda_{3,4} = -\mathrm{i}\sqrt{2}$. Hence there is no damping in the systems. By solving the subsidiary equations we find that the set of the invariants of X (first integrals) is given by

$$\{x_1^2 + x_2^2 + x_3^2 + x_4^2 - c_1,\ (x_1^2 + x_3^2)/2 - x_1x_3 + x_2^2 - c_2,\ (x_2^2 + x_4^2)/2 + x_2x_4 + x_1^2 - c_3\}. \tag{19}$$

The first expression is valid since the matrix of system (17) is skew-symmetric and hence represents an element in the Lie algebra so(4) (represented as matrices) which leaves length invariant. The invariants $\gamma_2(x)$ and $\gamma_3(x)$ describe an invariant manifold (integral manifold) of $\dot{x} = X(x)$ when we set $(x_1^2 + x_3^2)/2 - x_1x_3 + x_2^2 = c_2^2$ $(c_2 = \mathrm{i}\sqrt{2})$ and $(x_2^2 + x_4^2)/2 + x_2x_4 + x_1^2 = c_3^2$ $(c_3 = -\mathrm{i}\sqrt{2})$. Obviously, H is an invariant, too, and can be obtained as a linear combination of the invariants given above (19).

Now the second step is to obtain the vector field Y such that eq. (1) holds. In what follows, the argument of the functions f_1, f_2, f_3, and f_4, given by the invariants of X is omitted. We find

$$\begin{aligned} &\left[X, \sum_{i=1}^{4}\left(x_i \frac{\partial}{\partial x_i}\right)\right] = 0, \\ &[X, Q_{13} + Q_{24}] = 0, \\ &[X, Q_{12} - Q_{34}] = 0. \end{aligned} \tag{20}$$

Hence the vector field Y becomes

$$Y = f_1X + f_2\sum_{i=1}^{4} x_i \frac{\partial}{\partial x_i} + f_3(Q_{13} + Q_{24}) + f_4(Q_{12} - Q_{34}). \tag{21}$$

The corresponding autonomous system is

$$\begin{aligned} \dot{x}_1 &= (-x_2 - x_4)f_1 + x_1f_2 - x_3f_3 - x_2f_4, \\ \dot{x}_2 &= (x_1 - x_3)f_1 + x_2f_2 - x_4f_3 + x_1f_4, \\ \dot{x}_3 &= (x_2 - x_4)f_1 + x_3f_2 + x_1f_3 + x_4f_4, \\ \dot{x}_4 &= (x_1 + x_3)f_1 + x_4f_2 + x_2f_3 - x_3f_4. \end{aligned} \tag{22}$$

To be concrete, we set

$$\begin{aligned} &f_1 = 1, \quad f_2 = 4 - x_1^2 - x_2^2 - x_3^2 - x_4^2, \\ &f_3 = 1 - (x_1^2 + x_3^2)/2 + x_1 x_3 - x_2^2, \\ &f_4 = 1 - (x_2^2 + x_4^2)/2 - x_2 x_4 - x_1^2. \end{aligned} \tag{23}$$

The obtained system has only one critical point, namely $x = 0$. The intersection of the surfaces $f_2 = 0$, $f_3 = 0$, and $f_4 = 0$ leads to two closed curves, i.e. periodic solutions of the system (22) with the given functions. The periodic orbits can be given explicitly, namely

$$\begin{aligned} &x_1(t) = \cos \bar{t}, \quad x_2(t) = \cos \bar{t}, \quad x_3(t) = \cos \bar{t} + \sqrt{2} \sin \bar{t}, \\ &\qquad\qquad\qquad\qquad\qquad\qquad x_4(t) = -\cos \bar{t} + \sqrt{2} \sin \bar{t}, \\ &x_1(t) = \cos \bar{t}, \quad x_2(t) = -\cos \bar{t}, \quad x_3(t) = \cos \bar{t} - \sqrt{2} \sin \bar{t}, \\ &\qquad\qquad\qquad\qquad\qquad\qquad x_4(t) = \cos \bar{t} + \sqrt{2} \sin \bar{t}, \end{aligned} \tag{24}$$

where $\bar{t} = \sqrt{2}t$. These curves could just as well be periodic orbits as limit cycles of the system $\dot{x} = Y(x)$. In the present case the given periodic orbits are limit cycles. Consider the Liapunov function $V = (x_1^2 + x_2^2 + x_3^2 + x_4^2)/2$. It follows that

$$\dot{V} = (x_1^2 + x_2^2 + x_3^2 + x_4^2) f_2. \tag{25}$$

This quantity is positive definite within the sphere $x_1^2 + x_2^2 + x_3^2 + x_4^2 = 4$, and a well-known theorem assures us that the origin is unstable. Outside the sphere, the quantity $\dot{V}$ is negative. All trajectories inside and outside the sphere tend towards the limit cycles.

When the limit cycle is not reached there are entropy production rates. This means $\partial Y_1/\partial x_1 + \partial Y_2/\partial x_2 \neq 0$ and $\partial Y_3/\partial x_3 + \partial Y_4/\partial x_4 \neq 0$ ($x_1 = p_1$, $x_2 = q_1$, $x_3 = q_2$, $x_4 = p_2$). If a limit cycle arises in a dynamic system, then both negative damping (in the present case outside the sphere $x_1^2 + x_2^2 + x_3^2 + x_4^2 = 4$) and positive damping (inside the sphere $x_1^2 + x_2^2 + x_3^2 + x_4^2 = 4$) occur. When the limit cycle is reached (in the present case when $f_2 = 0$, $f_3 = 0$ and $f_4 = 0$ and therefore $Y = X$) the system is no longer dissipative (div $Y = 0$) and can be described by a hamiltonian function.

To sum up, suppose the linear system of differential equations $\dot{x} = X(x)$ has quadratic first integrals γ_i. If the vector fields Z^i commute with X, then $\dot{x} = Y(x)$ ($Y = f_1(\gamma_i)X + \Sigma f_i(\gamma_i)Z^i$) has orbits coinciding with those of $\dot{x} = X(x)$, and these will be limit cycles (more accurately, an attracting surface) if a Lyapounov function can be constructed from the f_i. Under these circumstances, the Liouville equation (conservation of probability fluid) may also have a Lyapounov function in the form of an entropy-like functional [(11) through (13)].

5. Conclusion

In the first part of the present paper we have shown that the concept of Lie derivative can be used to obtain the generalized Liouville equation. The requirement $L_X\Omega = 0$, where $X = X_1\partial/\partial x_1 + \cdots + X_n\partial/\partial x_n + \partial/\partial t$ and $\Omega = \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_n \wedge \mathrm{d}t$ yields the desired result. Now we are also able to treat dynamic systems which are not generated via a hamiltonian function. In particular we can study systems which include limit cycles. This has been done in the second part. We have investigated a certain class of autonomous systems of differential equations, namely such systems $\dot{x} = Y(x)$ which are generated via $[X, Y] = 0$, where X is a linear combination of the basis of the Lie algebra so(n) represented as $\{Q_{ij} = x_i\partial/\partial x_j - x_j\partial/\partial x_i\}$. Such vector fields play a central role in investigating dynamic systems possessing limit cycles. If and only if the limit cycle (or limit cycles) of the dynamic system $\dot{x} = Y(x)$ is reached, then the system is no longer dissipative and the system is described by $\dot{x} = X(x)$ with certain initial conditions given by the functions $f_2, \ldots, f_n$. Consequently, the limit cycle itself can be described by a hamiltonian function (div $X = 0$).

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Introduction to a Brownian Quasiparticle Model

P. Combis,[1] **J. Fronteau,**[1] **and A. Tellez-Arenas**[1]

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A description intermediate between the usual stochastic description of a Brownian particle and the deterministic description of a classical particle is proposed. It is based on a model which utilizes the notions of a current velocity and of an osmotic velocity, and which generates a random process which allows us to associate with any given initial and final conditions a unique differentiable trajectory. This intermediate description of the Brownian motion, in terms of quasiparticles with quasideterministic behavior, gives back the same mean and the same variance as does the usual stochastic description.

KEY WORDS: Brownian motion; Fokker–Planck equation; current velocity; osmotic velocity; quasideterministic behavior; quasiparticles.

1. INTRODUCTION

Before exposing the problem we are going to handle, let us summarize some results of stochastic physics. Let $X(t)$ be a process in $\mathbb{R}^n$ which satisfies a generalized Langevin equation of the form

$$dX(t) = D(X(t), t)\, dt + dW(t)$$

where $X(t)$ is a vector of $\mathbb{R}^n$, D a regular field of vectors, dt a macroscopically infinitesimal increment of time, and $W(t)$ a Wiener process, i.e., a process whose increments are Gaussian, with zero mean, and whose variance matrix $|t - s|[\sigma_{ij}^2]$, $i, j = 1,\dots, n$, is proportional to the time increment $|t - s|$. We call the matrix of diffusion the matrix $[M] = \frac{1}{2}[\sigma_{ij}^2]$. Given D, the probability density in $\mathbb{R}^n$, $f(X, t)$, satisfies the Fokker–Planck equation

$$\frac{\partial}{\partial t} f(X, t) = -\mathrm{div}_X(f(X, t)D(X, t)) + \mathrm{div}_X([M]\, \mathrm{grad}_X f(X, t)) \tag{1}$$

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[1] Laboratoire CAT, Département de Physique, UER Sciences Fondamentales et Appliquées, Université d'Orléans, Orléans, France.

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The conditional probability density $P(Xt \mid X_0 t_0)$ that the variable $X(t)$ takes the value X at time t, knowing that it has the value X_0 at time t_0, is the fundamental solution $G(X, t, X_0, t_0)$ of this equation, i.e., the solution that tends to $\delta(X - X_0)$ when t tends to zero ($t > t_0$).

In this paper we limit ourselves to a D field of vectors independent of time and linear in X. In this case, we can explicitly integrate the differential deterministic system

$$dX_t^D = D(X_t^D)\,dt$$

and we call $X_t^D(t - t_0, X_0)$ the solution that takes the value X_0 at time t_0. The conditional probability density is then a function of $t - t_0$, and we write it as $f^\delta(X, t - t_0, X_0)$:

$$P(Xt \mid X_0 t_0) = f^\delta(X, t - t_0, X_0), \qquad t > t_0$$

Finally, the mean of the process is equal to X_t^D,

$$E\{X(t)\} = \int X f^\delta(X, t - t_0, X_0)\,dX = X_t^D(t - t_0, X_0)$$

and the elements of its variance matrix are functions of $t - t_0$:

$$E\{(X_i(t) - X_{t,i}^D)(X_j(t) - X_{t,j}^D)\} = C_{ij}(t - t_0)$$

We are now in a position to expose the problem that is the object of this paper. Let us consider a Brownian particle submitted to a double initial and final condition: to leave X_0 at time t_0 and to arrive at X' at time t'. To this double condition there correspond an infinity of possible stochastic trajectories (nondifferentiable). Our aim is to build a model of quasiparticles which involves a sole differentiable trajectory, going from $(X_0 t_0)$ to $(X' t')$, and representing a certain mean behavior of the Brownian particle between those two points. This mean behavior must be such as to give back, by integrating over the final position X', the mean $X_t^D(t - t_0, X_0)$ and the variance matrix $[C_{ij}(t - t_0)]$ of the process $X(t)$ at time t, given the initial $(X_0 t_0)$ condition. Moreover, it must be the same thing for any initial $I(X_0)$ density. However, we do not ourselves impose any condition on the covariance at two different instants.

2. DESCRIPTION OF THE MODEL

The first idea which comes in mind is to take as a trajectory the partial mean of the process $X(t)$, which is calculated with the conditional probability density $P(Xt \mid X_0 t_0, X' t')$ to be at (Xt), knowing that we are at X_0 at time t_0 and at X' at time t' ($t' > t > t_0$),

$$Y(t, X', t', X_0, t_0) = \int X P(Xt \mid X_0 t_0, X' t')\,dX$$

We easily check that the mean of Y over the final condition X', which is calculated with the probability density $P(X't'|X_0t_0)$, is independent of t' and is equal to the mean X_t^D of the process $X(t)$. But we can check in particular cases (we handle in the appendix the simplest case, $n = 1$, $D = 0$) that the variance matrix of Y is not equal to the variance matrix of $X(t)$. Thus, the trajectory Y does not satisfy the criteria we have chosen. We now present a model which satisfies these criteria.

Our model is founded on the notions of the current velocity and of the osmotic velocity associated with the process $X(t)$ for the initial (X_0t_0) condition.(1) The current velocity $V(X, t - t_0, X_0)$ and the osmotic velocity $\Omega(X, t - t_0, X_0)$ are respectively the half sum and the half difference of the mean velocity departing from $X(t)$ (mean forward velocity) and of the mean velocity arriving at $X(t)$ (mean backward velocity). Therefore V and Ω are linked by the relation

$$V(X, t - t_0, X_0) = D(X) - \Omega(X, t - t_0, X_0)$$

Moreover, Ω is a function of the probability density

$$\Omega(X, t - t_0, X_0) = [M] \operatorname{grad}_X \log f^\delta(X, t - t_0, X_0)$$

and V satisfies the continuity equation in the Eulerian description.

Our idea introduces the preceding notions into a Lagrangian description. We consequently postulate a continuous dynamic evolution, which is described by the variable X_t,

$$\frac{d}{dt} X_t = V(X_t, t - t_0, X_0) = D(X_t) - [M] \operatorname{grad}_{X_t} \log f^\delta(X_t, t - t_0, X_0) \quad (2)$$

and which satisfies the continuity equation along the stream:

$$\frac{\partial}{\partial t} f^\delta(X_t, t - t_0, X_0) = -\operatorname{div}_{X_t}(f^\delta(X_t, t - t_0, X_0) V(X_t, t - t_0, X_0)) \quad (3)$$

We verify that the compatibility equation between (2) and (3) is just the Fokker–Planck equation (1) written for $X = X_t$.

In various particular cases, we have developed this model in the following way:

(a) We solve Eq. (1); for a field D independent of time and linear in X, the fundamental solution f^δ is a Gaussian function whose argument is a quadratic form of $(X - X_t^D)$, where $X_t^D(t - t_0, X_0)$ is the solution of the deterministic system $dX_t^D = D(X_t^D)\,dt$.

(b) We put this solution f^δ in (2), which thus becomes an explicit differential system, which we integrate, thus obtaining the general solution

$$X_t(t - t_0, \Lambda, X_0) = X_t^D(t - t_0, X_0) + [\phi(t - t_0)]\Lambda$$

where the vector Λ represents the n arbitrary constants of integration, and where $[\phi(t - t_0)]$ is an $n \times n$ matrix which vanishes for $t = t_0$.

(c) It appears that the Jacobian $J_{t'} = \mathscr{D}(X_{t'})/\mathscr{D}(\Lambda) = \det[\phi(t' - t_0)]$ is different from zero for $t' > t_0$; given a final condition $X_{t'} = X'$ at time t', we thus determine the vector Λ. This gives us a well-defined trajectory X_t going from $(X_0 t_0)$ to $(X't')$.

(d) We associate with this trajectory (and thus with the corresponding vector Λ) the probability density $f^{\delta}(X', t' - t_0, X_0)$ for arrival at $(X't')$ after leaving $(X_0 t_0)$. With this probability density, and by integration over X', it is then possible to calculate the mean and the variance matrix of X_t. These quantities, which are independent of t', are the same as those of the process $X(t)$. In fact, we use a law of distribution for Λ, such that

$$\rho(\Lambda, t' - t_0, X_0)\, d\Lambda = f^{\delta}(X', t' - t_0, X_0)\, dX'$$

and it appears that this law ρ is a function only of Λ, and that it has a Gaussian form. It is thus possible to introduce a random process $Z(t - t_0, \Lambda, X_0)$ in the following form:

$$\text{process } Z\colon \begin{cases} Z(t - t_0, \Lambda, X_0) = X_t^{D}(t - t_0, X_0) + [\phi(t - t_0)]\Lambda \\ \text{Gaussian distribution law } \rho(\Lambda) \end{cases}$$

and we check that the mean and the variance matrix, respectively, of this process Z are equal to those of the process $X(t)$.

(e) When X_0 becomes a random variable, denoted Ξ, with the (normalized) initial density $I(\Xi)$, we easily verify that the mean and the variance matrix of the process Z are still the same as those of the process $X(t)$. Indeed, in this case, the mean of $X(t)$ is

$$E\{X(t)\} = \iint X f^{\delta}(X, t - t_0, \Xi) I(\Xi)\, d\Xi\, dX$$

The transformation $(\Xi, X) \to (\Xi, \Lambda)$, such that $X = Z(t - t_0, \Lambda, \Xi)$, allows us to write the preceding integral as the mean of the process Z, calculated with the joint density $F(\Xi, \Lambda) = I(\Xi)\rho(\Lambda)$ for the independent variables Ξ and Λ. The same is true for the variance matrix.

To picture the method which has just been exposed, we are going to calculate explicitly a process Z. For simplicity, we limit ourselves to an example in $\mathbb{R}$.

3. EXAMPLE IN $\mathbb{R}$

If $X(t) = x(t) \in \mathbb{R}$ is the variable of position, Eq. (1) is reduced to an equation of the Smoluchowski type. For $D = ax + b$ and $[M] = \mu$, it is written

$$\frac{\partial}{\partial t} f(x, t) = -\frac{\partial}{\partial x}\{(ax + b) f(x, t)\} + \mu \frac{\partial^2}{\partial x^2} f(x, t)$$

and its fundamental solution is

$$f^{\delta}(x, t - t_0, x_0) = \{2\pi A(t - t_0)\}^{-1/2} \exp -\frac{(x - x_t^D)^2}{2A(t - t_0)}$$

with

$$A(t - t_0) = \frac{\mu}{a}(e^{2a(t-t_0)} - 1), \qquad x_t^D = x_0 e^{a(t-t_0)} + \frac{b}{a}(e^{a(t-t_0)} - 1)$$

Hence we deduce that x_t^D and $A(t - t_0)$ are, respectively, the mean and the variance of the process $x(t)$. Let us put this solution into the dynamic equation (2); we obtain the differential equation

$$\frac{dx_t}{dt} = ax_t + b + \frac{\mu}{A(t - t_0)}(x_t - x_t^D)$$

whose general solution is

$$x_t = x_t^D + \lambda[A(t - t_0)]^{1/2}; \qquad \lambda \text{ a constant of integration}$$

We notice that the A function vanishes for $t = t_0$, and thus x_t and x_t^D correspond to the same initial condition $(x_0 t_0)$.

The Jacobian $J_{t'} = \partial x_{t'}/\partial\lambda = [A(t' - t_0)]^{1/2}$ is different from zero for $t' > t_0$. Given a final condition $x_{t'} = x'$ at time t', we then determine the value of the constant λ associated with the point $(x't')$:

$$\lambda = (x' - x_{t'}^D)/[A(t' - t_0)]^{1/2}$$

We thus obtain a sole trajectory going from $(x_0 t_0)$ to $(x't')$:

$$x_t = x_t^D + \frac{x' - x_{t'}^D}{[A(t' - t_0)]^{1/2}}[A(t - t_0)]^{1/2}; \qquad t' > t > t_0$$

Let us associate with this trajectory the probability density for arrival at x' at time t'. It is then possible to calculate the mean and the variance of x_t by integration over x', but it is better to deduce for λ a probability density ρ defined by $\rho(\lambda, t' - t_0, x_0)\, d\lambda = f^{\delta}(x', t' - t_0, x_0)\, dx'$. Because of the expressions which have been found for λ and $J_{t'}$, it appears that ρ is a Gaussian function only of λ:

$$\rho(\lambda) = (2\pi)^{-1/2} e^{-\lambda^2/2}$$

The set of the trajectories x_t starting from $(x_0 t_0)$ and corresponding to all the possible $(x't')$ points can then be considered as a process $z(t - t_0, \lambda, x_0)$:

$$z(t - t_0, \lambda, x_0) = x_t^D(t - t_0, x_0) + \lambda[A(t - t_0)]^{1/2}; \qquad \rho(\lambda) = (2\pi)^{-1/2} e^{-\lambda^2/2}$$

We immediately check that the mean and the variance of this process z are respectively equal to the mean and the variance of the process $x(t)$:

$$\int z(t - t_0, \lambda, x_0)\rho(\lambda)\, d\lambda = x_t^D(t - t_0, x_0)$$

$$\int \{z(t - t_0, \lambda, x_0) - x_t^D(t - t_0, x_0)\}^2 \rho(\lambda)\, d\lambda = A(t - t_0)$$

Let us consider now the case of any (normalized) initial density $I(\xi) \neq \delta(\xi - x_0)$. The mean of the process $x(t)$ is then

$$E\{x(t)\} = \iint x\{2\pi A(t - t_0)\}^{-1/2} \times \left\{\exp - \frac{[x - x_t^D(t - t_0, \xi)]^2}{2A(t - t_0)}\right\} I(\xi)\, d\xi\, dx$$

The transformation $(\xi, x) \rightarrow (\xi, \lambda)$, such that $x = z(t - t_0, \lambda, \xi)$, leads to

$$E\{x(t)\} = \iint \{x_t^D(t - t_0, \xi) + \lambda[A(t - t_0)]^{1/2}\} \times (2\pi)^{-1/2} e^{-\lambda^2/2} I(\xi)\, d\xi\, d\lambda$$

In this formula, we recognize the mean of the process z calculated with the joint probability density for the two independent variables λ and ξ. The same is true for the variance. Moreover, due to the linearity of z with respect to λ and ξ, the calculation is achieved very easily:

$$E\{x(t)\} = x_t^D(t - t_0, \bar{\xi}); \qquad \bar{\xi} = \int \xi I(\xi)\, d\xi$$

$$E\{[x(t) - x_t^D(t - t_0, \bar{\xi})]^2\} = e^{2a(t-t_0)}\overline{(\xi - \bar{\xi})^2} + A(t - t_0)$$

It should be noted that the particular form of the process z (in which λ and ξ are separate and ρ is Gaussian) does not proceed from the simplicity of the given example. Indeed we still obtain this form (Λ and Ξ separate, ρ Gaussian) in more sophisticated linear cases [for example, $X(t)$ in phase space for any quadratic potential]. The results obtained above have therefore a rather broad meaning.

4. CONCLUDING REMARKS

In this paper, we have considered a Brownian particle described by a process $X(t)$ in a field D linear and independent of time. With the process $X(t)$, starting from $(X_0 t_0)$, we associate a description intermediate between the usual stochastic description (nondifferentiable trajectories)

$$dX(t) = D(X(t))\, dt + dW(t)$$

and the classical deterministic description

$$dX_t^D = D(X_t^D)\,dt$$

whose solution, for the initial condition (X_0t_0), is the mean of the previous process.

In this intermediate description, to any final point $(X't')$, $t' > t_0$, there corresponds a unique differentiable trajectory X_t going from (X_0t_0) to $(X't')$ and such that

$$dX_t/dt = D(X_t) - [M]\,\mathrm{grad}_{X_t} \log f^\delta(X_t, t - t_0, X_0)$$

To this trajectory we assign the probability density $f^\delta(X', t' - t_0, X_0)$ for arrival at $(X't')$. The set of the differentiable trajectories thus defined constitutes a process $(Z(t - t_0, \Lambda, X_0);\ \rho(\Lambda))$ whose mean and variance matrix are the same as those of the process $X(t)$ when (X_0t_0) is given. In the general case, when X_0 is a random variable denoted Ξ, with density $I(\Xi)$, the mean and the variance matrix of the process $Z(t - t_0, \Lambda, \Xi)$, calculated with the joint density $I(\Xi)\rho(\Lambda)$, are still the same as those of the process $X(t)$.

Thus, to the real Brownian particles, we associate quasiparticles whose behavior presents both a certain deterministic aspect (in such a way that any given initial and final conditions determine a sole trajectory) and a probabilistic aspect (in such a way that a probability is attached to each of the trajectories). However, the process Z which describes the behavior of these quasiparticles is not equivalent to the process $X(t)$: it does not give back the covariance of $X(t)$ at two different instants. Yet it presents the advantage of simplicity. In particular, it allows us to achieve easily the calculation of the mean and of the variance matrix of the process $X(t)$ for any given initial density.

Finally, we note that the notion of Brownian quasiparticles introduced here is of some interest in the context of the recent stochastic interpretation of quantum mechanics (see, e.g., Refs. 2–6).

APPENDIX

In the case $D = 0$, the process $X(t)$ is reduced to the Wiener process $W(t)$ and for $n = 1$ we denote it, as in the text, $x(t)$. The associated Fokker–Planck equation is the heat equation, whose fundamental solution is

$$P(xt|x_0t_0) = f^\delta(x, t - t_0, x_0) = \{4\pi(t - t_0)\mu\}^{-1/2} \exp -\frac{(x - x_0)^2}{4(t - t_0)\mu}$$

The mean and the variance of the process $x(t)$ are, respectively, x_0 and $2(t - t_0)\mu$. The process Y, which is introduced in the text, is written here

$$y(t, x', t', x_0, t_0) = \int x\, \frac{P(xt|x_0t_0)P(x't'|xt, x_0t_0)}{P(x't'|x_0t_0)}\, dx; \qquad t' > t > t_0$$

where $P(x't'|xt, x_0t_0) = P(x't'|xt) = f^{\delta}(x', t' - t, x)$ because of the Markovian and homogeneous nature of the process $x(t)$. Thus

$$y(t, x', t', x_0, t_0) = \frac{(t - t_0)x' + (t' - t)x_0}{t' - t_0}$$

The mean of the process y being equal to x_0, its variance is

$$E\{(y - x_0)^2\} = \int \left(\frac{(t - t_0)(x' - x_0)}{t' - t_0}\right)^2 f^{\delta}(x', t' - t_0, x_0)\, dx' = 2\mu \frac{(t - t_0)^2}{t' - t_0}$$

As stated in the text, the variance of the process y at time t is different from the variance $2(t - t_0)\mu$ of the process $x(t)$ at the same time.

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Lie-admissible structure of statistical mechanics

J. Fronteau and **A. Tellez-Arenas**
Département de Physique
Université d'Orléans
F-45045 Orléans Cedex, France

and

R.M. Santilli*
Department of Mathematics
Harvard University
Cambridge, Massachusetts 02138

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Abstract

The objective of this paper is to identify the algebraic structure of statistical mechanics for Newtonian systems as they actually occur in nature, that is, with forces nonderivable from a potential. For this objective, we first review the definition of dissipative forces, nonconservative forces, and, more generally, variationally nonselfadjoint forces, the latter being the forces which violate the integrability conditions for the existence of a potential. We then review Liouville's theorem in its original formulation, and show that this theorem is indeed capable of incorporating variationally nonselfadjoint forces. By using this background, we then pass to the identification of a number of properties of the statistical description of Newtonian systems of the class considered. Our major result consists of the proof of a theorem according to which the time evolution law of densities for the statistical description of variationally nonselfadjoint Newtonian systems can always be represented in terms of brackets verifying the laws of the Lie-admissible algebras. Since these algebras are an algebraic covering of the Lie algebras, the conventional Lie-algebra formulation of statistical mechanics is recovered as a subcase when all forces are derivable from a potential. This result establishes the direct universality of the Lie-admissible algebras in statistical mechanics, in the sense that these algebras occur without redefinition of the local variables and physical quantities, as well as they hold for all systems of the class considered. We then tackle the problem of quantization of the statistics of dissipative phenomena, with particular reference to an algebraic reinterpretation of the approach by Prigogine and his collaborators. The paper ends with a number of comments indicating the physical relevance of our analysis with respect to: (a) the relevance of dissipative forces in plasma physics, with particular reference to the problem of stability; (b) the remarkable capability of the Lie-admissible algebras of representing the forces of nature, with particular reference to the most general forces known at this time, the superposition of local forces derivable from a potential, the local forces nonderivable from a potential, and the nonlocal forces.

The present paper has been written in a rather detailed, self-contained form, readable by physicists and mathematicians who are not necessarily familiar with nonselfadjoint forces and Lie-admissible algebras. Those who are engaged in this field of research will kindly excuse unavoidable repetitions of elementary concepts.

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Lie-admissible structure of statistical mechanics

I. INTRODUCTION.

The history of the physical applications of the dissipative forces, the nonconservative forces or, in general, the forces nonderivable from a potential, is rather remarkable.

At the time of the inception of contemporary analytic mechanics, the forces nonderivable from a potential were rightly incorporated by Lagrange in his celebrated equations via external terms (Lagrange, 1788), e.g., for the case of one particle in a three-dimensional Euclidean space,

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{r}}} - \frac{\partial L}{\partial \vec{r}} = \vec{F}(t,\vec{r},\dot{\vec{r}}) \quad , \tag{I.1a}$$

$$L = T(\dot{\vec{r}}) - V(\vec{r}) \quad , \quad \vec{r} \equiv (x,y,z) \tag{I.1b}$$

where $\vec{F}$ represents the forces nonderivable from a potential. Hamilton's equations were then written (Hamilton, 1834) :

$$\begin{cases} \dot{\vec{r}} = \dfrac{\partial H}{\partial \vec{p}} \quad , \\ \dot{\vec{p}} = - \dfrac{\partial H}{\partial \vec{r}} + \vec{F} \quad , \end{cases} \tag{I.2a}$$

$$H = T(\vec{p}) + V(\vec{r}) \quad , \quad \vec{p} = \frac{\partial L}{\partial \dot{\vec{r}}} = m\dot{\vec{r}} \quad . \tag{I.2b}$$

As we shall review in this paper, Liouville's theorem was originally formulated in a way allowing full compatibility with Equations (I.1) and (I.2) (Liouville, 1838), thus allowing a statistical formulation for forces generally nonderivable from a potential.

In essence, these authors appear to have been fully aware of the fact that particles in our Earthly environment are subjected to forces which *are not*, in general, derivable from a potential (such as in the case of dissipative forces, or applied forces), without excluding the existence of particular Newtonian systems with forces entirely derivable from a potential.

Rather oddly, since the beginning of this century, Lagrange's equations have been "truncated", so to say, with the removal of the external terms, by acquiring the form almost universally used in contemporary physical literature

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{\vec{r}}} - \frac{\partial L}{\partial \vec{r}} = 0 \tag{I.3a}$$

$$L = T(\dot{\vec{r}}) - V(\vec{r}) \quad . \tag{I.3b}$$

As a result, Hamilton's equations were also "truncated", by acquiring the familiar form

$$\left\{ \begin{array}{l} \dot{\vec{r}} = \dfrac{\partial H}{\partial \vec{p}} \quad , \\ \\ \dot{\vec{p}} = - \dfrac{\partial H}{\partial \vec{r}} \quad , \end{array} \right. \tag{I.4a}$$

$$H = T(\vec{p}) + V(\vec{r}) \quad . \tag{I.4b}$$

Along similar lines, Liouville's theorem was also "truncated", as we shall see later on, via the removal of a term representative of the forces $\vec{F}$, by acquiring the conventional form compatible with Equations (I.4).

The historical reasons for the reduction of the fundamental analytic equations from their original form (I.1) and (I.2), to the simpler form (I.3) and (I.4) are unknown. Nevertheless, it is rather tempting to argue that this reduction is likely due to the rather dominating character in the research of this century of the physical systems representable via equations (I.3) and (I.4), such as the planetary system and the system of charged particles under the action of the Lorentz force. After all, the quantization of these systems produced the solution of the problem of the atomic structure, with a self-evident impact in the conceptual attitude of the researchers.

Lately, however, a number of seemingly independent motivations have promoted a sort of return "ad originem", that is, the study of the physical applications of forces nonderivable from a potential. Without any claim of completeness, we quote below the following cases.

- *Newtonian Mechanics*. The need to avoid an excessive approximation of the Newtonian reality (e.g., for system with holonomic mechanical constraints, thus producing dissipative effects) has forced the study of the methods for the treatment of forces nonderivable from a potential. These efforts can, at this moment, be classified into the so-called

(a) "Inverse Problem" of Newtonian Mechanics. It essentially consists of : (i) the integrability conditions for the existence of the conventional equations (I.3) and (I.4) -the so-called conditions of variational self-adjointness- ; (ii) the methods for the computation of a Lagrangian or a Hamiltonian from the equations of motion ; and (iii) the methods for transforming variationally nonselfadjoint systems into a form representable via equations (I.3) and (I.4) (see Santilli 1978a, 1980a and quoted references).

(b) "Lie-admissible Problem" of Newtonian Mechanics. It essentially consists of the direct study of the generalized analytic, algebraic, and geometrical properties of the original equations (I.1) and (I.2). In particular, the brackets of the time evolution law induced by equations (I.2), when properly written, characterize a covering of the Lie algebras called Lie-admissible algebras (see Santilli, 1978b and 1979a, and the reprint volumes Myung, Okubo and Santilli, 1978a and 1978b).

- *Statistical Mechanics and Thermodynamics*. A number of authors have initiated the interpretation of irreversible processes via the use of forces nonderivable from a potential and the study of the statistical/thermodynamical character of nonconservative mechanics (see, for instance, Guiaşu, 1966 ; Fronteau, 1966,1971 ; Roman & Santilli, 1969 ; Fronteau, 1975 ; Salmon, 1975,1977 ; Dobbertin, 1976 ; Enz, 1977 ; George, Henin, Mayné & Prigogine, 1978 ; Fronteau, 1979 ; Combis, Fronteau & Tellez-Arenas, 1979). It is shown in (Tellez-Arenas, Fronteau & Combis, 1979) that the use of nonselfadjoint interactions is in full agreement with the physical assumptions which constitute the foundations of statistical physics.

- *Astrophysics*. The flattening of a galaxy may be explained via a model which postulates inelastic collisions between the objects in the galaxy (Brahic, 1977).

- *Accelerator Theory*. Bremstrahlung is used to focus electrons (Kolomensky & Lebedev, 1962). Also, a comparable effect is obtained for heavy particles by cooling the beam with Coulomb collisions on an auxiliary electron beam, giving rise, on an average, to a frictional force (Budker et al, 1974).

- *Nuclear Physics*. The quantum mechanical study of dissipative effects has lately seen a considerable increase in nuclear physics (see, for instance, Nörenberg & Weidenmüller, 1976 ; Hasse, 1977, and quoted references). In connection with this discipline, a number of extensions of the Schrödinger equation have been proposed (see, for instance, Kostin, 1975 ; Fronteau & Tellez-Arenas, 1976 ; Yasue, 1977 ; Santilli, 1978d ; Yasue, 1978).

- *Hadron Physics*. The study of the old idea that the strong interactions are nonderivable from a potential has been recently intensified (Santilli, 1978d, 1978e, 1979a and 1980b ; see also Myung, Okubo and Santilli, 1978b and 1979).

In this paper, we shall first recall the notion of dissipative, nonconservative and, in general, variationally nonselfadjoint forces (Section II). We shall then review Liouville's theorem in its original formulation (Section III), and identify an algebraic character of classical statistical mechanics for forces nonderivable from a potential (Section IV). This will allow us to tackle the problem of quantization of the statistics of dissipative phenomena, and to propose a possible generalization of the conventional Lie formulation for the quantum evolution law (Section V). A number of comments on the possible relevance of this physically and algebraically broader approach to statistics will be also presented (Section VI).

II. DISSIPATIVE, NONCONSERVATIVE AND VARIATIONALLY NONSELFADJOINT FORCES.

1°) Dissipative systems.

Let us state as clearly as possible what we understand by "dissipation" of energy. We shall say that a system of particles (with no applied forces) is dissipative when the total energy $E_{tot} = E_{kin} + E_{pot}$ is monotonically nonincreasing in time (Santilli, 1978a, p.229), i.e.,

$$E_{tot}|_{t_1} \geqslant E_{tot}|_{t_2} \quad , \quad t_1 < t_2 \quad . \tag{II.1}$$

This definition is intended for conventional Newtonian systems, such as particles moving in our atmosphere, spinning tops with drag torques, systems with holonomic mechanical constraints, etc... In general, these systems are open, in the sense that they cannot be considered as isolated from their environment. The energy lost by a system is then acquired by its environment and cannot be recuperated via a variation of any potential. The monotonicity condition ensures the existence of dissipation at all times. The equality in condition (II.1) also allows the inclusion of the class of conservative systems as a particular case of the broader class of dissipative systems.

2°) Conservative systems.

We are now in a position to state what we understand by "conservation" of energy. First, it is trivially understood that for any closed system of particles (that is, systems which can be considered as isolated from their environment) the total energy is conserved. Nevertheless, this property alone is insufficient to identify the desired notion of conservation, and the following differentiation becomes essential.

(a) *Conservative systems without internal dissipative effects*.

Typically, these are systems of (point) particles moving in vacuum without collisions and with only action-at-a-distance forces derivable from a potential.

(b) *Conservative systems vith internal dissipative effects*.

Consider an open dissipative system such as a satellite in Earth's atmosphere. This system is subjected to forces derivable from a potential (the gravitational force) *and* forces nonderivable from a potential (polynomial expansions in the velocities). In the transition to the corresponding closed system comprising the original dissipative system and its environment (that is, the Earth with its atmosphere for the case at hand) the total energy is conserved. Nevertheless, the internal dissipative forces and effects persist. We simply have in this case mutual exchanges of energy between the components of the system via forces nonderivable from a potential. This second class of conservative systems is discussed in a separate paper of these Proceedings (Tellez-Arenas, Fronteau & Santilli, 1979).

3°) Nonconservative systems.

Finally, we are in a position to state what we understand by "nonconservation" of energy. Conservative and dissipative forces do not exhaust the forces of Newtonian Mechanics. A third relevant class is given by the so-called applied forces. These are external forces applied to the system considered (e.g., an oscillator) to preserve the motion for the desired period of time (without an external supply of energy, any motion in our environment decays in time). More generally, applied forces can supply an arbitrary amount of energy to the system considered. We reach in this way the following definition.

Nonconservative systems are generally open systems of particles (often called dynamical systems) subjected to a collection of conservative, dissipative, and applied forces for which the total energy can continuously but arbitrarily vary in time (Santilli, 1978a, p.233).

$$E_{tot}|_{t_1} \gtrless E_{tot}|_{t_2} \quad , \quad t_1 < t_2 \quad . \tag{II.2}$$

A typical example is given by the damped and forced oscillator, for which the variation of the energy in time is arbitrary, because dependent on the relationship of the dissipated and supplied energies.

In conclusion, a distinction among "conservative systems", "dissipative systems" and "nonconservative systems" is that :

- in the first case, the energy is conserved ;
- in the second case, the energy is nonincreasing in time ; and
- in the third case, the energy varies arbitrarily in time.

Almost needless to say, when the nonconservative (dynamical) systems are considered as a class, they are inclusive, as particular cases, of the dissipative and the conservative systems.

4°) Variationally nonselfadjoint forces.

The variational characterization of the forces for the systems considered is treated in detail in (Santilli, 1978a). We limit ourselves here to recall the notion of variationally selfadjoint and nonselfadjoint forces.

A Newtonian force $\vec{f}(t,\vec{r},\dot{\vec{r}})$, $\vec{r} \equiv (x,y,z)$, is called *variationally selfadjoint* when the following conditions are verified :

(a) The force $\vec{f}$ is of at least class C^1 in a (star shaped) neighborhood of its variables.

(b) The force $\vec{f}$ is at most linearly dependent on the velocity, i.e., of the type

$$f_i = \rho_{ij}(t,\vec{r})\,\dot{r}^j + \sigma_i(t,\vec{r}) \quad , \quad i = x,y,z \quad . \tag{II.3}$$

(c) All the following conditions of variational selfadjointness are verified in the neighborhood considered

$$\begin{aligned} &\rho_{ij} + \rho_{ji} = 0 \quad , \\ &\frac{\partial \rho_{ij}}{\partial r^k} + \frac{\partial \rho_{jk}}{\partial r^i} + \frac{\partial \rho_{ki}}{\partial r^j} = 0 \quad , \\ &\frac{\partial \rho_{ij}}{\partial t} = \frac{\partial \sigma_i}{\partial r^j} - \frac{\partial \sigma_j}{\partial r^i} \quad , \quad i,j,k = x,y,z \quad . \end{aligned} \tag{II.4}$$

Under these conditions, a potential function $U(t,\vec{r},\dot{\vec{r}})$ verifying the familiar rule

$$\vec{f} \equiv - \frac{\partial U}{\partial \vec{r}} + \frac{d}{dt} \frac{\partial U}{\partial \dot{\vec{r}}} \tag{II.5}$$

exists and can be computed from the force $\vec{f}$ via the methods of the Inverse Problem (Santilli, loc cit.). When at least one of conditions (II.3) and (II.4) is violated, the force is called *variationally nonselfadjoint*.

Notice that conditions (a), (b) and (c) above include the Lorentz force which, therefore, is variationally selfadjoint.

All conservative forces, (as those which govern the entire evolution of systems of the class 2°)a, are variationally selfadjoint, while dissipative forces are, in general, nonselfadjoint. With regards to applied forces, a number of them are selfadjoint (e.g., applied forces only dependent on time). However, applied forces are, in general, nonselfadjoint.

As a result, the notion of variationally nonselfadjoint forces constitutes a technical characterization of the most general possible, local, Newtonian forces, where the term "local" is intended to exclude integrodifferential forces, and the term "Newtonian" is intended to exclude acceleration dependent forces.

The notion of variational selfadjointness extends to systems of second-order ordinary differential equations, e.g., of the Newtonian form, in which case we shall write

$$[m\ddot{\vec{r}} - \vec{f}(t,\vec{r},\dot{\vec{r}})]_{SA} = 0 \qquad (II.6)$$

and provides the integrability conditions for the existence of the so-called direct analytic representation in terms of the (truncated) Lagrange's equations

$$\begin{aligned} &\frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{r}}} - \frac{\partial L}{\partial \vec{r}} \equiv [m\ddot{\vec{r}} - \vec{f}]_{SA} = 0 \\ &L = T(\dot{\vec{r}}) - U(t,\vec{r},\dot{\vec{r}}) \end{aligned} \qquad (II.7)$$

These systems are *highly restrictive* for the analysis of this paper. Indeed, they are a subclass of the most general possible, local, Newtonian systems

$$\left\{[m\ddot{\vec{r}} - f(t,\vec{r},\dot{\vec{r}})]_{SA} - \vec{F}(t,\vec{r},\dot{\vec{r}})\right\}_{NSA} = 0 \qquad (II.8)$$

where NSA stands for nonselfadjointness of the forces (and of the systems). For these latter systems, Lagrange's equations in their original conception (I.1) are directly applicable (that is, applicable without equivalence transformations) according to the rule

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\vec{r}}} - \frac{\partial L}{\partial \vec{r}} - \vec{F} \equiv \left\{[m\,\ddot{\vec{r}} - \vec{f}]_{SA} - \vec{F}\right\}_{NSA} \qquad \text{(II.9)}$$

Hamilton's equations with external terms representative of the nonselfadjoint forces are then directly applicable according to the scheme

$$\begin{aligned}
&\frac{d}{dt}(X^{\mu}) - (\omega^{\mu\nu})\,\frac{\partial H}{\partial X^{\nu}} - (F^{\mu}) \\
&= \begin{pmatrix} \dot{\vec{r}} \\ \dot{\vec{p}} \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} \partial H/\partial\vec{r} \\ \partial H/\partial\vec{p} \end{pmatrix} - \begin{pmatrix} 0 \\ \vec{F} \end{pmatrix} \\
&= \left\{\left[\begin{pmatrix} \dot{\vec{r}} \\ \dot{\vec{p}} \end{pmatrix} - \begin{pmatrix} \vec{p}/m \\ \vec{f}(\vec{r}) \end{pmatrix}\right]_{SA} - \begin{pmatrix} 0 \\ \vec{F}(t,\vec{r},\frac{\vec{p}}{m}) \end{pmatrix}\right\}_{NSA} \qquad \text{(II.10)} \\
&= 0
\end{aligned}$$

where, for simplicity but without loss of generality, we have considered the case when the selfadjoint force is only dependent on $\vec{r}$.

The statistical analysis of this paper is based on systems (II.10).

III. LIOUVILLE'S THEOREM IN ITS ORIGINAL FORMULATION.

In this section, we will recall Liouville's theorem in its original formulation

(Liouville, 1838) and show that it is indeed capable of incorporating variationally nonselfadjoint forces.

1°) Liouville's theorem.

Given a differential system

$$\frac{dX}{dt} - \mathcal{F}(X,t) = 0 \quad , \quad X \in \mathbb{R}^n \quad , \tag{III.1}$$

where the vector field $\mathcal{F}$ has only to satisfy usual regularity conditions which are unessential here, we consider the solution

$$X_t = X(t,X_0)$$

written in terms of the initial condition X_0.

The theorem of Liouville states that* the Jacobian J_t

$$J_t = \frac{D(X_t)}{D(X_0)}$$

satisfies the relation

$$\frac{d}{dt} \operatorname{Log} |J_t| = \operatorname{div}_X \mathcal{F} \tag{III.2}$$

where $\operatorname{div}_X \mathcal{F}$ is evaluated for $X = X_t$.

This result has an immediate geometrical interpretation. Denoting the element of volume in the X space at time t as dX_t, the time evolution of dX_t is governed by the Jacobian J_t, according to the rule

$$dX_t = \left|\frac{D(X_t)}{D(X_0)}\right| dX_0 = |J_t| \; dX_0 \quad . \tag{III.3}$$

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*Liouville's theorem is even a slightly more general result, since it is in fact related to the solution written in terms of the integration constants (Liouville, 1838 ; Tellez-Arenas, Fronteau & Combis, 1979), and not in terms of the initial conditions.

To appreciate the physical meaning of this rule, it is useful to identify (III.1) with the dynamics (II.10) in the case of a one particle Newtonian system with selfadjoint and nonselfadjoint forces :

$$X = \begin{pmatrix} r^i \\ p_i \end{pmatrix} \; ; \; \mathcal{F}(X,t) = \begin{pmatrix} p_i/m \\ f_i(\vec{r}) \end{pmatrix}_{SA} + \begin{pmatrix} 0 \\ F_i(t,\vec{r},\vec{p}/m) \end{pmatrix}_{NSA} \qquad \text{(III.4)}$$

$i = 1,2,3 = x,y,z$.

In this case, (III.2) becomes

$$\frac{d}{dt} \operatorname{Log} |J_t| = \frac{\partial}{\partial p_i} F_{i,NSA} \quad , \quad \text{(sum over i)} \quad . \qquad \text{(III.5)}$$

Thus, if there were only selfadjoint forces (Hamiltonian system), we would recover, from (III.5) and (III.3), the usual time conservation of the volume element in phase space. But the presence of *nonselfadjoint forces* has a fundamental consequence : the element of volume in the dynamical space *varies in time* according to the relation (III.5).

2°) Statistical application of Liouville's theorem.

The transition from the one particle dynamics to the statistical profile is realized through the introduction of a density $\rho(X,t)$. If there are neither creation nor annihilation of states during the time evolution, we can write the following conservation condition

$$\rho(X_t,t)\; dX_t = \rho(X_0,t_0)\; dX_0 \quad , \quad \forall\, t \qquad \text{(III.6)}$$

or

$$\rho(X_t,t)\; |J_t| = \text{constant} \quad .$$

Consequently, (III.2) becomes,

$$\frac{d}{dt} \operatorname{Log} \rho(X_t,t) = - (\operatorname{div}_X \mathcal{F})_{X=X_t} \qquad \text{(III.7)}$$

or, equivalently,

$$\frac{\partial}{\partial t} \rho + \operatorname{div}_X(\rho \mathcal{F}) = 0 \quad . \qquad \text{(III.8)}$$

Recall that, in (III.8), all terms are evaluated for $X = X_t$; moreover, (III.8), which appears as the equation of *continuity in the* X *space*, is often called the generalized Liouville equation but, in fact, it is nothing more than the *true Liouville equation* emerging from (III.2).

In the dynamical case (III.4), the relation (III.7) becomes

$$\frac{d}{dt} \operatorname{Log} \rho = - \frac{\partial}{\partial p_i} F_{i,NSA} \quad . \qquad \text{(III.9)}$$

Thus, if there are only selfadjoint forces, the density ρ is a constant of motion, as well known. However, if nonselfadjoint forces are introduced, the density ρ varies with time.

Note also that (III.9), or (III.8), is equivalent to the relation

$$\frac{\partial}{\partial t} \rho + [\rho,H] + F_{i,NSA} \frac{\partial \rho}{\partial p_i} + \rho \frac{\partial}{\partial p_i} F_{i,NSA} = 0 \qquad \text{(III.10)}$$

which, for $\vec{F}_{NSA} \equiv 0$, reduces to the usual conservative ("truncated") Liouville equation

$$\frac{\partial}{\partial t} \rho + [\rho,H] = 0 \quad . \qquad \text{(III.11)}$$

Thus, the transition from the selfadjoint case to the nonselfadjoint case introduces two supplementary terms . The first one, $F_{i,NSA} \frac{\partial \rho}{\partial p_i}$, modifies each Hamiltonian trajectory, and the second one, which is essential from a statistical viewpoint, $\rho \frac{\partial}{\partial p_i} F_{i,NSA}$, modifies the dynamical space itself, in the vicinity of the actual trajectory. The influence of these two terms on the algebraic structure of statistical mechanics will be studied in the following sections.

It should finally be noted that the meaning of the original Liouville's theorem has been brought to light more than one decade ago (Fronteau, 1965) and that at the same time Liouville's demonstration was rediscovered as a new one (Guiaşu, 1966). Note also that the Liouville equation, with a Lie-admissible structure, has been derived by (Roman & Santilli, 1969) for a particular case of forces nonderivable from a potential. However, different authors working on nonselfadjoint forces continue to ignore today the original work by Liouville and to propose some proofs of the Liouville equation (Gerlich, 1973 ; Enz, 1977 ; Steeb, 1979).

IV. THE LIE-ADMISSIBLE STRUCTURE OF CLASSICAL STATISTICAL MECHANICS.

1°) Conservative statistical mechanics.

Let us first review the Lie algebra structure of the conventional case of statistical mechanics for conservative forces. For clarity, we shall limit ourselves to a presentation as elementary as possible.

1.a) *One particle evolution*.

The equations of motion in first-order form (vector field on the cotangent bundle), for a Newtonian particle under the action of conservative forces, are given by

$$\dot{X}^\mu - \Xi^\mu(X) = 0 \quad , \quad (X^\mu) = \begin{pmatrix} \vec{r} \\ \\ \vec{p} \end{pmatrix} , \quad (\Xi^\mu) = \begin{pmatrix} \vec{p}/m \\ \\ \vec{f}(\vec{r}) \end{pmatrix} , \qquad \text{(IV.1)}$$

$\mu = 1,2,3,4,5,6$.

and admit the following direct representation in terms of the conventional (that is, "truncated") Hamilton's equations

$$\dot{X}^{\mu} - \omega^{\mu\nu}\frac{\partial H}{\partial X^{\nu}} \equiv \dot{X}^{\mu} - \Xi^{\mu}(X) = 0 \tag{IV.2a}$$

$$(\omega^{\mu\nu}) = \begin{pmatrix} 0_{3\times3} & 1_{3\times3} \\ -1_{3\times3} & 0_{3\times3} \end{pmatrix} \quad . \tag{IV.2b}$$

These assumptions imply that the brackets [A,H] of the time evolution law of functions $A(\vec{r},\vec{p})$ in the phase space of the (canonically conjugate) variables $\vec{r}$ and $\vec{p}$, i.e., the conventional Poisson brackets,

$$\dot{A} = [A,H] = \frac{\partial A}{\partial X^{\mu}}\,\omega^{\mu\nu}\,\frac{\partial H}{\partial X^{\nu}} \equiv \frac{\partial A}{\partial \vec{r}}\cdot\frac{\partial H}{\partial \vec{p}} - \frac{\partial A}{\partial \vec{p}}\cdot\frac{\partial H}{\partial \vec{r}} \quad , \tag{IV.3}$$

verify the Lie algebra laws

$$[A,B] + [B,A] = 0 \quad , \tag{IV.4a}$$

$$[[A,B],C] + [[B,C],A] + [[C,A],B] = 0 \quad . \tag{IV.4b}$$

For later use, it should be recalled here that the brackets [A,B], first of all, verify the conditions to qualify them as the product of an "algebra" as commonly understood, that is, they verify the distributive and scalar rules

$$[A,B+C] = [A,B] + [A,C] \quad , \quad [A+B,C] = [A,C] + [B,C] \tag{IV.5a}$$

$$[\alpha A,B] = [A,\alpha B] = \alpha[A,B] \qquad \alpha = \text{Number} \quad . \tag{IV.5b}$$

Secondly, the brackets [A,B] characterize a nonassociative algebra, i.e.,

$$[[A,B],C] \neq [A,[B,C]] \quad . \tag{IV.6}$$

Thirdly, this nonassociative algebra is a Lie algebra, on account of the verification of properties (IV.4) for all functions on phase space (satisfying certain smoothness conditions unessential for our analysis).

1.b) *Statistical evolution.*

The restriction of the forces to be conservative, and the representation of the equations of motion via the "truncated" Hamilton's equations has the following primary implications from a statistical viewpoint.

First of all, we have the trivial property

$$\mathrm{div}_X \; \Xi(X) = \frac{\partial}{\partial \vec{r}} \cdot \frac{\partial H}{\partial \vec{p}} + \frac{\partial}{\partial \vec{p}} \left(- \frac{\partial H}{\partial \vec{r}} \right) \equiv 0 \quad . \tag{IV.7}$$

Secondly, the time evolution law of densities $\rho(t,\vec{r},\vec{p})$ is given by the conventionally used Liouville's equation

$$\begin{aligned} \frac{d}{dt} \rho &= \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial \vec{r}} \cdot \frac{\partial H}{\partial \vec{p}} - \frac{\partial \rho}{\partial \vec{p}} \cdot \frac{\partial H}{\partial \vec{r}} \\ &= \frac{\partial \rho}{\partial t} + [\rho, H] = 0 \end{aligned} \tag{IV.8}$$

and, as such, it exhibits a Lie algebra structure.

Thirdly, the structure of the product of the Lie algebra of the one particle evolution, equation (IV.3), coincides with the product of the Lie algebra of the statistical evolution, equations (IV.8).

The same algebraic structure, at both the one particle level and the statistical level, is preserved for the more general class of variationally selfadjoint forces, that is, the forces verifying the integrability conditions for the existence of a potential.

2°) Nonconservative statistical mechanics.

As stressed in Section II, the variationally selfadjoint forces do not exhaust, by far, the forces of Newtonian Mechanics. To avoid unnecessary and excessive physical restrictions, we therefore consider a Newtonian particle under the action of the most general possible, local, Newtonian forces. These forces can be decomposed, according to Equations (II. 8) into a term which is variationally selfadjoint (derivable from a potential) and a term which is variationally nonselfadjoint (nonderivable from a potential).

2.a) *One particle evolution.*

The first-order (vector field) form of the equations of motion are now given by

$$\dot{X}^{\mu} - \Xi^{\mu}(X) - F^{\mu}_{NSA}(t,X) = 0 \quad , \quad (X^{\mu}) = \begin{pmatrix} \vec{r} \\ \\ \vec{p} \end{pmatrix} , \quad (\Xi^{\mu}) = \begin{pmatrix} \vec{p}/m \\ \\ \vec{f}_{SA}(\vec{r}) \end{pmatrix} , \quad (F^{\mu}_{NSA}) = \begin{pmatrix} 0 \\ \\ \vec{F}_{NSA} \end{pmatrix}$$

$\mu = 1,2,3,4,5,6.$ (IV.9)

where, for simplicity but without loss of generality, we have considered the subcase when the selfadjoint force is only dependent on $\vec{r}$ (but the nonselfadjoint force is unrestricted). Equations (IV.9) admit a representation in terms of Hamilton's equations in their original form according to Equations (II.10), i.e.,

$$\dot{X}^{\mu} - \omega^{\mu\nu} \frac{\partial H}{\partial X^{\nu}} - F^{\mu}_{NSA} \equiv \dot{X}^{\mu} - \Xi^{\mu}(X) - F^{\mu}_{NSA}(t,X) = 0 \quad . \qquad \text{(IV.10)}$$

A primary implication of this physically and mathematically broder setting is the following. The brackets AxH of the emerging time evolution law

$$\dot{A}(X) = \dot{A}(\vec{r},\vec{p})$$

$$= \frac{\partial A}{\partial \vec{r}} \cdot \frac{\partial H}{\partial \vec{p}} - \frac{\partial A}{\partial \vec{p}} \cdot \frac{\partial H}{\partial \vec{r}} + \frac{\partial A}{\partial \vec{p}} \cdot \vec{F}_{NSA} \qquad \text{(IV.11)}$$

$$= \frac{\partial A}{\partial X^{\mu}} \omega^{\mu\nu} \frac{\partial H}{\partial X^{\nu}} + \frac{\partial A}{\partial X^{\mu}} F^{\mu}_{NSA} = [A,H] + \frac{\partial A}{\partial X^{\mu}} F^{\mu}_{NSA} \overset{\text{def}}{=} A \times H$$

do not characterize an algebra any more, because they violate the right distributive and the scalar law (Santilli, 1978b, p.300).

$$\begin{aligned} &A \times (B + C) \neq A \times B + A \times C \\ &(\alpha A) \times B \neq A \times (\alpha B) \quad . \end{aligned} \tag{IV.12}$$

Nevertheless, for all systems considered, one has $\partial H/\partial p_i \neq 0$ for all $i = 1,2,3 = x,y,z$, and we can always rewrite the nonselfadjoint forces in the form

$$F^{\mu}_{NSA} = T^{\mu\nu} \frac{\partial H}{\partial X^{\nu}} \quad , \qquad T^{\mu\nu} = T^{\nu\mu} \tag{IV.13}$$

with the trivial, diagonal, algebraic solution

$$(T^{\mu\nu}) = \begin{pmatrix} 0_{3\times3} & 0_{3\times3} \\ 0_{3\times3} & s_{3\times3} \end{pmatrix} \quad s_{3\times3} = \begin{pmatrix} F_{1,NSA}/(\partial H/\partial p_1) & 0 & 0 \\ 0 & F_{2,NSA}/(\partial H/\partial p_2) & 0 \\ 0 & 0 & F_{3,NSA}/(\partial H/\partial p_3) \end{pmatrix} \tag{IV.14}$$

Representation (IV.10) now reads

$$\begin{aligned} &\dot{X}^{\mu} - S^{\mu\nu}(t,X) \frac{\partial H(X)}{\partial X^{\nu}} \\ \equiv\ &\dot{X}^{\mu} - \Xi^{\mu}(X) - F^{\mu}_{NSA}(t,X) \\ &(S^{\mu\nu}) = (\omega^{\mu\nu}) + (T^{\mu\nu}) = \begin{pmatrix} 0_{3\times3} & 1_{3\times3} \\ -1_{3\times3} & s_{3\times3} \end{pmatrix} \\ &\det\,(S^{\mu\nu}) = 1 \neq 0 \end{aligned} \tag{IV.15}$$

and the brackets of the time evolution law acquire the form

$$\dot{A}(X) = \frac{\partial A}{\partial X^{\mu}} S^{\mu\nu} \frac{\partial H}{\partial X^{\nu}} = \frac{\partial A}{\partial r^i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial r^i} + \frac{\partial A}{\partial p_i} s_{ij} \frac{\partial H}{\partial p_j} \overset{\text{def}}{=} (A,H) \tag{IV.16}$$

For given Hamiltonian H and nonconservative forces $\vec{F}_{NSA}$ (i.e., for a *given* matrix $s_{3x3}(t,\vec{r},\vec{p})$), these brackets (A,B) verify the following properties (Santilli, loc. cit. p.311, and 1978c, p.1294).

(i) The brackets (A,B) characterize an algebra, that is, they verify the left and right distributive and scalar law

$$(A,B+C) = (A,B) + (A,C) \quad , \quad (A+B,C) = (A,C) + (B,C) \qquad \text{(IV.17a)}$$

$$(\alpha A,B) = (A,\alpha B) = \alpha(A,B) \quad , \quad \alpha = \text{number} \quad . \qquad \text{(IV.17b)}$$

(ii) The algebra characterized by the brackets (A,B) is nonassociative (as for the case of the Lie algebra), i.e.,

$$((A,B),C) \neq (A,(B,C)) \qquad \text{(IV.18)}$$

(iii) The brackets (A,B) characterize an algebraic covering of the Lie algebras called Lie-admissible algebras. These algebras, in the Newtonian realization considered here, are characterized by the law

$$\begin{aligned} &((A,B),C) + ((B,C),A) + ((C,A),B) \\ &+ (C,(B,A)) + (B,(A,C)) + (A,(C,B)) \\ &- (A,(B,C)) - (B,(C,A)) - (C,(A,B)) \\ &- ((C,B),A) - ((B,A),C) - ((A,C),B) = 0 \quad . \end{aligned} \qquad \text{(IV.19)}$$

The product (A,B) is neither totally symmetric nor totally antisymmetric. Nevertheless, when such a product is totally antisymmetric, the Lie algebra law (IV.4a) is trivially verified, and law (IV.19) reduces to four times Jacobi's law (IV.4b). A first interpretation of the covering nature of the Lie-admissible algebras over the Lie algebras can then be expressed by saying that the former admit the latter as a particular case. A second interpretation of this covering profile is provided by the property that the reduction of the product (A,B) to a totally antisymmetric form, i.e., [A,B], is representative of the null value of the nonselfadjoint forces in equations (IV.16). Thus, the algebraic property of the Lie-admissible algebras of being a covering of the Lie algebra possesses a direct and immediate physical interpretation in terms of the nature of the forces acting in the time evolution law. In particular, the forces nonderivable from a potential are embedded into the algebraic product (.,.) and are represented by the departure of this product from the Lie product [.,.].

These ideas can be equivalently expressed by saying that the product (A,B) is Lie-admissible because the so-called attached product

$$[A,B]^{-} = (A,B) - (B,A) = 2[A,B] \tag{IV.20}$$

is Lie, that is, it verifies laws (IV.4).

2.b) *Statistical evolution.*

The extension of the preceding algebraic structure to statistical mechanics, through Liouville's theorem, is rather intringuing. (Note that this study of the algebraic structure of nonconservative mechanics is apparently considered in this article for the first time).

First, for the sake of clarity, let us note that the variables $\vec{r}$ and $\vec{p}$ *do not span a phase space* for systems (IV.15) because they are no longer canonically conjugate. They span a more general space called *dynamical space* (Santilli, 1978b and 1979a). The conventional phase space, however, is admitted as a particular case, trivially, when all forces are derivable from a potential.

The time evolution of densities $\rho(t,\vec{r},\vec{p})$ in this broader dynamical space is now given (see (III.9)) by

$$\frac{d\rho}{dt} = - \rho \frac{\partial}{\partial X^{\mu}} \left(\Xi^{\mu} + F^{\mu}_{NSA} \right) = - \rho \frac{\partial}{\partial p_i} F_{i,NSA} \tag{IV.21}$$

that is

$$\frac{\partial\rho}{\partial t} + (\rho,H) + \rho\,\frac{\partial}{\partial p_i}\,F_{i,NSA} = 0 \qquad \text{(IV.22)}$$

where, of course, we have now made full use of Liouville's theorem in its original formulation (equation (III.2) and then (III.7)).

An inspection of equations (IV.22) indicates the emergence of a *first layer of Lie-admissible algebras*, in the sense that the Lie-admissible one particle Newtonian product now enters into the definition of the time evolution law of densities. However, this product alone does not characterize the entire time evolution law of densities, trivially, because of the presence of the *additional term* $\rho\,\frac{\partial}{\partial p_i}\,F_{i,NSA}$. Indeed, this agrees with the physical meaning of density, whose variation along any given trajectory is closely related to the variation of the element of volume in the vicinity of the trajectory considered (see Section III).

3°) Algebraic structure of nonconservative statistical mechanics.

We will now show that the study of the algebraic structure of nonconservative statistical mechanics reveals a *second layer of Lie-admissible algebras*, capable of providing the *complete* algebraic representation of the time evolution law of densities, equation (IV.22). To identify this second layer, the notion of *isotopy* is needed.

3.a) *The notion of Lie-admissible isotopy.*

Let U be an algebra with elements a,b,c,... over a field $\mathcal{F}$ (here assumed of characteristic zero) and abstract product ab. An isotopic mapping of the algebra U or an U-isotope is an algebra, say, U^*, which coincides with U as vector space (that is, the elements of U and U^* coincide), but whose product $a*b$ is given by any modification of the product ab, via elements of U, which is such as to preserve the algebraic law of U (that is, if U is associative, or Lie, or Jordan, etc..., U^* is also associative, or Lie, or Jordan, etc..., respectively). For studies on this notion of isotopy, see (Santilli, 1978b and 1979a). For more recent studies, see the contribution to these proceedings (Myung & Santilli, 1979). An example of Newtonian isotopy is provided by the Lie algebra isotope (Santilli, 1978b)

$$[A,B] = \frac{\partial A}{\partial X^\mu}\,\omega^{\mu\nu}\,\frac{\partial B}{\partial X^\nu} \rightarrow [A,B]^* = \frac{\partial A}{\partial X^\mu}\,\Omega^{\mu\nu}(X)\,\frac{\partial B}{\partial X^\nu} \qquad \text{(IV.23a)}$$

$$(\Omega^{\mu\nu}) = \left(\left\|\frac{\partial R_\nu(X)}{\partial X^\mu} - \frac{\partial R_\mu(X)}{\partial X^\nu}\right\|^{-1}\right)^{\mu\nu} = \omega^{\mu\nu} + h^{\mu\nu}(X) \qquad \text{(IV.23b)}$$

which characterizes the transition from Hamilton's equations to the so-called Birkhoff's equations.

In this paper, we are interested in the *Lie-admissible isotopy*, that is, any modification of the product (A,B) which satisfies the following rules :

(i) the base manifold with local coordinates $\vec{r}$ and $\vec{p}$ is unchanged.

(ii) the vector space of the algebra (here given by functions of the $(\vec{r},\vec{p})$-coordinates) is also unchanged.

(iii) the isotopy occurs via a modification of the structure of the product (A,B) in terms of elements of the vector space.

(iiii) the new product $(A,B)^*$ verifies the Lie-admissible laws (IV.17,18,19).

Writing the new product $(A,B)^*$ in the following way,

$$(A,B) = \frac{\partial A}{\partial X^\mu}\,S^{\mu\nu}(t,X)\,\frac{\partial B}{\partial X^\nu} \rightarrow (A,B)^* = \frac{\partial A}{\partial X^\mu}\,S^{*\mu\nu}(t,X)\,\frac{\partial B}{\partial X^\nu} \qquad \text{(IV.24)}$$

one of the simplest possible realizations of the Lie-admissible isotopies in one particle Newtonian mechanics is given by

$$(S^{\mu\nu}) = \begin{pmatrix} 0_{3\times3} & 1_{3\times3} \\ -1_{3\times3} & s_{3\times3} \end{pmatrix} \rightarrow S^{*\mu\nu} = \begin{pmatrix} 0_{3\times3} & 1_{3\times3} \\ -1_{3\times3} & (s+s^{*})_{3\times3} \end{pmatrix} \qquad \text{(IV.25)}$$

$$s = s^{T} \qquad\qquad s^{*} = s^{*T}$$

that is, it is provided by the addition to the symmetric matrix (s_{ij}) of a new symmetric matrix (s^{*}_{ij}) defined in the same variables.

3.b) *The Lie-admissible isotopy associated with nonconservative statistical mechanics.*

The central theorem which shows the isotopic character of the time evolution law for densities, i.e., equation (IV.22), is obtained by means of the following result, which is easily verified : *assuming that the density* $\rho(t,\vec{r},\vec{p})$ *and the Hamiltonian* $H(\vec{r},\vec{p})$ *always depend on all components of* $\vec{p}$, *the divergence term* $\rho \frac{\partial}{\partial p_i} F_{i,NSA}$ *in Liouville's theorem* (IV.21) *always admits the representation*

$$\rho \frac{\partial}{\partial p_i} F_{i,NSA} = \frac{\partial \rho}{\partial p_i} s^{*}_{ij} \frac{\partial H}{\partial p_j} \qquad \text{(IV.26a)}$$

$$s^{*}_{3\times3} = \begin{pmatrix} s^{*}_{11} & 0 & 0 \\ 0 & s^{*}_{22} & 0 \\ 0 & 0 & s^{*}_{33} \end{pmatrix}, \quad s^{*}_{ii} = \overbrace{\rho \frac{\partial}{\partial p_i} F_{i,NSA} \Big/ \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial p_i}}^{\text{no sum here}} \qquad \text{(IV.26b)}$$

$$\rho \frac{\partial}{\partial p_i} F_{i,NSA} = \frac{\partial \rho}{\partial X^{\mu}} T^{*\mu\nu} \frac{\partial H}{\partial X^{\nu}}, \quad (T^{*\mu\nu}) = \begin{pmatrix} 0_{3\times3} & 0_{3\times3} \\ 0_{3\times3} & s^{*}_{3\times3} \end{pmatrix} .$$

As a result, the time evolution law of densities, equation (IV.22), can always be written in the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial r^{i}} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial r^{i}} + \frac{\partial \rho}{\partial p_i} s_{ij} \frac{\partial H}{\partial p_j} + \frac{\partial \rho}{\partial p_i} s^{*}_{ij} \frac{\partial H}{\partial p_j}$$

$$= \frac{\partial \rho}{\partial t} + (\rho, H) + \frac{\partial \rho}{\partial p_i} s^{*}_{ij} \frac{\partial H}{\partial p_j} = \frac{\partial \rho}{\partial t} + (\rho, H)^{*} = 0 \quad . \qquad \text{(IV.27)}$$

For a given statistical system (i.e., for *given* matrices s and s*), the new brackets $(A,B)^*$ are such that

$$(A,B)^* - (B,A)^* = (A,B) - (B,A) = 2[A,B] \tag{IV.28}$$

which proves that the new product $(A,B)^*$ is Lie-admissible and thus that it is an isotope of (A,B).

This algebraic property has the following direct physical interpretation. As indicated earlier, the one particle Newtonian product (A,H) is neither totally symmetric, nor totally antisymmetric. As such, it can be decomposed into a totally symmetric and a totally antisymmetric part according to

$$\left.\begin{aligned} (A,H) &= \frac{\partial A}{\partial X^\mu} S^{\mu\nu}(t,X) \frac{\partial H}{\partial X^\nu} \\ &= \frac{\partial A}{\partial X^\mu} \omega^{\mu\nu} \frac{\partial H}{\partial X^\nu} + \frac{\partial A}{\partial X^\mu} T^{\mu\nu}(t,X) \frac{\partial H}{\partial X^\nu} \\ &= [A,H] + \{A,H\} \end{aligned}\right\} \tag{IV.29}$$

$$\omega^{\mu\nu} = - \omega^{\nu\mu} \quad , \quad T^{\mu\nu}(t,X) = T^{\nu\mu}(t,X)$$

$$[A,H] = - [H,A] \quad , \quad \{A,H\} = \{H,A\} \quad .$$

The nonselfadjoint forces $\vec{F}_{NSA}$ are entirely represented by the symmetric part, according to the rule (IV.13) or

$$(S^{\mu\nu} - \omega^{\mu\nu}) \frac{\partial H}{\partial X^\nu} = T^{\mu\nu} \frac{\partial H}{\partial X^\nu} = F^\mu_{NSA} \quad . \tag{IV.30}$$

It is in this sense that, as indicated earlier, the forces of the one particle Newtonian reality are embedded into the structure of the algebraic product. In the transition to the statistical profile, this situation persists, in the sense that the isotopically mapped product $(\rho,H)^*$ is also neither totally antisymmetric nor totally symmetric and admits the decomposition

$$\begin{aligned} (\rho,H)^* &= \frac{\partial\rho}{\partial X^\mu}\, S^{*\mu\nu}(t,X)\, \frac{\partial H}{\partial X^\nu} \\ &= \frac{\partial\rho}{\partial X^\mu}\, \omega^{\mu\nu}\, \frac{\partial H}{\partial X^\nu} + \frac{\partial\rho}{\partial X^\mu}\, T^{\mu\nu}(t,X)\, \frac{\partial H}{\partial X^\nu} + \frac{\partial\rho}{\partial X^\mu}\, T^{*\mu\nu}(t,X)\, \frac{\partial H}{\partial X^\nu} \qquad \text{(IV.31)} \\ &= [\rho,H] + \{\rho,H\} + \{\rho,H\}^* \quad , \qquad T^{*\mu\nu} = T^{*\nu\mu} \quad . \end{aligned}$$

The totally antisymmetric part, $[\rho,H]$, of this product represents the conventional Liouville's case for conservative forces. The symmetric part is made up of two terms, the first, $\{\rho,H\}$, of one particle Newtonian origin, and the second, $\{\rho,H\}^*$, of statistical origin. As a result, the divergence term $\rho \frac{\partial}{\partial p_i} F_{i,NSA}$ of Liouville's theorem in its original formulation becomes embedded into the structure of the algebraic product, via a symmetric term which is additive to the one particle Newtonian term.

These results can be expressed via the following theorem, which we shall refer as *the theorem of direct universality of the Lie-admissible structure of statistical mechanics*, where the term "direct" stands to indicate that the Lie-admissible algebras occurs *without* redefinition of the equations of motion, of the Hamiltonian and of the local variables, and the term "universality" stands to indicate that the Lie-admissible structure is possible for *all* Newtonian systems of the class considered.

THEOREM. *The time evolution law of densities for the statistical description of variationally nonselfadjoint Newtonian systems always admit a Lie-admissible structure according to equation* (IV.27).

4°) Résumé of Section IV.

We can resume this section by saying that the admission of the most general possible local Newtonian forces (the variationally nonselfadjoint forces) has the following primary implications :

(a) It is naturally compatible with Liouville's theorem in its original formulation, rather than the reduced version of this theorem used in most of the contemporary literature.

(b) It implies the necessary violation of the Lie algebra structure of conventional statistical mechanics for conservative forces, under the condition that the equations of motion, the Hamiltonian (defined as the total physical energy, kinetic plus potential) and the local variables are preserved (see Appendix for comments when this condition is relaxed).

(c) It implies the emergence of the Lie-admissible covering of the Lie algebras.

(d) The products of the one particle Newtonian description, (A,H), and of the statistical description, $(\rho,H)^*$, are both Lie-admissible. Yet the latter is physically broader than the former, in the sense that it contains an additional term representative of the time variation of the volume element in the dynamical space (Lie-admissible isotopy). This feature is completely absent in the conventional, Lie, statistical description. Indeed, in this case, the structure of the one particle Newtonian product [A,H] from equation (IV.3) and that of the statistical product $[\rho,H]$ from equation (IV.8), coincide.

(e) The forces $\vec{F}_{NSA}$ nonderivable from a potential and the divergence term $\rho\frac{\partial}{\partial p_i}F_{i,NSA}$ of Liouville's theorem are directly represented in the structure of the Lie-admissible product and, more specifically, are expressed by its symmetric parts.

V. THE LIE-ADMISSIBLE STRUCTURE OF QUANTUM STATISTICAL MECHANICS.

Another reason for our interest in the Lie-admissible formulation of statistics rests on possible contributions to the problem of quantization. This is another field of physics which has lately seen outstanding advances, particularly in the case of dissipative forces (see, for instance, George et al, 1978, and quoted references). However, most of these efforts are still based on the quantum mechanical form of Liouville's equation (IV.8), that is, the so-called Liouville-von Neumann equation

$$i\,\frac{\partial\hat{\rho}}{\partial t} - \hat{L}\,\hat{\rho} = 0 \quad , \quad \hbar = 1 \quad , \tag{V.1a}$$

$$\hat{L}\,\hat{\rho} = [\hat{H},\hat{\rho}] = \hat{H}\hat{\rho} - \hat{\rho}\,\hat{H} \quad , \quad \hat{\rho},\ \hat{L},\ \hat{H} = \text{Q.M. operators} \ . \tag{V.1b}$$

Dissipative forces are then treated via a careful use of *nonunitary* transformations (see George et al, loc. cit.).

There is no doubt that this approach constitutes a genuine advancement over conventional, quantum mechanical treatment of statistics and, as such it is indeed able to accomodate forces more general than the simplistic forces $\vec{f} = -\partial V/\partial\vec{r}$. The aspect in which we are interested is whether there exist a still more *general formulation* of the quantum mechanical treatment of the statistics of dissipative phenomena.

1°) Preliminary remarks.

There is little doubt that the *nonunitary* transformations play a fundamental role for the description of dissipative phenomena. Our view on this aspect can be presented as follows. One of the crucial implications of the presence of external terms nonderivable from a potential in the time evolution law (i.e., the transition from the "truncated" Hamilton's equations to their original form,or from (IV.3) to (IV.16)) is that the *time evolution of the system is no longer a canonical transformation* as in conventional conservative mechanics. Instead, such a transformation is canonical-admissible (Santilli, 1978b, p.325 ; see also the contribution to these

Proceedings by Kobussen & Santilli, 1979) in the sense that the time evolution, from X at time 0 to X' at time t,

$$\begin{aligned} X'^{\mu} &= X^{\mu} + \frac{t}{1}\dot{X}^{\mu} + \frac{t^2}{2!}\ddot{X}^{\mu} + \dots \\ &= X^{\mu} + \frac{t}{1}(X^{\mu},H) + \frac{t^2}{2!}((X^{\mu},H),H) + \dots = e^{t(\cdot,H)}\, X^{\mu} \\ &= e^{tS^{\alpha\beta}(0,X)\,\frac{\partial H(X)}{\partial X^{\beta}}\,\frac{\partial}{\partial X^{\alpha}}}\, X^{\mu} \end{aligned} \tag{V.2}$$

violates the condition for a transformation to be canonical, that is, it does not preserve the fundamental Poisson brackets,

$$\omega^{\mu\nu} = [X^{\mu},X^{\nu}] \rightarrow \omega'^{\mu\nu} = [X'^{\mu},X'^{\nu}] = \frac{\partial X'^{\mu}}{\partial X^{\alpha}}\,\omega^{\alpha\beta}\,\frac{\partial X'^{\nu}}{\partial X^{\beta}} \neq \omega^{\mu\nu} \tag{V.3a}$$

$$\omega^{\mu\nu} = \begin{pmatrix} [r^i,r^j] & [r^i,p_j] \\ [p_i,r^j] & [p_i,p_j] \end{pmatrix} = \begin{pmatrix} 0_{3\times3} & 1_{3\times3} \\ -1_{3\times3} & 0_{3\times3} \end{pmatrix} . \tag{V.3b}$$

Clearly, if the time evolution is *not canonical* at the classical one particle Newtonian level, its quantum mechanical image is necessarily *nonunitary* in order to preserve the correspondence principle. This illustrates the necessity of performing the transition from the conventional unitary transformations to the more general class of nonunitary transformations for any effective quantum mechanical description of dissipativity. This aspect is fully in line with the approach by (George et al, loc. cit.).

There are, however, other, rather crucial implications of the full technical treatment of dissipative forces. That which is most relevant for this paper is the property that, at the Newtonian level, the product of the time evolution law is necessarily *non-Lie*, under the condition of being referred to the *physical, total,* (i.e., kinetic plus potential) energy. (Santilli, 1978b, 1978c, 1978d, 1979a and

1979b). This can be trivially seen from the fact that the Lie product is totally antisymmetric. Suppose that the brackets of the time evolution under genuine dissipative forces (that is, nonselfadjoint forces),

$$\mathring{A}(X) = \frac{\partial A}{\partial X^{\mu}} \mathring{X}^{\mu} \overset{\text{def}}{=} A \,.\, H \qquad (V.4)$$

characterize an algebra (i.e., they verify conditions (IV.5)) and suppose that H(X) represents the physical, total energy of the system. Due to the antisymmetric nature of the Lie product, the Lie realization of law (V.4) would imply the property

$$\mathring{H}(X) = H.H \equiv 0 \quad , \quad H(X) = \text{constant} \qquad (V.5)$$

which is contrary to physical evidence, as well as contrary to the necessary condition for the system to be dissipative (Definition of Section II).

As a result, a quantum mechanical description of the statistical mechanics of dissipative systems based on the conventional Lie algebra product for the time evolution law, equation (V.1), is open to generalizations, particularly under the condition of compliance with the correspondence principle.

We are referring here to the expectation that, if the product of the time evolution law is non-Lie at the Newtonian level, it is expected to remain non-Lie at the quantum mechanical level, thus yielding a generalization of law (V.1). Nevertheless, Lie's formulations of this topic are not excluded here and, before introducing the non-Lie formulation, it may be useful to recall the Lie aspect of the problem (see also appendix).

2°) Lie formulation.

As was recalled in 1°), a necessary condition for mathematical and physical consistency in this case, i.e., Lie formulation, is that the function H *does not* represent the actual, nonconserved, physical, total energy. Instead, it is an "auxiliary function" (in the language of Santilli, 1979c) assisting in the treatment of the problem. This aspect too is in line with the approach by Prigogine and his collaborators (George et al, loc. cit.).

We will now show that, in fact, a second necessary condition is that the product of the time evolution law *is not* the conventional, trivial Lie-product $\hat{A}\hat{B}-\hat{B}\hat{A}$, but instead it is given by the more general isotope

$$[\hat{A},\hat{B}]^{*} = \hat{A}\,\hat{C}\,\hat{B} - \hat{B}\,\hat{C}\,\hat{A} \quad , \quad \hat{C} = \text{fixed} \quad . \tag{V.6}$$

This latter aspect can be directly seen via the use of the nonunitary transformations. Suppose that the system is indeed described at a given value of time by the trivial Lie product $\hat{A}\hat{H}-\hat{H}\hat{A}$, where $\hat{H}$ is the "auxiliary operator" conventionally called the Hamiltonian. As indicated earlier, a necessary condition for the time evolution of this system under genuine dissipative forces is that the time transformation is not unitary. A most significant class of nonunitary transformations is given by the so-called unitary-admissible transformations (Santilli, 1978d)

$$\hat{A} \rightarrow \hat{A}' = e^{it\hat{H}\hat{S}}\,\hat{A}\,e^{-it\hat{R}\hat{H}} \tag{V.7}$$

$$\hat{H} = \hat{H}^{\dagger} \ , \quad \hat{R} \neq \hat{R}^{\dagger} \ , \quad \hat{S} \neq \hat{S}^{\dagger} \ , \quad [\hat{H}\hat{S},\hat{R}\hat{H}] \neq 0 \quad . \tag{V.8}$$

To appreciate the physical meaning of transformations (V.7), note that they yield immediately

$$i\dot{\hat{A}} = i \lim_{t\to 0} \frac{\hat{A}'-\hat{A}}{t} = (\hat{A}\hat{R}\hat{H} - \hat{H}\hat{S}\hat{A}) = (\hat{A},\hat{H})$$

where $(\hat{A},\hat{H})$ is Lie-admissible. Since Lie-admissibility is associated with nonselfadjoint forces, it appears clearly that (V.7) represents evolution under the influence of such forces. These transformations (V.7) are said unitary-admissible in the sense that they are nonunitary, yet they trivially recover the conventional unitary transformations at the values $\hat{R}=\hat{S}=\hat{1}$. Also, transformations (V.7) are a quantum mechanical image of the Newtonian transformations (V.2).

Consider now the unitary-admissible transformations of the Liouville-von Neumann equation. It is easily seen that, under these transformations, this equation is transformed into a *Lie isotope* according to the rule

$$i \frac{\partial \hat{\rho}}{\partial t} - [\hat{H},\hat{\rho}] = 0 \rightarrow i \frac{\partial \hat{\rho}'}{\partial t} - [\hat{H}',\hat{\rho}']^* = 0 \tag{V.9a}$$

$$\hat{\rho}' = \hat{\theta}\,\hat{\rho}\,\hat{\theta}' \ , \quad \hat{H}' = \hat{\theta}\,\hat{H}\,\hat{\theta}' \ , \quad \hat{\theta} = e^{it\hat{H}\hat{S}} \ , \quad \hat{\theta}' = e^{-it\hat{R}\hat{H}} \tag{V.9b}$$

$$[\hat{H}',\hat{\rho}']^* = \hat{H}'\,\hat{C}\hat{\rho}' - \hat{\rho}'\,\hat{C}\hat{H}' \ , \quad \hat{C} = e^{it\hat{R}\hat{H}}\, e^{-it\hat{H}\hat{S}} \quad . \tag{V.9c}$$

Indeed

$$\begin{aligned} e^{it\hat{H}\hat{S}}\, [\hat{H},\hat{\rho}]\, e^{-it\hat{R}\hat{H}} &= e^{it\hat{H}\hat{S}}\, \hat{H}\, e^{-it\hat{R}\hat{H}}\, e^{it\hat{R}\hat{H}}\, e^{-it\hat{H}\hat{S}}\, e^{it\hat{H}\hat{S}}\, \hat{\rho}\, e^{-it\hat{R}\hat{H}} \\ &- e^{it\hat{H}\hat{S}}\, \hat{\rho}\, e^{-it\hat{R}\hat{H}}\, e^{it\hat{R}\hat{H}}\, e^{-it\hat{H}\hat{S}}\, e^{it\hat{H}\hat{S}}\, \hat{H}\, e^{-it\hat{R}\hat{H}} \\ &= \hat{H}'\, e^{it\hat{R}\hat{H}}\, e^{-it\hat{H}\hat{S}}\, \hat{\rho}' - \hat{\rho}'\, e^{it\hat{R}\hat{H}}\, e^{-it\hat{H}\hat{S}}\, \hat{H}' = [\hat{H}',\hat{\rho}']^* \end{aligned} \tag{V.10}$$

Thus, not only $\hat{H}$ *does not* represent the total physical energy, but the product of the time evolution law *is not* the trivial Lie product.

This yields the Lie algebra preserving generalization of Heisenberg's (and of the Liouville - von Neumann) equations proposed by Santilli (Santilli, 1978d, p.752, and 1979c), which is such that the Lie isotopic structure is preserved :

$$i\, \dot{\hat{X}}^{\mu} - [\hat{B},\hat{X}^{\mu}]^* = 0 \quad , \quad i \frac{\partial \hat{\rho}}{\partial t} - [\hat{B},\hat{\rho}]^{**} = 0 \tag{V.11a}$$

$$[\hat{X}^{\mu},\hat{X}^{\nu}]^* = \hat{X}^{\mu}\,\hat{C}\,\hat{X}^{\nu} - \hat{X}^{\nu}\,\hat{C}\,\hat{X}^{\mu} = \hat{\Omega}^{\mu\nu}(t,\hat{X}) \tag{V.11b}$$

$$(\Omega^{\mu\nu}) = (\hat{\Omega}^{\mu\nu})_{\hbar=0} = \left(\left\| \frac{\partial R_{\nu}}{\partial X^{\mu}} - \frac{\partial R_{\mu}}{\partial X^{\nu}} \right\|^{-1} \right)^{\mu\nu} \quad . \tag{V.11c}$$

Indeed, these equations now preserve their structure under arbitrary unitary-admissible transformations (remember that Heisenberg's equations (and the Liouville - von Neumann) equations preserve their structure only under unitary transformations).

Note also that the notation $\hat{B}$ is introduced here, instead of $\hat{H}$, to recall that the "auxiliary operator", or "Birkhoffian" $\hat{B}$, does not represent the total physical energy.

To be specific in this rather crucial point, it should be again stressed here that, when the time evolution is expressed in terms of the conventional, quantum mechanical, Lie product $\hat{A}\hat{H} - \hat{H}\hat{A}$, and $\hat{H}$ is the total, physical energy $\hat{T} + \hat{V}$, all forces are entirely derivable from a potential. On the contrary, when the Lie product is generalized to the form $\hat{A}\,\hat{C}\hat{H}$ - $\hat{H}\,\hat{C}\,\hat{A}$, genuine nonselfadjoint forces occur under the correspondence limit, but, as indicated earlier, the operator $\hat{H}$ (conventionally called the Hamiltonian) cannot be the total, physical, nonconserved energy. If not taken into account, this latter point may be misleading, particularly with respect to the rather crucial problem of the physical interpretation of the algorithms at hand.

In conclusion, it appears that the inspection from an algebraic viewpoint of the quantum mechanical, statistical approach to dissipative forces by Prigogine and his collaborators (Mayne et al, loc. cit., and quoted papers) reveals the existence of a reinterpretation in terms of an isotope of the Lie algebra, along the lines of the Lie algebra preserving generalization of Heisenberg's (and Liouville's von Neumann) equations proposed by Santilli (Santilli, loc. cit.). This point is not purely formal. Indeed, it allows the computation of the classical limit of the equations and the verification of the existence of genuine dissipative forces nonderivable from a potential. For the method how to compute this classical limit for equations (V.11), see (Santilli, 1978a, particularly Chart 4.9).

3°) Lie-admissible formulation.

The difficulties associated with the physical interpretation of $\hat{H}$ in the Lie formulation are easily remedied by the Lie-admissible algebras. Suppose that the non-Lie algebra of the time evolution (V.4) is Lie-admissible. This algebra, as by now familiar, admits a product which is neither totally antisymmetric nor totally symmetric. As such, it is indeed capable of representing the actual evolution in time of the energy according to the rule (IV.16)

$$\dot{H} = (H,H) = \frac{\partial H}{\partial X^{\mu}} S^{\mu\nu}(t,X) \frac{\partial H}{\partial X^{\nu}} = \frac{\partial H}{\partial p_i} F_{i,NSA} \neq 0 \qquad \text{(V.12)}$$

by therefore bypassing inconsistency (V.5). Indeed, (V.12) is nothing but the usual classical rule giving the time variation of the total energy $H = T(\vec{p}) + V(\vec{r})$ of a system under the influence of nonselfadjoint forces : $dH = d\vec{r}.\vec{F}_{NSA}$ and thus $\dot{H} = \dot{\vec{r}}.\vec{F}_{NSA}$.

Once the algebra is non-Lie at the Newtonian level, we expect that it is non-Lie also at the quantum mechanical level, in order to preserve a direct physical significance of all the algorithms at hand, including, and most importantly, the preservation of the physical meaning of the operator $\hat{H}$ as the total, nonconserved, physical energy.

This yields the Lie-admissible generalization of Heisenberg's equations proposed by Santilli (Santilli, 1978d and 1979b ; see also the contributed paper to these proceedings, Santilli 1979c)

$$i\, \dot{\hat{X}}^{\mu} - (\hat{H},\hat{X}^{\mu}) = 0 \quad , \qquad \text{(V.13a)}$$

$$(\hat{X}^{\mu},\hat{X}^{\nu}) = \hat{X}^{\mu}\, \hat{R}\, \hat{X}^{\nu} - \hat{X}^{\nu}\, \hat{S}\, \hat{X}^{\mu} = \hat{S}^{\mu\nu}(t,\hat{X}) \qquad \text{(V.13b)}$$

$$(S^{\mu\nu} - S^{\nu\mu}) = (\hat{S}^{\mu\nu} - \hat{S}^{\nu\mu})_{\hbar=0} = \left(\left\| \frac{\partial R_{\nu}}{\partial X^{\mu}} - \frac{\partial R_{\mu}}{\partial X^{\nu}} \right\|^{-1} \right)^{\mu\nu} \qquad \text{(V.13c)}$$

which preserves the Lie-admissible character under arbitrary unitary-admissible transformations, and which verifies a generalized version of the correspondence principle, yielding equations of type (IV.15).

The point we intended for this paper is that, in the transition from the quantum mechanical equations (V.13) to the statistical profile, the Lie-admissible product $(\hat{H},\hat{X})$, in view of section IV.3, *is not* expected to be preserved. Instead, we expect the emergence of the Lie-admissible, quantum mechanical isotopy

$$i \frac{\partial \hat{\rho}}{\partial t} - (\hat{H},\hat{\rho})^* = 0 \quad , \tag{V.14a}$$

$$(\hat{H},\hat{\rho})^* = \hat{H}\,\hat{R}^*\hat{\rho} - \hat{\rho}\,\hat{S}^*\hat{H} \quad , \tag{V.14b}$$

$$\hat{R}^* = \hat{R} + \hat{R}' \quad , \quad \hat{S}^* = \hat{S} + \hat{S}' \quad \text{or} \quad \hat{R}^* = \hat{R}\,\hat{R}' \quad , \quad \hat{S}^* = \hat{S}\,\hat{S}' \quad .$$

This isotopy is necessary in order to comply with the correspondence principle in the following sense. At the classical, Lie-admissible, statistical level (Section IV), we have identified the necessary emergence of an isotopy of the one particle Newtonian product in order to truly perform the transition to the statistical profile. If the same Lie-admissible product apply for both the quantum mechanical, generalized, Heisenberg's level (V.13) and the corresponding statistical level, such a description would necessarily violate the correspondence principle. Indeed, its classical limit would not represent a genuine statistical framework, because it would not represent the crucial divergence term $\rho\, \partial F_{i,NSA}/\partial p_i$ originating from Liouville's theorem in its original formulation.

It is appropriate here to indicate that a considerable advance in the study of equations (V.13) and (V.14) has been achieved at this workshop. For instance, these Lie-admissible equations can be treated via conventional Hilbert spaces, although interpreted as two-sided, left and right modules, *and not* in their one-sided interpretation of conventional quantum mechanics (Santilli, 1979c). Nevertheless, it should be equally indicated here that a considerable way remains yet to be covered in order to reach the necessary technical maturity for the treatment, understanding, and applications of Lie-admissible equations (V.13) and (V.14).

VI. CONCLUDING REMARKS.

As indicated in the introduction, most of contemporary theoretical physics is still dominated by the forces derivable from a potential, by their representation in terms of the conventional analytic equations in the "truncated" forms (I.3) and (I.4), and by the underlying Lie algebra structure. It may therefore be of some value to present a few remarks aiming at the identification of the physical relevance of our results, as well as at the indication of further, possible, developments.

As is well known, a most significant part of statistical mechanics is plasma physics. This discipline has lately seen truly remarkable progresses, mainly motivated by energy-related issues. Yet, it appears that the physical relevance for this field of physics of nonconservative forces in general, and that of dissipative forces in particular, is not sufficiently stressed in the literature, nor adequately treated as yet on technical grounds.

A certain number of experimental facts, interpreted by means of the definition of dissipativity of Section II, suggest the following remark : *dissipation of energy often implies a contraction effect in the emitting matter*. The most banal of these facts is to be found in quantum physics. A transition from a given bound state to a more bound state of the same system via the emission of quanta of energy often corresponds to a reduction of the mean spatial extension of the system.

Along similar lines, we have already indicated in Section I the focusing effect of electron Bremstrahlung (see, for instance, Kolomensky & Lebedev, 1962). This effect results in a volume reduction in dynamical space. Likewise, focusing of a heavy beam may be obtained by "friction" on an auxiliary electron beam (see, for instance, Budker et al, 1974). Finally, astrophysicists have recently shown, using a numerical model, that inelastic collisions between celestial objects imply a clustering of these objects (see Brahic, 1977). There certainly exist examples of this type in other parts of physics.

In conclusion, it appears that dissipation, if properly identified on physical grounds and adequately treated on mathematical grounds, can provide a relevant, if not crucial role, in stability problems in plasma physics and, more specifically, in the clustering of plasmas. In turn, this aspect is linked to the fundamental role of dissipative forces in the evolution of the physical world at the one particle Newtonian level,at the quantum mechanical level and at the statistical/thermodynamical level.

This idea is, by no means, new. H. Poincaré (Poincaré, 1911), commenting on the cosmological theory by R. du Ligondes, wrote :

> "Evolution is produced by these collisions ; if there were neither collision nor passive resistance (i.e., friction), or even if bodies were perfectly elastic, these projectiles could move about indefinitely, without showing any tendency to cluster, in spite of the attractive forces between them".

Despite the loss of almost three-quarter of a century in the study of this rather fundamental physical aspect, it appears that physicists have finally initiated its comprehensive study. However, apart from specialized contributions on the topic, the phenomenon "dissipation-contraction", that we associate with the time evolution of the element of volume in the dynamical space, according to (III.5), does not appear to be clearly identified and treated in the existing literature at large. We feel that it is useful to draw attention to this point. We also feel that the noninitiated reader should not be surprised by the rather deep methodological implications of the full treatment of the phenomenon considered, such as the abandonment of the familiar Lie algebras in favor of the covering Lie-admissible algebras.

A final remark may be useful to indicate another reason of our interest in the Lie-admissible approach to statistical mechanics. In this paper we have reached an algebraic characterization of statistical mechanics under a rather general class of forces, the variationally nonselfadjoint forces. Nevertheless, *these forces do not exhaust the forces of nature*. A still more general class of forces is given by the *nonlocal forces*, that is, the forces composed by :

- a local-differential, selfadjoint part ;
- a local-differential, nonselfadjoint part ; and
- an integral, nonselfadjoint part ;

according to the scheme

$$\vec{F}_{tot}(t,\vec{r},\dot{\vec{r}}) = \vec{f}_{SA}(t,\vec{r},\dot{\vec{r}}) + \vec{F}_{NSA}(t,\vec{r},\dot{\vec{r}}) + \iiint \vec{U}(t,\vec{r},\vec{r}\,',\dot{\vec{r}},\dot{\vec{r}}\,',\ldots)\, dV'.$$

It goes without saying that the applicability of Lie algebras for the time evolution under these nonlocal forces is in doubt.

Even though numerous physical systems can be effectively described by the local terms only, there exist systems in nature which demand the use of nonlocal forces for a more adequate treatment. Also, local, nonselfadjoint, forces are often an approximation of true nonlocal forces under the reduction to a point-like treatment of the "particles" still capable of accounting for their extended character. This is typically the case of the dissipative motion of extended bodies in a resistive medium (e.g., a satellite in Earth's atmosphere).

The remark intended for this paper is that *the Newtonian realization of the Lie-admissible algebras appears to be fully capable of incorporating nonlocal forces*. Indeed, in all equations (II.10), (III.5), (IV.15) and (IV.30), the external forces have been left undefined in their actual structure (whether local or nonlocal) precisely in view of this potentiality. It is at this point that the Newtonian notion of Lie-admissibility acquires its full light. Recall that non-Lie brackets (A,H) are Lie-admissible when the attached brackets $[A,H]^- = (A,H) - (H,A)$ are Lie. Suppose now that the nonselfadjoint forces responsible for the transition of the time evolution law, from the Lie brackets [A,H] to the Lie-admissible brackets (A,H), are purely nonlocal. We then reach the remarkable property that the "Lie contents" of the brackets (A,H), given by the antisymmetric part $\frac{1}{2}[A,H]^{-}$, is representative of the local component of the system, while its departure from the Lie algebra character, given by the symmetric part $\frac{1}{2}((A,H)+(H,A))$, is representative of the nonlocal component of the same system.

It is hoped that these remarks illustrate the usefulness of abandoning conventional Lie algebra formulations of (classical and quantum) mechanics in favor of the covering Lie-admissible formulations, as well as they illustrate the truly remarkable capability of representation of the forces of nature which are offered by the Lie-admissible algebras.

APPENDIX

It may be of some value to illustrate in more detail the fact that, *for the case of local forces*, the Lie-admissible structure according to the theorem of section IV.3 is *not the unique* possible algebraic structure for nonconservative statistical mechanics.(For the case of nonlocal forces, the technical difficulties for the use of any algebra other than the Lie-admissible algebras are so great to render meaningless at this time the search of any alternative to the Lie-admissible algebras. Thus, we limit the present analysis to the case of local forces).

The topic under consideration has been treated in detail in the forthcoming monograph (Santilli, 1980a) and we restrict ourselves here to only a brief, nontechnical, summary.

The problem under consideration is whether (local) equations of motion with nonselfadjoint forces in their first-order form

$$\dot{X}^{\mu} - \tilde{\Xi}^{\mu}(t,X) = 0 \quad , \quad \mu = 1,2,3,4,5,6 \tag{A.1a}$$

$$(X^{\mu}) = \begin{pmatrix} \vec{r} \\ \vec{p} \end{pmatrix} , \quad (\tilde{\Xi}^{\mu}) = \begin{pmatrix} \vec{p}/m \\ \vec{f}_{SA}(t,\vec{r},\vec{p}) + \vec{F}_{NSA}(t,\vec{r},\vec{p}) \end{pmatrix} \tag{A.1b}$$

admit a representation with analytic equations *other* than the Lie-admissible ones of equations (IV.15). The answer to this question is affirmative. Among the various analytic equations which might be considered, most relevant are the so-called Birkhoff's equations which, for the case of autonomous systems, are characterized by the rules

$$\Omega_{\mu\nu}(X) \; \tilde{\Xi}^{\nu}(X) = \frac{\partial B(X)}{\partial X^{\mu}} \tag{A.2a}$$

$$\Omega_{\mu\nu}(X) = \frac{\partial R_{\nu}(X)}{\partial X^{\mu}} - \frac{\partial R_{\mu}(X)}{\partial X^{\nu}} \tag{A.2b}$$

$$\det (\Omega_{\mu\nu}) \neq 0$$

yielding the analytic equations (Birkhoff's equations)

$$\dot{X}^{\mu} - \Omega^{\mu\nu}(X)\,\frac{\partial B(X)}{\partial X^{\nu}} = 0 \qquad (A.3)$$

$$(\Omega^{\mu\nu}(X)) = (\|\Omega_{\mu\nu}\|^{-1})^{\mu\nu}$$

and the time evolution law

$$\dot{A}(X) = \frac{\partial A}{\partial X^{\mu}}\,\Omega^{\mu\nu}(X)\,\frac{\partial B}{\partial X^{\nu}} \overset{\text{def}}{=} [A,B]^{*} \quad . \qquad (A.4)$$

The important part of this alternative is that the brackets $[A,B]^{*}$ of equations (A.4) do indeed verify the Lie algebra laws (IV.4). As a matter of fact, they represent the most general possible, Newtonian, regular, realization of the Lie algebra product.

Another important aspect of this alternative is that such a Birkhoffian representation of the systems considered always exists (under certain smoothness and regularity conditions unessential here).

Upon transition to the statistical aspect via the use of the original Liouville's theorem, we then reach the following alternative to equations (IV.22) (for autonomous systems)

$$\frac{\partial \rho}{\partial t} + [\rho,B]^{*} + \rho\,\frac{\partial}{\partial p_i}\,F_{i,NSA} = 0 \quad . \qquad (A.5)$$

A number of remarks are essential here to put this methodological alternative in its proper perspective.

First of all it should be restressed that the "truncated" Hamilton's equations are *strictly inapplicable*, in general, for representations (A.2), under the condition that the local variables $\vec{r}$ are the coordinates of the *actual experimental setting* (if this condition is relaxed, a universality theorem of Hamiltonian formulations exists). This point is important to stress that the conventional Liouville's equation (IV.8) must necessarily be abandoned for the statistics of nonselfadjoint forces (under the condition of preservation of the reference frame used in actual experiments). The only alternative left under these conditions is what type of generalization should be used.

Secondly, it is unknown at this moment whether, despite the generalized structure of the Lie product as per equation (A.4), the Lie algebra can indeed describe the complete time evolution law (A.5), as it is the case of the Lie-admissible algebras via the notion of isotopy (section IV.3). The problem consists of the study whether the additional scalar term $\rho \frac{\partial}{\partial p_i} F_{i,NSA}$ of equation (A.5) always admits a Lie algebra representation of the type

$$[\rho,B]^* + \rho \frac{\partial}{\partial p_i} F_i = [\rho,B]^{**} = \frac{\partial \rho}{\partial X^\mu} \Omega'^{\mu\nu} \frac{\partial B}{\partial X^\nu} \qquad \text{(A.6a)}$$

$$(\Omega'^{\mu\nu}) = \left(\left\| \frac{\partial R'_\nu}{\partial X^\mu} - \frac{\partial R'_\mu}{\partial X^\nu} \right\|^{-1} \right)^{\mu\nu} \qquad \text{(A.6b)}$$

thus yielding the isotopy

$$[\rho,B]^* \rightarrow [\rho,B]^{**} \quad . \qquad \text{(A.7)}$$

It should be indicated here that equations (A.6b) constitute the necessary and sufficient condition for the brackets $[\rho,B]^{**}$ to be Lie.

Thirdly, even though the existence of the Birkhoffian representation (A.2) is ensured by the existence theorems of the Inverse Problem, its actual computation in practice is so complex, even for low dimensionality and simple nonselfadjoint forces, to discourage the most devoted Lie scalar, in the language of (Santilli, 1978c, p.1312). Assuming that such a Birkhoffian representation exists, one still remains with the problem of establishing the existence of the isotopy (A.6). Assuming that such an existence can be guaranteed, one then remains with the rather substantial problem of its explicit computation in the needed closed form.

The need for the explicit knowledge in the closed form of the generalized Lie tensors $\Omega^{\mu\nu}$ and $\Omega'^{\mu\nu}$ and of the Birkhoffian B should be stressed here. Indeed, without such knowledge, the treatment would be purely formal (e.g., for the problem of quantization).

These technical difficulties are due to the need of solving *partial differential equations* for the computation of these functions. This situation should be compared to the universality and simplicity of the corresponding results for the Lie-admissible algebras, equations (IV.14) and (IV.26). Indeed, these results are valid for *all* the Newtonian systems of the class considered.

Also, as indicated in Section V, the function B *cannot* represent a physical quantity and it is, instead, an auxiliary function. The total, physical, energy must be separately defined. This implies the fact that the *time evolution law cannot be defined in terms of the energy whenever the brackets are Lie.*

And last, but not least, *the entire methodological context of the Inverse Problem is inapplicable in its currently available form (Santilli, 1978a and 1980) for the case of nonlocal forces, while the applicability of the Lie-admissible approach persists.*

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A Stochastic Approach to Nonequilibrium Thermodynamics of Chemical Reaction System

K. Ishida
Department of Applied Chemistry, Ibaraki University, Hitachi, Japan

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Nonequilibrium thermodynamics is formulated by combining the nonlinear Fokker-Planck equation with the so-called Gibbs entropy postulate. The entropy production thus derived consists of two parts: one is of the same form as the usual entropy production and the other is the fluctuating part attendant on it. The evolution criterion can easily be verified in the stochastic framework. For illustration the system governed by the linear Fokker-Planck equation is in detail discussed.

1. Introduction

The thermodynamics of chemical reaction system far from equilibrium has extensively been developed by Prigogine and his co-workers [1]. The stochastic approach to chemical kinetics [1–4], however, has been studied almost independently of the nonequilibrium thermodynamics. Except the attempts by a few authors [5, 6], we have little knowledge of those to connect the stochastic property of chemical reaction with its nonequilibrium thermodynamics.

We denote by $P(\mathbf{X}, t)$ the probability distribution for finding the numbers of molecules of d chemically reacting constituents to be $\mathbf{X}=(X_1, X_2, \ldots, X_d)$ at time t. The behavior of chemical process, on the assumption that it is Markovian, is described by the master equation (ME) of birth-and-death type governing the time evolution of $P(\mathbf{X}, t)$. The chemical ME represents the mascroscopic rate equation in the space of stochastic variables, which assume the realized values $(X_1, X_2, \ldots, X_d)$ at time t. The clue to incorporate the stochastic behavior of chemical process into the framework of nonequilibrium thermodynamics is to find a thermodynamic quantity closely related to the probability distribution. Such a relation is given by the so-called Gibbs entropy postulate [7], which defines entropy in terms of the probability distributions over all possible reaction states. The stochastic process of chemical reaction has no notion of force. The Gibbs entropy postulate, however, makes it possible to introduce the force corresponding to the reaction rate (flow) derived from the chemical ME. To investigate this problem, in Sect. 2, we do not start with the chemical ME itself but with the nonlinear Fokker-Planck equation (FPE) obtained as an asymptotic representation of it in the limit of large system size [8].

On the basis of the Gibbs entropy postulate, we define the entropy difference, which is the entropy measured from its steady-state value. Its time derivative is evaluated in such a way that a generalized force can naturally be introduced in the course of transformation of the nonlinear FPE. It is then shown that the time derivative of the entropy difference consists of two parts. One is the linear part of entropy production. This is expressed in terms of the probability-flux differences and the definite generalized forces at steady state. The other is the nonlinear part of entropy production. This is due to the deviation of the generalized forces from their steady-state values. Its stochastic expression in the neighborhood of steady state is of the same form as that by which Schlögl [5] has made the information-theoretical approach to nonlinear thermodynamics of open system.

The nonlinear part of entropy production, which is of central interest in this paper, can also be split into two parts: the systematic part concerning the average motion and the fluctuating part attendant of it. This state of affairs, in Sect. 3, is illustrated by the system with Gaussian distribution. In the neighborhood of

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steady state, the systematic part is just the same as the so-called excess entropy production and the fluctuating part plays a subsidiary role in discussing the stability of the steady state.

In Sect. 4 the excess entropy production is dealt with from the stochastic standpoint. Then the irreversible circulation of fluctuations [9] appears of itself in the derivation of evolution criterion in terms of excess flows and excess forces.

2. Derivation of Entropy Production

We consider a system in which a sequence of chemical reactions occurs under the conditions as follows. The system as a whole is at mechanical equilibrium and its temperature and volume are maintained constant. The initial reactants A are converted into the final products M via the intermediates X. The system is so well stirred that all the chemical species can uniformly be distributed in space. The concentrations of A and M in the system, so as to remain unchanged in time, are controlled by each external reservoir with constant chemical potential. The intermediates X are open to both A and M subject to such a time-independent condition.

For the numbers of reacting molecules we use the same symbols as those of chemical species, and let us denote by $W(\mathbf{X}\to\mathbf{X}+\mathbf{r}_\rho)\equiv W(\mathbf{X},\mathbf{r}_\rho)$ the transition probability for the numbers of reacting molecules to pass from $\mathbf{X}$ to $\mathbf{X}+\mathbf{r}_\rho$ in a unit time due to a ρ-th reaction. The jump $\mathbf{r}_\rho$ is a set of integers $r_{i\rho}$, which may be positive, negative or zero. The birth-and-death ME describing the time evolution of the probability distribution $P(\mathbf{X},t)$ is then given by

$$\frac{\partial}{\partial t}P(\mathbf{X},t)=\sum_{\mathbf{r}_\rho}\{W(\mathbf{X}-\mathbf{r}_\rho,\mathbf{r}_\rho)\,P(\mathbf{X}-\mathbf{r}_\rho,t)$$
$$-W(\mathbf{X},\mathbf{r}_\rho)\,P(\mathbf{X},t)\}. \tag{2.1}$$

We now define intensive variables by $\mathbf{x}=\mathbf{X}/V$, where V is the size (volume) of the system under consideration. In the limit of large system size ($\mathbf{X}\to\infty$, $V\to\infty$, $\mathbf{X}/V=$finite), $\mathbf{x}$ becomes continuous. The realizations of the chemical birth-and-death process described by (2.1), therefore, tend to continuous path.

Horthemke and Brenig [8] have recently derived a nonlinear FPE by analyzing the behavior of fluctuations in the chemical birth-and-death process in the limit of large system size. The derivation is based on the theories of diffusion processes and Ito stochastic differential equation [10]. Such a procedure makes it possible to overcome the difficulty associated with the truncation of the Kramers-Moyal expansion. They have thus shown that the most general asymptotic representation of Eq. (2.1) in the limit of large system size is the nonlinear FPE.

$$\frac{\partial}{\partial t}p(\mathbf{x},t)=-\frac{\partial}{\partial \mathbf{x}}\cdot\{\mathbf{f}(\mathbf{x})\,p(\mathbf{x},t)\}$$
$$+\frac{1}{2V}\frac{\partial^2}{\partial\mathbf{x}\,\partial\mathbf{x}}:\{\mathbf{B}(\mathbf{x})\,p(\mathbf{x},t)\}. \tag{2.2}$$

In this equation $p(\mathbf{x},t)=V^d P(\mathbf{X},t)$, and the drift vector $\mathbf{f}(\mathbf{x})$ and the diffusion matrix $\mathbf{B}(\mathbf{x})$, which is symmetric and non-negative definite, respectively, are the values in the thermodynamic limit of the first- and second-moment of the jump $\mathbf{r}_\rho/V$ with respect to the transition probability expressed in terms of $\mathbf{X}/V$.

Horsthemke and Brenig have demonstrated by some simple model reactions that the nonlinear FPE approach is in good agreement with the birth-and-death ME formalism in contrast to the van Kampen approach [11]. We now try to formulate the nonequilibrium thermodynamics of the open reaction-system subject to the nonlinear FPE (2.2).

According to the Gibbs entropy postulate, we introduce the entropy change $S(t)-S_{eq}$ produced in the interior of a system by irreversible processes, which induce the deviation of nonequilibrium probability distribution $p(\mathbf{x},t)$ from its equilibrium one $p_{eq}(\mathbf{x})$. It is defined by

$$S(t)-S_{eq}=-\int d\mathbf{x}\,p(\mathbf{x},t)\ln\{p(\mathbf{x},t)/p_{eq}(\mathbf{x})\}, \tag{2.3}$$

where Boltzmann's constant is assumed equal to unity and $d\mathbf{x}=dx_1\,dx_2\ldots dx_d$. On the probability distribution we impose the natural boundary condition which means that $p(\mathbf{x},t)$ vanishes for $\mathbf{x}\to\pm\infty$. Since, however, the numbers of reacting molecules are nonnegative, we define $p(\mathbf{x},t)=0$ for $-\infty<\mathbf{x}<0$. The local equilibrium is implicitly assumed through (2.3), which involves the fact that the probability distribution preserves invariably its form in the time evolution of system. Such a probability distribution is said to be invariant with respect to reversible motion in the sense of stochastic dynamics. This reversibility invariance gives a justification of the macroscopic approximation by the local equilibrium for a certain class of systems called hydrodynamic system [5b]. Otherwise, it is impossible to define the force corresponding to the thermodynamic force in the ordinary nonequilibrium thermodynamics constructed on the assumption of local equilibrium.

Assuming the existence of a unique steady state, we have $\Delta S(t)=S(t)-S_0$, as the deviation of $S(t)$ from its steady-state value S_0:

$$\Delta S(t)=-K(p,p_0)-\int d\mathbf{x}\,\Delta p\ln(p_0/p_{eq}). \tag{2.4}$$

where

$$K(p, p_0) = \int d\mathbf{x}\, p(\mathbf{x}, t) \ln \{p(\mathbf{x}, t)/p_0(\mathbf{x})\} \geqq 0 \tag{2.5}$$

and

$$\Delta p = p(\mathbf{x}, t) - p_0(\mathbf{x}).$$

The $K(p, p_0)$ is called Kullback information [12] or information gain [13] of $p(\mathbf{x}, t)$ with respect to $p_0(\mathbf{x})$. Using $K(p, p_0)$, Schlögl has attempted to formulate the information-theoretical nonequilibrium thermodynamics of open systems [5].

Differentiating (2.4) with respect to t, we obtain

$$\frac{d}{dt}\Delta S(t) = -\frac{d}{dt}K(p, p_0) - \int d\mathbf{x}\, \frac{\partial \Delta p}{\partial t} \ln (p_0/p_{\mathrm{eq}}). \tag{2.6}$$

In order to investigate thermodynamically the time evolution of the reaction system governed by the nonlinear FPE (2.2), we start with the transformation of the first term on the r.h.s. of (2.6) into a thermodynamic expression. To this end we write (2.2) in the form

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial \mathbf{x}} \cdot (p\mathbf{F}) \tag{2.7}$$

or

$$-\frac{\partial}{\partial t}\ln p = \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{F} + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{x}} \ln p, \tag{2.8}$$

where

$$\mathbf{F} = \mathbf{f} - \frac{1}{2V}\left\{\frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{B} + \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{x}} \ln p_0 + \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{x}} \ln (p/p_0)\right\}. \tag{2.9}$$

We now define a generalized force $\mathbf{X}$ by

$$\mathbf{X} = -\frac{\partial}{\partial \mathbf{x}} \ln \{p(\mathbf{x}, t)/p_{\mathrm{eq}}(\mathbf{x})\}. \tag{2.10}$$

This $\mathbf{X}$ should not be confused with the symbol $\mathbf{X}$ for a set of numbers of reacting molecules in (2.1). If, for instance, the probability distribution for an open system in which chemical reactions are taking place is Poissonian, this force is in complete agreement with the chemical affinity expressed in terms of chemical potentials [14]. For the deviation of $\mathbf{X}$ from its steady-state value $\mathbf{X}_0$, we have

$$\Delta\mathbf{X} = -\frac{\partial}{\partial \mathbf{x}} \ln \{p(\mathbf{x}, t)/p_0(\mathbf{x})\}. \tag{2.11}$$

By subtracting (2.8) at the steady state from (2.8) itself, we can derive, taking (2.11) into consideration,

$$-\frac{\partial}{\partial t}\ln (p/p_0) = -\mathbf{F} \cdot \Delta\mathbf{X} + \frac{1}{2V}\left\{\frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{B} \cdot \Delta\mathbf{X}) + \Delta\mathbf{X} \cdot \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{x}} \ln p_0\right\}. \tag{2.12}$$

Multiplying both sides of (2.7) by $\ln (p/p_0)$ and those of (2.12) by p and adding the two, we obtain

$$-\frac{\partial}{\partial t}\{p \ln (p/p_0)\} = \frac{\partial}{\partial \mathbf{x}} \cdot [p\{\mathbf{F} \ln (p/p_0) - \mathbf{B} \cdot \Delta\mathbf{X}\}] + \frac{1}{2V} p\, \Delta\mathbf{X} \cdot \mathbf{B} \cdot \Delta\mathbf{X}. \tag{2.13}$$

On integrating this and taking account of

$$\int d\mathbf{x}\, \frac{\partial}{\partial \mathbf{x}} \cdot [p\{\mathbf{F} \ln (p/p_0) - \mathbf{B} \cdot \Delta\mathbf{X}\}] = 0,$$

we find

$$-\frac{d}{dt}K(p, p_0) = \frac{1}{2V}\int d\mathbf{x}\, p\, \Delta\mathbf{X} \cdot \mathbf{B} \cdot \Delta\mathbf{X} \geqq 0. \tag{2.14}$$

The inequality [6] is due to the fact that the diffusion matrix $\mathbf{B}$ is positive definite.

To deal with chemical reactions, however, it is to be desired that one derives an alternative expression in terms of $\mathbf{F}$ and $\Delta\mathbf{X}$. This is motivated by the fact as follows. The $\mathbf{F}$ given by (2.9) contains explicitly the force difference $\Delta\mathbf{X}$ and the drift vector $\mathbf{f}$, which is related to the deterministic rate equation $d\bar{\mathbf{x}}/dt = \mathbf{f}(\bar{\mathbf{x}})$ for the most probable path $\bar{\mathbf{x}}(t)$. When we multiply both sides of (2.12) by p and perform integration by parts, we find, taking account of $\int d\mathbf{x}\, p\partial \ln (p/p_0)/\partial t = (d/dt)\int d\mathbf{x}\, p = 0$,

$$\int d\mathbf{x}\, p\mathbf{F} \cdot \Delta\mathbf{X} = \frac{1}{2V}\int d\mathbf{x}\, p\, \Delta\mathbf{X} \cdot \mathbf{B} \cdot \Delta\mathbf{X}. \tag{2.15}$$

We therefore have as the alternative to (2.14)

$$-\frac{d}{dt}K(p, p_0) = \int d\mathbf{x}\, p\, \mathbf{F} \cdot \Delta\mathbf{X} \geqq 0, \tag{2.16}$$

where, in reference to the probabilistic continuity equation (2.7),

$$p\mathbf{F} = p\mathbf{f} - \frac{1}{2V}\frac{\partial}{\partial \mathbf{x}} \cdot (p\mathbf{F}) \tag{2.17}$$

is called the probability flux in the space of stochastic variables. If (2.17) is substituted into the r.h.s. of (2.16), the following equation is finally obtained,

$$-\frac{d}{dt}K(p, p_0) = \langle \mathbf{f} \cdot \Delta\mathbf{X} \rangle + \frac{1}{2V}\left\langle \mathbf{B} : \frac{\partial}{\partial \mathbf{x}} \Delta\mathbf{X} \right\rangle, \tag{2.18}$$

where

$$\langle \cdot \rangle = \int d\mathbf{x}\, p(\mathbf{x}, t)(\cdot)$$

and

$$\mathbf{B} : \frac{\partial}{\partial \mathbf{x}} \Delta\mathbf{X} = \sum_{i=1}^{d} \sum_{j=1}^{d} B_{ij}\, \partial(\Delta X_i)/\partial x_j.$$

In this stage, comparing both terms on the r.h.s. of (2.6) to each other, we observe what thermodynamic character each term has. Substituting (2.7) and its steady-state equation into the second term and performing integration by parts, we obtain the expression in terms of the probability-flux differences $\Delta(p\mathbf{F}) = p\mathbf{F} - (p\mathbf{F})_0$ and the generalized forces $\mathbf{X}_0$ at the steady state,

$$-\int d\mathbf{x}\,\frac{\partial \Delta p}{\partial t}\ln(p_0/p_{\mathrm{eq}}) = \int d\mathbf{x}\,\Delta(p\mathbf{F})\cdot\mathbf{X}_0. \tag{2.19}$$

Let us now limit ourselves to the immediate neighborhood of the steady state. We then find that the l.h.s of (2.19), that is, the linear part of the entropy production in the Schlögl's information-theoretical approach [5a] can be assigned to the first-order quantity δP of the entropy production variation $\Delta P = \delta P + (1/2)\delta^2 P + \ldots$ around the steady state, where P is the entropy production introduced in nonequilibrium thermodynamics [1b]. In contrast to this, equation (2.16) or (2.18), the l.h.s. of which is the nonlinear part of the Schlögl's expression for entropy production, is assigned to the second-order quantity $(1/2)\delta^2 P$, that is, to the excess entropy production in terms of excess flows and excess forces in respect to the steady state.

The nonequilibrium-thermodynamic study of stability of steady state is based on the excess entropy production. What we are really interested in, therefore, is the nonlinear part of the Schlögl's expression for entropy production. In the present framework it is the entropy production arising from the force differences $\Delta\mathbf{X}$. From now on, denoting it by $\Delta_{\mathbf{X}}\mathscr{P}$, we use in place of (2.18)

$$\Delta_{\mathbf{X}}\mathscr{P} = \langle \mathbf{f}\cdot\Delta\mathbf{X}\rangle + \frac{1}{2V}\left\langle \mathbf{B} : \frac{\partial}{\partial\mathbf{x}}\Delta\mathbf{X}\right\rangle \geqq 0. \tag{2.20}$$

The first term on the r.h.s. is attributed to the systematic part of reaction processes and the second one to the fluctuating part.

We see from (2.5) and (2.16) that except at the steady state the sign of $-dK(p, p_0)/dt = \Delta_{\mathbf{X}}\mathscr{P}$ is always opposite to that of $-K(p, p_0)$. According to the Liapunov's theorems [15], then, the steady-state probability distribution $p_0(\mathbf{x})$ is asymptotically stable and $-K(p, p_0)$ is a Liapunov function for the nonlinear FPE (2.2). As far as we are concerned in the nonequilibrium thermodynamics on the basis of the Gibbs entropy postulate, we are compelled to restrict ourselves to such systems that it is possible to assume an asymptotically stable probability distribution.

In what follows we shall derive the evolution criterion in the present framework. To consider the temporal change of $\Delta_{\mathbf{X}}\mathscr{P}$, we return to the original expression $\Delta_{\mathbf{X}}\mathscr{P} = -\int d\mathbf{x}(\partial p/\partial t)\ln(p/p_0)$. We then obtain

$$\frac{d(\Delta_{\mathbf{X}}\mathscr{P})}{dt} = -\int d\mathbf{x}\,\frac{\partial p}{\partial t}\frac{\partial}{\partial t}\ln(p/p_0)$$
$$-\int d\mathbf{x}\,\frac{\partial^2 p}{\partial t^2}\ln(p/p_0). \tag{2.21}$$

The first integral on the r.h.s. of this equation is always negative definite except at the steady state, because of

$$-\int d\mathbf{x}\,\frac{\partial p}{\partial t}\frac{\partial}{\partial t}\ln(p/p_0) = -\int d\mathbf{x}\,p\left\{\frac{\partial}{\partial t}\ln(p/p_0)\right\}^2 < 0.$$

If, however, we use (2.7) in the first integral and perform integration by parts, we obtain

$$-\int d\mathbf{x}\,\frac{\partial p}{\partial t}\frac{\partial}{\partial t}\ln(p/p_0) = \int d\mathbf{x}\,p\mathbf{F}\cdot\Delta\dot{\mathbf{X}} < 0, \tag{2.22}$$

where $\Delta\dot{\mathbf{X}} = \partial\Delta\mathbf{X}/\partial t$. The r.h.s. of this equation represents the temporal change of $\Delta_{\mathbf{X}}\mathscr{P}$ in such a way that the probability flux $p\mathbf{F}$ is held constant and only the force differences $\Delta\mathbf{X}$ are varied. Let us indicate this by $d_{\mathbf{X}}(\Delta_{\mathbf{X}}\mathscr{P})/dt$. We thus obtain, using (2.17),

$$\frac{d_{\mathbf{X}}(\Delta_{\mathbf{X}}\mathscr{P})}{dt} = \langle \mathbf{f}\cdot\Delta\dot{\mathbf{X}}\rangle + \frac{1}{2V}\left\langle \mathbf{B} : \frac{\partial}{\partial\mathbf{x}}\Delta\dot{\mathbf{X}}\right\rangle < 0. \tag{2.23}$$

This equation, though involving the fluctuating part, is of the form similar to the evolution criterion introduced by Glansdorff and Prigogine [1]. It may here be remarked incidentally that the second integral on the r.h.s. of (2.21) represents the temporal change of $\Delta_{\mathbf{X}}\mathscr{P}$ due to the change of the probability flux $p\mathbf{F}$;

$$-\int d\mathbf{x}\,\frac{\partial^2 p}{\partial t^2}\ln(p/p_0) = \frac{d_{p\mathbf{F}}(\Delta_{\mathbf{X}}\mathscr{P})}{dt}$$
$$= \int d\mathbf{x}\,\frac{\partial}{\partial t}(p\mathbf{F})\cdot\Delta\mathbf{X}.$$

We bring this section to a close with the consideration on the behavior of (2.20) in the neighborhood of the average $\langle\mathbf{x}\rangle$. The obtained results will be made available in the next section. We start with the derivation of the kinetic equations for the average $\langle\mathbf{x}\rangle$ and the variance $\boldsymbol{\sigma} = \langle\mathbf{x}\mathbf{x}\rangle - \langle\mathbf{x}\rangle\langle\mathbf{x}\rangle$, where is a dyadic product, i.e., a matrix with elements $x_i x_j$. It follows directly from (2.2) that

$$\frac{d}{dt}\langle\mathbf{x}\rangle = \langle\mathbf{f}(\mathbf{x})\rangle \tag{2.24}$$

and

$$\frac{d}{dt}\boldsymbol{\sigma} = \langle(\mathbf{x} - \langle\mathbf{x}\rangle)\mathbf{f}(\mathbf{x})\rangle$$
$$+ \langle(\mathbf{x} - \langle\mathbf{x}\rangle)\mathbf{f}(\mathbf{x})\rangle^{t} + \frac{1}{V}\langle\mathbf{B}(\mathbf{x})\rangle, \tag{2.25}$$

where T indicates transpose matrix. Expanding $f_i(\mathbf{x})$ around the average $\langle\mathbf{x}\rangle$, we obtain the power series in terms of $\Delta\mathbf{x}=\mathbf{x}-\langle\mathbf{x}\rangle$,

$$f_i(\mathbf{x})-f_i(\langle\mathbf{x}\rangle)+\sum_{j=1}^{d}\left(\frac{\partial f_i}{\partial x_j}\right)_{\langle\mathbf{x}\rangle}\Delta x_j$$
$$+\tfrac{1}{2}\sum_{j=1}^{d}\sum_{k=1}^{d}\left(\frac{\partial^2 f_i}{\partial x_j\partial x_k}\right)_{\langle\mathbf{x}\rangle}\Delta x_j\Delta x_k+O(\Delta x_j\Delta x_k\Delta x_l). \tag{2.26}$$

We have also for $B_{ij}(\mathbf{x})$ the similar expansion in power series. Using these expansion equations in (2.24) and (2.25), we find

$$\frac{d}{dt}\langle x_i\rangle=f_i(\langle\mathbf{x}\rangle)$$
$$+\tfrac{1}{2}\sum_{j=1}^{d}\sum_{k=1}^{d}\left(\frac{\partial^2 f_i}{\partial x_j\partial x_k}\right)_{\langle\mathbf{x}\rangle}\sigma_{ij}+O(\langle\Delta x_j\Delta x_k\Delta x_l\rangle) \tag{2.27}$$

and

$$\frac{d}{dt}\sigma_{ij}=\sum_{k=1}^{d}\left\{\left(\frac{\partial f_i}{\partial x_k}\right)_{\langle\mathbf{x}\rangle}\sigma_{jk}+\left(\frac{\partial f_j}{\partial x_k}\right)_{\langle\mathbf{x}\rangle}\sigma_{ik}\right\}$$
$$+\frac{1}{V}\left\{B_{ij}(\langle\mathbf{x}\rangle)+\tfrac{1}{2}\sum_{k=1}^{d}\sum_{l=1}^{d}\left(\frac{\partial^2 B_{ij}}{\partial x_k\partial x_l}\right)_{\langle\mathbf{x}\rangle}\sigma_{kl}\right\}$$
$$+O(\langle\Delta x_j\Delta x_k\Delta x_l\rangle). \tag{2.28}$$

Exactly similar procedure applied to (2.20) gives us

$$\Delta_{\mathbf{X}}\mathscr{P}=\sum_{i=1}^{d}\bar{J}_i\Delta\bar{X}_i+\sum_{i=1}^{d}\sum_{j=1}^{d}(\tfrac{1}{2}\dot{\sigma}_{ij}-\alpha_{ij})\left(\frac{\partial\Delta X_i}{\partial x_j}\right)_{\langle\mathbf{x}\rangle}$$
$$+\sum_{i=1}^{d}\sum_{j=1}^{d}\left[f_i(\langle\mathbf{x}\rangle)\tfrac{1}{2}\sum_{k=1}^{d}\left(\frac{\partial}{\partial x_k}\left(\frac{\partial\Delta X_i}{\partial x_j}\right)\right)_{\langle\mathbf{x}\rangle}\sigma_{jk}\right.$$
$$+\frac{1}{2V}\sum_{k=1}^{d}\sum_{l=1}^{d}\left\{\left(\frac{\partial B_{ij}}{\partial x_k}\right)_{\langle\mathbf{x}\rangle}\left(\frac{\partial}{\partial x_l}\left(\frac{\partial\Delta X_i}{\partial x_j}\right)\right)_{\langle\mathbf{x}\rangle}\right.$$
$$\left.\left.+\tfrac{1}{2}B_{ij}(\langle\mathbf{x}\rangle)\left(\frac{\partial^2}{\partial x_k\partial x_l}\left(\frac{\partial\Delta X_i}{\partial x_i}\right)\right)_{\langle\mathbf{x}\rangle}\right\}\sigma_{kl}\right]$$
$$+O(\langle\Delta x_j\Delta x_k\Delta x_l\rangle). \tag{2.29}$$

In this equation, $\Delta\bar{X}_i=\Delta X_i(\langle\mathbf{x}\rangle)$, $\bar{J}_i=d\langle x_i\rangle/dt$ and $\dot{\sigma}_{ij}=d\sigma_{ij}/dt$ have been substituted respectively for (2.27) and (2.28), in which the higher order terms $O(\langle\Delta x_j\Delta x_k\Delta x_l\rangle)$ are truncated, and the irreversible circulation of fluctuations [9] defined by

$$\alpha_{ij}=\tfrac{1}{2}\sum_{k=1}^{d}\left\{\left(\frac{\partial f_i}{\partial x_k}\right)_{\langle\mathbf{x}\rangle}\sigma_{jk}-\left(\frac{\partial f_j}{\partial x_k}\right)_{\langle\mathbf{x}\rangle}\sigma_{ik}\right\} \tag{2.30}$$

has been introduced.

3. The System Subject to Linear FPE

For an understanding of (2.29) we consider the system that $\mathbf{x}$ is so distributed around its average $\langle\mathbf{x}\rangle$ that $\mathbf{x}-\langle\mathbf{x}\rangle$ is of the order of magnitude of $V^{-1/2}$. It is then possible to write (2.27) and (2.28) in the closed forms independent of each other as follows:

$$\frac{d}{dt}\langle\mathbf{x}\rangle=\mathbf{f}(\langle\mathbf{x}\rangle), \tag{3.1}$$

which is the rate equation for the most probable path, and

$$\frac{d}{dt}\sigma=\gamma\cdot\sigma+(\gamma\cdot\sigma)^T+\frac{1}{V}\bar{\mathbf{B}}, \tag{3.2}$$

where γ is the matrix with elements $\gamma_{ij}=(\partial f_i/\partial x_j)_{\langle\mathbf{x}\rangle}$ and $\bar{\mathbf{B}}=\mathbf{B}(\langle\mathbf{x}\rangle)$. As will later be shown in a concrete form, such truncatins of higher order terms are legitimate, if the system just considered assumes an asymptotically stable steady state. The equation (3.2) is derived from the linear FPE,

$$\frac{\partial}{\partial t}p(\mathbf{x},t)=-\frac{\partial}{\partial\mathbf{x}}\cdot\{\gamma\cdot(\mathbf{x}-\langle\mathbf{x}\rangle)p(\mathbf{x},t)\}\cdot$$
$$+\frac{1}{2V}\frac{\partial^2}{\partial\mathbf{x}\partial\mathbf{x}}:\{\bar{\mathbf{B}}p(\mathbf{x},t)\}. \tag{3.3}$$

We can also obtain this linear FPE, together with (3.1), by means of the system size expansion [11, 16] of the birth-and-death ME (2.1).

To the same degree of approximation as (3.1) and (3.2), the equation (2.29) reduces to

$$\Delta_{\mathbf{X}}\mathscr{P}=\bar{\mathbf{J}}\cdot\Delta\bar{\mathbf{X}}+\tfrac{1}{2}\dot{\sigma}:\left(\frac{\partial}{\partial\mathbf{x}}\Delta\mathbf{X}\right)_{\langle\mathbf{x}\rangle}. \tag{3.4}$$

We have here used the fact that the term $\alpha:(\partial\Delta\mathbf{X}/\partial\mathbf{x})_{\langle\mathbf{x}\rangle}$ vanishes because of $\alpha_{ij}=-\alpha_{ji}$ and $\partial\Delta X_i/\partial x_j=\partial\Delta X_j/\partial x_i$. The irreversible circulation of fluctuations, α, is given by

$$\alpha=\tfrac{1}{2}\{(\gamma\cdot\sigma)^T-\gamma\cdot\sigma\}. \tag{3.5}$$

Let us now consider the behavior of this equation in the immediate neighborhood of the steady state. The flow $\bar{\mathbf{J}}$ vanishes at the steady state, that is, $\bar{\mathbf{J}}_0=\mathbf{f}(\langle\mathbf{x}\rangle_0)=0$. We therefore have the excess flow

$$\delta\bar{\mathbf{J}}=\gamma_0\cdot\delta\langle\mathbf{x}\rangle, \tag{3.6}$$

where $\gamma_0=\gamma(\langle\mathbf{x}\rangle_0)$ and $\delta\langle\mathbf{x}\rangle=\langle\mathbf{x}\rangle-\langle\mathbf{x}\rangle_0$. Corresponding to $\delta\bar{\mathbf{J}}$, the force difference $\Delta\bar{\mathbf{X}}$ is replaced by $\delta\bar{\mathbf{X}}$. We thus obtain the excess entropy production $\delta_{\mathbf{X}}\mathscr{P}$,

$$\delta_{\mathbf{X}}\mathscr{P}=\delta\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}+\tfrac{1}{2}\dot{\sigma}:\left(\frac{\partial}{\partial\mathbf{x}}\delta\mathbf{X}\right)_{\langle\mathbf{x}\rangle}. \tag{3.7}$$

where

$$\dot{\sigma}=\gamma_0\cdot\sigma+(\gamma_0\cdot\sigma)^T+\frac{1}{V}\mathbf{B}_0. \tag{3.8}$$

On the r.h.s. of (3.7), the first term is the excess entropy production concerning the most probable motion and the second term is that due to the fluctuations of excess flows and excess forces.

The solution of the linear FPE (3.3) is given by the Gaussian distribution,

$$p(\mathbf{x},t)=(2\pi/V)^{-d/2}(\det\sigma)^{-1/2} \times \exp\left\{-\frac{V}{2}\sigma^{-1}:(\mathbf{x}-\langle\mathbf{x}\rangle)(\mathbf{x}-\langle\mathbf{x}\rangle)\right\}. \tag{3.9}$$

Since the approximation $\int_0^{\infty}\simeq\int_{-\infty}^{\infty}$ holds for the Gaussian distribution, the natural boundary condition defined in the preceding section is consistently used. According to (2.11), the excess force $\delta\mathbf{X}$ derived from (3.9) takes the form

$$\delta\mathbf{X}=V\{\sigma^{-1}\cdot(\mathbf{x}-\langle\mathbf{x}\rangle)-\sigma_0^{-1}\cdot(\mathbf{x}-\langle\mathbf{x}\rangle_0)\}. \tag{3.10}$$

We therefore have

$$\left(\frac{\partial}{\partial\mathbf{x}}\delta\mathbf{X}\right)_{\langle\mathbf{x}\rangle}=V(\sigma^{-1}-\sigma_0^{-1}). \tag{3.11}$$

Substituting this into (3.7), we obtain

$$\delta_{\mathbf{X}}\mathscr{P}=\delta\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}+V\tfrac{1}{2}\dot{\sigma}:(\sigma^{-1}-\sigma_0^{-1})\geqq 0. \tag{3.12}$$

The positiveness of $\delta_{\mathbf{X}}\mathscr{P}$, which originates in that of (2.20), can be ensured by the following two factors. (i) When $\delta\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}>0$, the steady state is asymptotically stable. This is based on the thermodynamic criterion for the stability of steady state [1]. (ii) The inequality

$$\frac{V}{2}\dot{\sigma}:(\sigma^{-1}-\sigma_0^{-1})>0 \tag{3.13}$$

always holds for the case under consideration, as it can easily be verified below. All the variances tend toward their steady-state values, that is, if $\dot{\sigma}<0$, $\sigma>\sigma_0$, or if $\dot{\sigma}>0$, $\sigma<\sigma_0$. The example will be given in Appendix.

Let us apply exactly the same procedure as the derivation of the inequality (2.14) to the linear FPE (3.3) in the immediate neighborhood of the steady state. We then obtain, to the same degree of approximation as (3.8),

$$-\frac{d}{dt}K(p,p_0)=\frac{1}{2V}\int d\mathbf{x}\,p\,\delta\mathbf{X}\cdot\bar{\mathbf{B}}_0\cdot\delta\mathbf{X}>0 \tag{3.14}$$

except at the steady state. If, on the other hand, the linear FPE (3.3) and both Gaussian distribution (3.9) and its stationary one are substituted into the integrand of $-\int d\mathbf{x}(\partial p/\partial t)\ln(p/p_0)$, which is equal to the l.h.s. of (3.14), then after straightforward calculation we can find, using (3.8),

$$-\frac{d}{dt}K(p,p_0)=V\tfrac{1}{2}\dot{\sigma}:(\sigma^{-1}-\sigma_0^{-1})>0. \tag{3.15}$$

When the steady state is unstable, the fluctuations $\mathbf{x}-\langle\mathbf{x}\rangle$ are anomalously enhanced up to order unity near the instability point and the probability distribution becomes non-Gaussian, even if it were initially Gaussian. That is to say, the form of the probability distribution is not invariant in the temporal evolution of system. It is then impossible to define the force difference such as (3.10) (or (2.11)), so that (3.12) remains no longer valid. From the stochastic point of view, therefore, it is concluded that the stability condition (3.14) or (2.14) holds only for the systems assuming the probability distribution invariant in time.

4. Excess Entropy Production. $\delta\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}$

The so-called excess entropy production has in detail been studied by Glansdorff and Prigogine [1] in relation to the evolution criterion in terms of excess flows and excess forces. In this section, however, we consider it in the present framework.

We denote by $\delta_{\mathbf{X}}\mathscr{P}'$ the excess entropy production $\delta\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}$ for the most probable path;

$$\delta_{\mathbf{X}}\mathscr{P}'=\delta\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}. \tag{4.1}$$

The excess flow $\delta\bar{\mathbf{J}}$ has already been given by (3.6). The excess force $\delta\bar{\mathbf{X}}$ is, according to (3.10),

$$\delta\bar{\mathbf{X}}=-V\sigma_0^{-1}\cdot\delta\langle\mathbf{x}\rangle. \tag{4.2}$$

It follows at once from (3.5) and (3.8) at steady state that

$$\gamma_0=-\left(\frac{1}{2V}\bar{\mathbf{B}}_0+\boldsymbol{\alpha}_0\right)\cdot\sigma_0^{-1}. \tag{4.3}$$

Substituting this into (3.6) and taking (4.2) into account, we obtain the linear relation between $\delta\bar{\mathbf{J}}$ and $\delta\bar{\mathbf{X}}$,

$$\delta\bar{\mathbf{J}}=\mathbf{L}_0\cdot\delta\bar{\mathbf{X}}, \tag{4.4}$$

where we have introduced the phenomenological coefficient defined by

$$\mathbf{L}_0=V^{-1}\left(\frac{1}{2V}\bar{\mathbf{B}}_0+\boldsymbol{\alpha}_0\right)>0. \tag{4.5}$$

The positiveness of $\mathbf{L}_0$ is due to the fact that $\bar{\mathbf{B}}_0$ and $\boldsymbol{\alpha}_0$ are always positive definite. In addition $\bar{\mathbf{B}}_0$ is symmetric, so that $\boldsymbol{\alpha}_0$ is the antisymmetric part of $\mathbf{L}_0$:

$$\boldsymbol{\alpha}_0=V\tfrac{1}{2}(\mathbf{L}_0-\mathbf{L}_0^t) \tag{4.6}$$

Using (4.4) in (4.1), we obtain

$$\delta_{\mathbf{X}}\mathscr{P}' = \delta\bar{\mathbf{X}}\cdot\mathbf{L}_0\cdot\delta\bar{\mathbf{X}} > 0. \tag{4.7}$$

This is the stability condition for small disturbances of the most probable path near the steady state.
We now consider the time change of $\delta_{\mathbf{X}}\mathscr{P}'$. It can be written in the form

$$\frac{d(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = \frac{d_{\mathbf{X}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} + \frac{d_{\mathbf{J}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt}, \tag{4.8}$$

where

$$\frac{d_{\mathbf{X}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = \delta\bar{\mathbf{J}}\cdot\dot{\delta}\bar{\mathbf{X}} \tag{4.9}$$

and

$$\frac{d_{\mathbf{J}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = \dot{\delta}\bar{\mathbf{J}}\cdot\delta\bar{\mathbf{X}}. \tag{4.10}$$

The differentiation of (4.2) with respect to time leads to

$$\dot{\delta}\bar{\mathbf{X}} = -V\sigma_0^{-1}\cdot\delta\bar{\mathbf{J}},$$

where $\delta\bar{\mathbf{J}} = (d/dt)\,\delta\langle\mathbf{x}\rangle$. Using this in (4.9), we obtain

$$\frac{d_{\mathbf{X}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = -V\delta\bar{\mathbf{J}}\cdot\sigma_0^{-1}\cdot\delta\bar{\mathbf{J}} < 0.$$

If, however, we substitute (4.4) and its time derivative into (4.9) and (4.10), respectively, and take (4.5) into consideration, we obtain

$$\frac{d_{\mathbf{X}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = V^{-1}\delta\bar{\mathbf{X}}\cdot\left(\frac{1}{2V}\bar{\mathbf{B}}_0 - \boldsymbol{\varkappa}_0\right)\cdot\dot{\delta}\bar{\mathbf{X}}$$

and

$$\frac{d_{\mathbf{J}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = V^{-1}\delta\bar{\mathbf{X}}\cdot\left(\frac{1}{2V}\bar{\mathbf{B}}_0 + \boldsymbol{\varkappa}_0\right)\cdot\dot{\delta}\bar{\mathbf{X}}.$$

From these two equations we can deduce

$$\frac{d_{\mathbf{X}}(\delta_{\mathbf{X}}\mathscr{P}')}{dt} = \frac{1}{2}\frac{d(\delta_{\mathbf{X}}\mathscr{P}')}{dt} - V^{-1}\delta\bar{\mathbf{X}}\cdot\boldsymbol{\varkappa}_0\cdot\dot{\delta}\bar{\mathbf{X}} < 0. \tag{4.11}$$

This is the evolution criterion in terms of the excess flows and the excess forces. For two-variable reaction systems, the second term on the r.h.s. of (4.11) is written in the form

$$\delta\bar{\mathbf{X}}\cdot\boldsymbol{\varkappa}_0\cdot\dot{\delta}\bar{\mathbf{X}} = \varkappa_0(\delta\bar{X}_1\,\dot{\delta}\bar{X}_2 - \dot{\delta}\bar{X}_1\,\delta\bar{X}_2),$$

where

$$\boldsymbol{\varkappa}_0 = \varkappa_0\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

This indicates that the irreversible circulation of fluctuations is closely related to the areal velocity $(1/2)(\delta\bar{X}_1\,\dot{\delta}\bar{X}_2 - \dot{\delta}\bar{X}_1\,\delta\bar{X}_2)$ around the steady state on the force plane $(\bar{X}_1, \bar{X}_2)$.

5. Final Remark

The formal derivation of the entropy production (2.20) from the nonlinear FPE (2.2), to be sure, is possible without recourse to the local equilibrium assumption [6], but it is really on this assumption to make the quantity $-\partial\ln(p/p_0)/\partial\mathbf{x}$ physically meaningful.
The formula (3.12) of the excess entropy production associated with the linear FPE (3.3) is adaptable to such systems that the steady state chosen as a reference state is stable. Whereas, then, the variances assume the finite values of the order of magnitude of V^{-1}, they tend to diverge near an unstable steady state, so that the formula (3.12) breaks down. As a device to overcome the difficulty of divergence of the variances, there is the scaling theory of transient phenomena proposed by Suzuki [17] for the macrovaribles near the instability point. In the present framework, however, we have no knowledge of how to define the force near the instability point.

Appendix

The reaction scheme of Prigogine-Lefever-Nicolis model [18] is as follows:

$$A \to X$$
$$B + X \to Y + D$$
$$2X + Y \to 3X$$
$$X \to E.$$

The concentrations of A, B, D and E are controlled from the outside and are maintained constant in time. If all the rate constants are assumed equal to unity, the birth-and-death ME is given by

$$\begin{aligned}\frac{\partial}{\partial t}P(X,Y,t) &= AP(X-1,Y,t) - AP(X,Y,t)\\ &+ V^{-1}B(X+1)P(X+1,Y-1,t) - V^{-1}BXP(X,Y,t)\\ &+ V^{-2}(X-1)(X-2)(Y+1)P(X-1,Y+1,t)\\ &- V^{-2}X(X-1)YP(X,Y,t)\\ &+ (X+1)P(X+1,Y,t) - XP(X,Y,t).\end{aligned} \tag{A.1}$$

Denoting the intensive macrovariables by $a = A/V$, $b = B/V$, $x = X/V$ and $y = Y/V$, we obtain for the drift vector $\mathbf{f}(\mathbf{x})$ and the diffusion matrix $\mathbb{B}(\mathbf{x})$

$$\mathbf{f}(\mathbf{x})=\begin{bmatrix} a-bx+x\left(x-\frac{1}{V}\right)y-x \\ bx-x\cdot\left(x-\frac{1}{V}\right)y \end{bmatrix}$$

$$\simeq\begin{bmatrix} a-bx+x^2y-x \\ bx-x^2y \end{bmatrix} \tag{A.2}$$

and

$$\mathbb{B}(\mathbf{x})=\begin{bmatrix} a+bx+x^2y+x & -bx-x^2y \\ -bx-x^2y & bx+x^2y \end{bmatrix}. \tag{A.3}$$

In the neighborhood of the steady state ($\langle x\rangle_0=a$, $\langle y\rangle_0=a/b$), the kinetic equations of $\delta\langle\mathbf{x}\rangle=\langle\mathbf{x}\rangle-\langle\mathbf{x}\rangle_0$ and σ are given by (3.6) and (3.8), respectively, in which

$$\gamma_0=\begin{bmatrix} b-1 & a^2 \\ -b & -a^2 \end{bmatrix} \tag{A.4}$$

and

$$\bar{\mathbb{B}}_0=\begin{bmatrix} 2a(b+1) & -2ab \\ -2ab & 2ab \end{bmatrix}. \tag{A.5}$$

It follows from the normal mode analysis that if $b_c(=a^2+1)>b$, the steady state is asymptotically stable. In the case of $2a>b_c-b>0$, setting $\omega=\{a^2-(b_c-b)^2/4\}^{1/2}$, we find that the solutions of (3.6) and (3.8) are written in the forms

$$\delta\langle\mathbf{x}\rangle=\exp\{-\tfrac{1}{2}(b_c-b)t\}\left\{(\cos\omega t)\,\mathbf{E}+\frac{\sin\omega t}{\omega}\left(\gamma_0+\frac{b_c-b}{2}\mathbf{E}\right)\right\}\cdot(\delta\langle\mathbf{x}\rangle)_i \tag{A.6}$$

and

$$\begin{aligned}\sigma=\sigma_0&+\exp\{-(b_c-b)t\}\\ &\times\left\{\left(\cos\omega t+\frac{b_c-b}{2\omega}\sin\omega t\right)\mathbf{E}+\frac{\sin\omega t}{\omega}\gamma_0\right\}\cdot(\sigma_i-\sigma_0)\\ &\times\left\{\left(\cos\omega t+\frac{b_c-b}{2\omega}\sin\omega t\right)\mathbf{E}+\frac{\sin\omega t}{\omega}\gamma_0^T\right\}.\end{aligned} \tag{A.7}$$

Here the subscript i indicates the initial state, $\mathbf{E}$ is unit matrix, and the variance σ_0 at the steady state is given by

$$\sigma_0=\begin{bmatrix} a(b_c+b)/V(b_c-b) & -2ab/V(b_c-b) \\ -2ab/V(b_c-b) & b(b_c+b)/Va(b_c-b) \end{bmatrix}. \tag{A.8}$$

Equation (A.7) satisfies the inequality (3.13), because of either $\dot{\sigma}<0$ for $\sigma_i>\sigma>\sigma_0$ or $\dot{\sigma}>0$ for $\sigma_i<\sigma<\sigma_0$.

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Kenzi Ishida
Department of Applied Chemistry
Ibaraki University
Nakanarusawa-machi 4-12-1
Hitachi-shi, Ibaraki
Japan 316

IRREVERSIBILITY AND ENVIRONMENTAL FORCES

SALMON Jean
Conservatoire National des Arts et Métiers
292, rue Saint-Martin, 75141 PARIS CEDEX 03

Abstract

Irreversibility in fluids is traditionally introduced by means of Boltzmann's postulate of molecular chaos.

We suggest another way, based on a non-Hamiltonian microdynamics characterized by environmental forces dependent on the velocities.

I – Introduction

The fundamental system of equations of classical statistical mechanics is reversible because it is based on Hamiltonian equations. It brings about the temporal invariance of the entropy of an isolated system which is contrary to the second principle of thermodynamics away from equilibrium.

It was Boltzmann who broke this irreversibility on establishing a kinetic equation ensuring the increase in entropy away from equilibrium and allowing the determination of the transport coefficients [1,2].

We suggest another way, based on the introduction of a non-Hamiltonian micro-dynamics bringing in two opposing environmental forces, one of damping and one of diffusion. A kinetic equation of the Fokker-Planck-Frey-Salmon type is thus obtained and leads to a correct result with respect to the entropy and to a determination of the viscosity coefficient of a dilute gas in good agreement with experiment.

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II' – The B.B.G.K.Y. System and Boltzmann's Equation

Let us consider a dilute gas made up of molecules of mass m. t designates the time and $\vec{x}_1, \vec{x}_2, \vec{w}_1, \vec{w}_2$ the position and velocity vectors of the number 1 and 2 particles. $\vec{X}_1$ and $\vec{X}_2$ are the external forces deriving from a potential φ_0, $\vec{X}_{12}$ and $\vec{X}_{21}$ are the interaction forces deriving from a potential φ.

The single and double distribution functions are shown by the symbols F_1 and F_{12}. The low value of the particle density allows us to neglect the triple collisions, and, in these conditions, the system of the first two BBGKY equations is written:

$$\frac{\partial F_1}{\partial t} + \vec{w}_1 \cdot \frac{\partial F_1}{\partial \vec{x}_1} + \frac{\vec{X}_1}{m} \cdot \frac{\partial F_1}{\partial \vec{w}_1} + \int \frac{\vec{X}_{12}}{m} \cdot \frac{\partial F_{12}}{\partial \vec{w}_1} \, \underline{dx}_2 \, \underline{dw}_2 = 0 \tag{1}$$

$$\frac{\partial F_{12}}{\partial t} + \vec{w}_1 \cdot \frac{\partial F_{12}}{\partial \vec{x}_1} + \vec{w}_2 \cdot \frac{\partial F_{12}}{\partial \vec{x}_2} + \frac{(\vec{X}_1 + \vec{X}_2)}{m} \cdot \frac{\partial F_{12}}{\partial \vec{w}_1} + \frac{(\vec{X}_2 + \vec{X}_{21})}{m} \cdot \frac{\partial F_{12}}{\partial \vec{w}_2} = 0 \tag{2}$$

This reversible system is incompatible with the second principle of thermodynamics. To obtain the transport coefficients, the collisions are considered as local and instantaneous whereas the external forces are considered as weak compared to the interaction forces, whence, on setting:

$$\vec{x}_{12} = \vec{x}_2 - \vec{x}_1 \tag{3}$$

we have the following equation in which the integral is only stretched to the interaction domain of the number 1 and 2 particles:

$$\frac{\partial F_1}{\partial t} + \vec{w}_1 \cdot \frac{\partial F_1}{\partial \vec{x}_1} = \int (\vec{w}_2 - \vec{w}_1) \cdot \frac{\partial F_{12}}{\partial \vec{x}_{12}} \, \underline{dx}_{12} \, \underline{dw}_2 \tag{4}$$

Let us designate by O the centre of the interaction sphere and by $Oxyz$ a system of axes such that the vector $g_{12} = \vec{w}_2 - \vec{w}_1$ is parallel to, and in the same direction as, Oz. Let us consider a straight line parallel to Oz and lying at a distance b from O. This line cuts the interaction sphere at the points A_E and A_S as well as the plane xOy at the point A of the polar co-ordinates b and ε (Fig. 1):

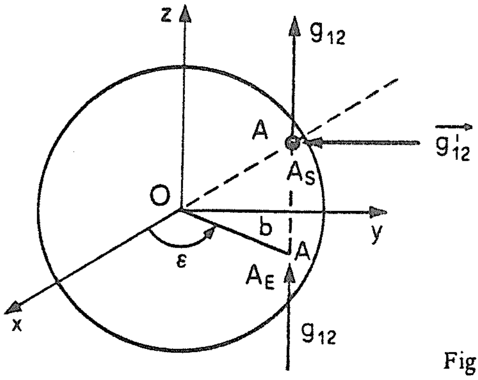

Fig. 1

The point A_E corresponds to the beginning of a collision and the point A_S to the end of a collision, whence:

$$\int\!\!\int\!\!\int (\vec{w}_2 - \vec{w}_1)\cdot \frac{\partial F_{12}}{\partial \vec{x}_{12}}\, \underline{dx}_{12} = \int\!\!\int g_{12}\left[F_{12}(Z_S) - F_{12}(Z_E)\right] b\, db\, d\varepsilon \tag{5}$$

The changing of t in $-t$ and consequently, $\vec{w}_1$ into $\vec{w}_2$ will change the sign of the two sides of the equation (4) if Oz does not change direction. On the other hand, if Oz is made to take the same direction as $\vec{g}_{12}$, only the sign of the left-hand side of (4) will be modified and irreversibility is introduced.

The equation (4) contains both F_1 and F_{12}. The postulate of molecular chaos ensures closure on imposing the loss of information of the particules, thus:

$$Z = Z_E \qquad F_{12} = F_1(\vec{w}_1)\, F_2(\vec{w}_2) \tag{6}$$

$$Z = Z_S \qquad F_{12} = F_1(\vec{w}'_1)\, F_2(\vec{w}'_2) \tag{7}$$

$\vec{w}'_1$ and $\vec{w}'_2$ corresponding to the velocities at the beginning of a collision which lead to the velocities $\vec{w}_1$ and $\vec{w}_2$ at the end of a collision according to the reversible laws of motion of the two bodies. On using (6) and (7), the equation obtained is that of Boltzmann:

$$\frac{\partial F_1}{\partial t} + \vec{w}_1\cdot\frac{\partial F_1}{\partial \vec{x}_1} = \int\!\!\int\!\!\int\!\!\int\!\!\int g_{12}\left[F_2(\vec{w}'_2)F_1(\vec{w}'_1) - F_2(\vec{w}_2)F_1(\vec{w}_1)\right] b\, db\, d\varepsilon\, \underline{dw}_2 \tag{8}$$

The importance of this equation is considerable. On the one hand, the entropy of an isolated system cannot decrease:

$$(9) \qquad S_1 = -K_0 \int \left[\log F_1\right] F_1 \, \underline{dw}_1 \, \underline{dx}_1 \ ; \qquad \frac{\partial S_1}{\partial t} \geqslant 0 \quad (\, K_0 \text{ Boltzmann's constant})$$

on the other hand, the theoretical determination of the kinetic viscosity coefficient μ is obtained on solving the equation (8).

Let us designate by $-K_0 T_i$ the minimum value of the interparticle potential and by σ the distance which makes the latter vanish. The deviation χ, corresponding to an impact parameter b and to a relative velocity $g = g_{12}$ is:

$$(10) \qquad \chi = \pi - 2b \int_{r_d}^{\infty} \left[1 - \frac{b^2}{r^2} - \frac{4\varphi}{mg^2}\right]^{-\frac{1}{2}} \frac{dr}{r^2}$$

(r_d being the root of the quantity in brackets).

From (10) we calculate the integrals:

$$(11) \qquad Q_\ell(g) = \frac{2}{\left[1 - \frac{1}{2}\left(\frac{1+(-1)^\ell}{1+\ell}\right)\right]} \int_0^{\infty} \left(1 - \cos^\ell \chi\right) \frac{b\,db}{\sigma^2}$$

$$(12) \qquad \Omega^{\ell,s} = \frac{2}{s+1\,!} \left(\frac{T_i}{T}\right)^{s+2} \int_0^{\infty} \left(\frac{m}{4K_0T_i}\right)^{s+2} Q_\ell(g)\, g^{2s+3}\, e^{-\frac{mg^2}{4K_0T}}\, dg\,.$$

The expression for the viscosity coefficient is then[2]:

$$(13) \qquad \mu = \frac{5}{16} \frac{\left(\pi m K_0 T\right)^{1/2}}{\pi \sigma^2 \Omega^{2,2}} \left[1 + \frac{3}{196}\left(8\, \frac{\Omega^{2,3}}{\Omega^{2,2}} - 7\right)^2\right]$$

An effective potential is that suggested by H.J.M. Hanley and M. Klein[3,4]

$$(14) \qquad \varphi = -K_0T_i \left[\frac{6+2\gamma}{m_0-6}\left(\frac{d\sigma}{r}\right)^{m_0} - \frac{\left[m_0 - \gamma(m_0-8)\right]}{m_0-6}\left(\frac{d\sigma}{r}\right)^6 - \gamma\left(\frac{d\sigma}{r}\right)^8\right]$$

The agreement with experimental results for Argon is excellent[5]:

$$m = 6{,}633\ 10^{-26}\,\text{kg} \ ; \quad T_i = 152{,}8\,\text{K} \ ; \quad \sigma = 3{,}297\ 10^{-10}\,\text{m} \ ; \quad \gamma = 3$$

$$K_0 = 1{,}3804\ 10^{-23} \ ; \quad \mu \text{ in } 10^{-6} \text{ poise} \ ; \quad m_0 = 11\,.$$

Table I

T K	μ_{exp}	μ_{th}	$\Delta\mu / \mu$
298,16	227,5	226,3	0,5 %
463,16	232,4	323,1	0,1 %
783,16	471,5	468,4	0,6 %
973,16	546,3	547,7	0,2 %

III – A NON-HAMILTONIAN MICRO-DYNAMICS

Since 1975, we have suggested a hypothesis introducing the irreversibility at the level of the molecular interaction[6,7]. Instead of first of all respecting the postulates of Hamiltonian mechanics and then breaking the past-future symmetry as we have shown in the preceding paragraph, we have chosen to add non-Hamiltonian terms to the fundamental equation of dynamics. The first which seems to impose itself is a damping term $\vec{X}_{12F}$ of the form:

$$\vec{X}_{12F} = -\beta\left[(\vec{w}_1-\vec{v}_1)-(\vec{w}_2-\vec{v}_2)\right] \tag{15}$$

$$n_1 = \int F_1\, \underline{dw}_1 \qquad n_2 = \int F_2\, \underline{dw}_2 \tag{16}$$

$$n_1\vec{v}_1 = \int F_1\, \vec{w}_1\, \underline{dw}_1 \qquad n_2\vec{v}_2 = \int F_2\, \vec{w}_2\, \underline{dw}_2 \tag{17}$$

This damping term must be compensated by a diffusion term in velocity space $\vec{X}_{12d}$ ensuring the continuation of the motion and the velocity at the thermodynamic equilibrium, which leads to the expression:

$$\vec{X}_{12d} = \beta\left[\frac{K_0T}{m}\left(\frac{\partial}{\partial \vec{w}_2} - \frac{\partial}{\partial \vec{w}_1}\right)\log F_{12}\right] \tag{18}$$

The ensemble $\vec{X}_{12F} + \vec{X}_{12d}$ represents an environmental force. The term must vanish for an interparticle Coulomb potential for particles of the same charge in the absence of a neutralizing bottom. Thus β should be proportional to the Laplacien $\Delta\varphi$ of φ. Lastly, the results obtained by means of the hypothesis of linear relaxation show that β must be the product of $\Delta\varphi$ by the average half-duration of the crossing time of the particle of velocity g and of reduced mass $m/2$ through the repulsive part of the interparticle potential of quantum origin.

We thus arrive at an equation of dynamics of the form:

$$m\frac{d\vec{w}_1}{dt} = \vec{X}_{1T} = -\frac{\partial\varphi}{\partial\vec{x}_1} - \tau\Delta\varphi\left[(\vec{w}_1-\vec{v}_1)-(\vec{w}_2-\vec{v}_2)+\frac{K_0T}{m}\left(\frac{\partial}{\partial\vec{w}_1}-\frac{\partial}{\partial\vec{w}_2}\right)\log F_{12}\right] \tag{19}$$

The true Liouville equation is written:

$$\frac{\partial F_{12}}{dt}+\vec{w}_1\cdot\frac{\partial F_{12}}{d\vec{x}_1}+\vec{w}_2\cdot\frac{\partial F_{12}}{d\vec{x}_2}+\frac{\partial}{\partial\vec{w}_1}\cdot\frac{(\vec{X}_{1T}F_{12})}{m}+\frac{\partial}{\partial\vec{w}_2}\cdot\frac{(\vec{X}_{2T}F_{12})}{m}=0 \tag{20}$$

whence, on fully writing out the irreversibility kinetic equation governing F_{12} :

$$\begin{aligned}
&\frac{\partial F_{12}}{\partial t}+\vec{w}_1\cdot\frac{\partial F_{12}}{\partial\vec{x}_1}+\vec{w}_2\cdot\frac{\partial F_{12}}{\partial\vec{x}_2}-\frac{1}{m}\frac{\partial\varphi}{\partial\vec{x}_1}\cdot\frac{\partial F_{12}}{\partial\vec{w}_1}-\frac{1}{m}\frac{\partial\varphi}{\partial\vec{x}_2}\cdot\frac{\partial F_{12}}{\partial\vec{w}_2}=\\
&\frac{\tau\Delta\varphi}{m}\left[\frac{\partial}{\partial\vec{w}_1}\cdot\left[(\vec{w}_1-\vec{v}_1)F_{12}-(\vec{w}_2-\vec{v}_2)F_{12}+\frac{K_0T}{m}\left(\frac{\partial F_{12}}{\partial\vec{w}_1}-\frac{\partial F_{12}}{\partial\vec{w}_2}\right)\right]\right]+\\
&+\frac{\tau\Delta\varphi}{m}\left[\frac{\partial}{\partial\vec{w}_2}\cdot\left[(\vec{w}_2-\vec{v}_2)F_{12}-(\vec{w}_1-\vec{v}_1)F_{12}+\frac{K_0T}{m}\left(\frac{\partial F_{12}}{\partial\vec{w}_2}-\frac{\partial F_{12}}{\partial\vec{w}_1}\right)\right]\right]
\end{aligned} \tag{21}$$

If two particles are in presence, the distribution functions are the Dirac type, thus Maxwellian at zero temperature. The irreversible term disappears and the traditional motion of the two bodies is re-established. Let us return to the case of a population of particles and in right-hand side of the equation (21) let us use the approximation:

$$F_{12} = F_1 F_2 e^{-\frac{\varphi}{K_0T}} \tag{22}$$

For a dilute gas, the position of the functions F_1 and F_2 varies little within the interaction sphere. Let us multiply (21) by $\underline{dx_2}$, $\underline{dw_2}$ and integrate. We then have the Frey-Salmon kinetic equation[8,9] :

$$\frac{\partial F_1}{\partial t} + \vec{w}_1 \cdot \frac{\partial F_1}{\partial \vec{x}_1} + \frac{\vec{X}_1}{m} \cdot \frac{\partial F_1}{\partial \vec{w}_1} = \frac{n K_0 T Z B}{2m} \frac{\partial}{\partial \vec{w}_1} \cdot \left[(\vec{w}_1 - \vec{v}_1) F_1 + \frac{K_0 T}{m} \frac{\partial F_1}{\partial \vec{w}_1} \right] \quad (23)$$

$$B = \frac{8\pi}{3 K_0^2 T^2} \int_0^\infty \left(\frac{d\varphi}{dr} \right)^2 e^{-\frac{\varphi}{K_0 T}} r^2 dr = \frac{8}{3 K_0 T} \int \Delta \varphi e^{-\frac{\varphi}{K_0 T}} r^2 dr \quad (24)$$

The non-decrease is entropy S_1 is ensured. Indeed, on designating the Maxwellian distribution by F_1^M, it follows that:

$$S_1 = -K_0 \int F_1 \log F_1 \underline{dx}_1 \underline{dw}_1 \quad F_1 = F_1^M h \quad \frac{\partial S_1}{\partial t} = \frac{n K_0^3 T^2}{2 m^2} \tau B \int \left(\frac{\partial h_1}{\partial \vec{w}_1} \right)^2 \frac{F_1^M}{h_1} \underline{dx}_1 \underline{dw}_1 \geq 0 \quad (25)$$

The expression for the viscosity coefficient is:

$$\mu = \frac{m}{\tau B} \quad (26)$$

with for τ : (Fig. 2)

$$\tau = \int_0^\sigma \int_0^\infty \left[\int_0^\sigma \left(g^2 \left(1 - \frac{b^2}{r^2} \right) - \frac{4}{m} \varphi(r) \right)^{1/2} dr \right] \left[\frac{2\pi b}{r \sigma^2} \left(\frac{m}{4\pi K_0 T} \right)^{3/2} e^{-\frac{m g^2}{4 K_0 T}} 4\pi g^2 \, db \, dg \right] \quad (27)$$

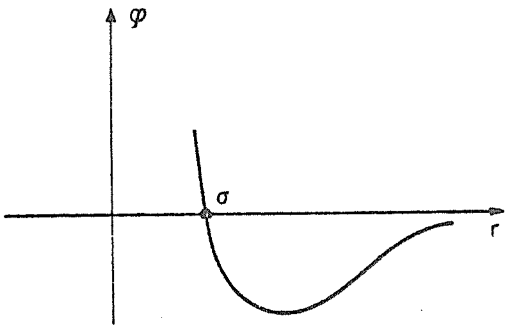

Fig. 2

For a sutherland potential:

$$r < \sigma \qquad \varphi = \infty \qquad r > \sigma \qquad \varphi = -K_0 T_i f_0\left(\frac{r}{\sigma}\right) \qquad f_0(1) = 1 \tag{28}$$

The calculation is made on considering the vertical straight line as the limit of an oblique straight line:

$$r \leqslant 0 \qquad \varphi = -K_0 T_i \quad \frac{r-a}{\sigma-a} \qquad a \longrightarrow \sigma \tag{29}$$

The final result is:

$$\mu = \frac{g}{32}\left(\frac{mK_0T}{\pi}\right)^{1/2}\frac{1}{\sigma^2}\,e^{-\frac{T_i}{T}} \tag{30}$$

Agreement with experiment is better than 1% from 300 to 2200 K for Argon[10]

$$\sigma = 2{,}829\ 10^{-10}\,\mathrm{m} \ ; \qquad T_i = 110{,}8\ \mathrm{K} \ ; \qquad m = 6{,}633\ 10^{-16}\,\mathrm{kg}.$$

Table 2

T K	$10^5\mu_{th}$ Pa.s	$10^5\mu_{exp}$ Pa.s	$\lvert \Delta\mu / \mu \rvert$
250	1,926	1,949	0,012
300	2,272	2,272	0,00
500	3,400	3,365	0,01
700	4,286	4,25	0,008
1000	5,372	5,35	0,004
1600	7,083	7,100	0,002
2200	8,463	8,510	0,006

IV – The Fine Entropy Method

The idea of the fine entropy method has been introduced by J. Fronteau[11,12] and defined as being the logarithm of the distribution function. A molecule of fluid, subjected to an external force $\vec{X}$ and to its close environment, is assumed to obey the following law of motion:

$$m\frac{d\vec{w}}{dt} = \vec{X} - \alpha\left(\vec{w} - \vec{v}\right) - \alpha\frac{K_0T}{m}\,\vec{\nabla}_w \log F = \vec{X}_T \tag{31}$$

in which the gradient of the fine entropy is brought in as a generator of disorder to oppose the state of rest towards which the molecule was tending in the absence of X.

The true Liouville equation,

$$\frac{\partial F}{\partial t} + \vec{w} \cdot \frac{\partial F}{\partial \vec{x}} + \frac{\partial}{\partial \vec{w}} \cdot \left(\frac{\vec{X}_T}{m} F \right) = 0 \qquad (32)$$

associated with the equation (30), allows us to recover an equation of the type (23)[12]:

$$\frac{\partial F}{\partial t} + \vec{w} \cdot \frac{\partial F}{\partial \vec{x}} + \frac{\vec{X}}{m} \cdot \frac{\partial F}{\partial \vec{w}} = \frac{\alpha}{m} \left[3F + (\vec{w} - \vec{v}) \cdot \frac{\partial F}{\partial \vec{w}} + \frac{K_0 T}{m} \Delta_w F \right] \qquad (33)$$

P. Combis, J. Fronteau and A. Tellez-Arenas[13] have also studied the motion of a one dimension Brownian quasi-particle at position x and velocity v. On designating the damping coefficient by ν, the equation of motion is written, in a uniform and constant external force $-mg$, as:

$$m \frac{dv}{dt} = -mg - \nu m v - \nu K_0 T \frac{\partial}{\partial v} \log f \qquad (34)$$

and leads, with (32), to the density probability equation f :

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \frac{\partial}{\partial v} (\nu v + g) f - \frac{\sigma^2}{2} \frac{\partial^2 f}{\partial v^2} = 0 \qquad (35)$$

$$\sigma^2 = 2 \nu \frac{K_0 T}{m} \qquad (36)$$

For an initial position x_0 and an initial velocity v_0 ... i.e. for a f function equal to $\delta(x - x_0) \delta(v - v_0)$ at zero time ... the equation (35) has the explicit solution[14]:

$$f = \frac{1}{2\pi (A)^{1/2}} \exp - \frac{1}{2A} \left[A_{vv} (x - \bar{x})^2 - 2 A_{xv} (x - \bar{x})(v - \bar{v}) + A_{xx} (v - \bar{v})^2 \right] \qquad (37)$$

with:

$$A_{xx} = \frac{\sigma^2}{2\nu^3}\left[2\nu t - 3 + 4e^{-\nu t} - e^{-2\nu t}\right] \tag{38}$$

$$A_{xv} = \frac{\sigma^2}{2\nu^2}\left(1 - e^{-\nu t}\right)^2 \tag{39}$$

$$A_{vv} = \frac{\sigma^2}{2\nu}\left[1 - e^{-2\nu t}\right] \tag{40}$$

$$A = A_{xx}A_{vv} - \left(A_{xv}\right)^2 \tag{41}$$

$$\overline{x} = x_0 + \frac{v_0}{\nu}\left(1 - e^{-\nu t}\right) - \frac{g}{\nu^2}\left(\nu t - 1 + e^{-\nu t}\right) \tag{42}$$

$$\overline{v} = v_0 e^{-\nu t} - \frac{g}{\nu}\left(1 - e^{-\nu t}\right) \tag{43}$$

The quantity $(x - \overline{x})^2$ has, for an average value:

$$\overline{\left(x - \overline{x}\right)^2} = \frac{\sigma^2}{2\nu^3}\left[2\nu t - 3 + 4e^{-\nu t} - e^{-2\nu t}\right] \tag{44}$$

thus, for large t, the following formula which is well verified by experiment:

$$\frac{\overline{\left(x - \overline{x}\right)^2}}{t} = \frac{\sigma^2}{\nu^2} = \frac{2K_0T}{m\nu} \tag{45}$$

V — Conclusion

We have taken up the problem of irreversibility starting from an equation of irreversibility motion. To the usual force deriving from a position potential, we have added two non-Hamiltonian forces or environmental forces. The first is an usual damping force and the second is a force proportional to the gradient in the velocity space of the logarithm of the distribution function.

We thus obtain an irreversible kinetic equation which allows us to take account of the viscosity coefficient of a dilute gas and of the laws of Brownian motion.

Consequently, we have associated non-Hamiltonian forces with dissipative structures.

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Inverse Liouville problem

M. Grmela
Centre de Recherche de
Mathématiques Appliquées
Université de Montréal
Montréal, P.Q., H3C 3J7, Canada

and

J. Fronteau and **A. Tellez-Arenas**
Département de Physique
Université d'Orléans
F-45046 Orléans Cedex, France

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Abstract

Liouville's theorem, in its original form (1838), allows us to derive a kinetic equation from any given dynamics, whether conservative or not. In this article we study the inverse problem: given a kinetic equation, to find quasi-particle dynamics (generally non-conservative) which, via Liouville's theorem, generates precisely this equation. The mathematical problem thus presented allows an infinite number of solutions. In fact, physically, we are allowed, by what we call the principle of correspondence, to retain one particular non-conservative set of dynamics, namely that which becomes conservative when statistical equilibrium is reached. From this viewpoint, we give the solution to the inverse Liouville problem for a very general class of kinetic equations. This solution has a direct physical interpretation in terms of current velocity. We consider in particular the cases of the Boltzmann and Fokker-Planck equations.

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Inverse Liouville problem

I. INTRODUCTION.

The following problem has been recently studied in (Frisch, Forgacs and Chui, 1979) : given a kinetic equation

$$\frac{\partial f}{\partial t} = \mathcal{R}(f) \qquad (I.1)$$

where $f(\underline{r},\underline{v},t)$ is the one-particle distribution, $\underline{r}$ is the position coordinate, $\underline{v}$ is the velocity, to determine a Hamilton function $H(\underline{r},\underline{v},t)$ such that, if $f(\underline{r},\underline{v},t)$ is a solution of (I.1), then the same $f(\underline{r},\underline{v},t)$ is also a solution of

$$\frac{\partial f}{\partial t} = -\frac{1}{m}\left(\frac{\partial f}{\partial r_i}\frac{\partial H}{\partial v_i} - \frac{\partial f}{\partial v_i}\frac{\partial H}{\partial r_i}\right) \quad . \qquad (I.2)$$

The summation convention was used in (I.2), $i = 1,2,3$, and m is the mass of a particle. Frisch, Forgacs and Chui considered the case where (I.1) becomes the Fokker-Planck equation and, for the fundamental solution corresponding to a quadratic potential, they found the Hamiltonian $H(\underline{r},\underline{v},t)$ explicitly.

The particular case of the Fokker-Planck equation brings to light, in our opinion, the deficiencies of the above method. Frisch, Forgacs and Chui start with a non-Hamiltonian evolution in an infinite dimensional dynamical space (the kinetic equation (I.1)). Via the Liouville equation (I.2), they look for Hamiltonian dynamics in a finite dimensional phase space, that are equivalent to the original kinetic equation (I.1) in a weak sense only. By the weak equivalence we mean that the Liouville equation (I.2) corresponding to the Hamiltonian dynamics that are found is not necessarily strictly equivalent to the kinetic equation (I.1) ; only the solutions of (I.1) have to be also solutions of (I.2). On the other hand, the Hamiltonian found in (Frisch, Forgacs and Chui, 1979) for the case of the Fokker-Planck equation does not have a physical meaning. Besides, this deficiency is of a general nature. Indeed, (Santilli, 1978) has recently considered the problem of reformulating non-Hamiltonian dynamics in a finite dimensional dynamical space as Hamiltonian dynamics in a finite dimensional phase space. The reformulation is possible under very general circumstances, but the Hamiltonian obtained after the reformulation does not, however, have a physical meaning.

In this paper we shall consider the inverse Liouville problem for a large class of kinetic equations of type (I.1), but we shall look for <u>non-Hamiltonian</u> dynamics (I.3) in a finite dimensional dynamical space,

$$\begin{aligned} \dot{\underline{r}} &= \underline{V}_r(f;\underline{r},\underline{v},t) \\ \dot{\underline{v}} &= \underline{V}_v(f;\underline{r},\underline{v},t) \end{aligned} \tag{I.3}$$

dynamics that are strictly equivalent to (I.1) via the general Liouville equation (I.4)

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial r_i}(f\,V_{r,i}) - \frac{\partial}{\partial v_i}(f\,V_{v,i}) \quad . \tag{I.4}$$

By "strictly equivalent" we mean that (I.1) and (I.4) are <u>identical equations</u>. Note that (I.4), which takes into account general non-selfadjoint forces (I.3), gives rise to an algebraic Lie-admissible formulation of statistical mechanics (Fronteau, Tellez-Arenas and Santilli, 1979). Note also that there exists a confusion in the literature about the exact meaning of the expression "Liouville equation". We have therefore added to this article an appendix devoted to this concept. In conclusion, the problem that we call the "Inverse Liouville Problem" is the following : given (I.1), find (I.3) such that (I.4) is equivalent to (I.1). We shall see that the time evolution equations (I.3) have a natural physical interpretation.

A few remarks about this problem are in order. In this paper, we solve the inverse Liouville problem for (I.1) being a rather general gain-loss balance kinetic equation. Simple physical argument allows us to select "good", physically interesting, time evolution equations (I.3) among many possible equations (I.3) for which (I.4) is identical to a given kinetic equation (I.1). It is important to note that the equations (I.3) are unusual time evolution equations: the vector field (I.3) depends on the function f that can only be obtained as a solution of (I.4). Thus (I.3) and (I.4) have to be considered together. The virtual particle evolving in time according to (I.3) has been referred to as a quasiparticle (Combis, Fronteau and Tellez-Arenas, 1979 ; Tellez-Arenas, Fronteau and Combis , 1979), i.e., a mathematical object representing a certain average behaviour of the real body.

In studying the inverse Liouville problem we have the following objectives : (i) The quasiparticle representation (I.3) of kinetic equations of type (I.1) provides a new view of the non-Hamiltonian, non-conservative structure of phenomenological equations of macroscopic physics. (ii) Physical experience associated with particle dynamics and stochastic processes might help to construct extension of the well-established kinetic equation (e.g., the Boltzmann equation) by constructing first the vector field (I.3) and then arriving at the kinetic equation via the Liouville equation (I.4). (iii) Finally, the reformulation (I.3) and (I.4) of (I.1) might be useful in solving the kinetic equation (I.1).

II. SOLUTION OF THE INVERSE LIOUVILLE PROBLEM FOR A CLASS OF KINETIC EQUATIONS.

1°) The kinetic equations considered.

We shall now specify more explicitly the class of the kinetic equations that will be considered. According to (Grmela and Iscoe, 1978 ; Grmela, 1979), the right hand side of (I.1) is decomposed uniquely into two parts,

$$\mathcal{R}(f) = \mathcal{R}^{-}(f) + \mathcal{R}^{+}(f) \qquad \text{(II.1)}$$

where

$$\mathcal{R}^{\pm}(f) = \frac{1}{2}\,[\mathcal{R}(f) \pm J\,\mathcal{R}(J\,f)\,] \qquad \text{(II.2)}$$

and

$$J\,f(\underline{r},\underline{v},t) = f(\underline{r},-\underline{v},t) \quad . \qquad \text{(II.3)}$$

It will be seen in the remainder of the article that, in the time evolution law for f, $\mathcal{R}^{+}(f)$ represents all the phenomena that are associated with collisions between particles. $\mathcal{R}^{+}(f)$ is thus called the non-conservative part of the statistical operator $\mathcal{R}(f)$, and, conversely, $\mathcal{R}^{-}(f)$ is called the conservative part of $\mathcal{R}(f)$.

Note first of all that the solution of the inverse Liouville problem for $\mathcal{R}(f)$ is immediately obtained from the solutions for $\mathcal{R}^{-}(f)$ and $\mathcal{R}^{+}(f)$. Indeed .

$$\mathcal{R}^{-}(f) = -\frac{\partial}{\partial r_i}\,(f\,V^{-}_{r,i}) - \frac{\partial}{\partial v_i}\,(f\,V^{-}_{v,i})$$

$$\mathcal{R}^{+}(f) = -\frac{\partial}{\partial r_i}\,(f\,V^{+}_{r,i}) - \frac{\partial}{\partial v_i}\,(f\,V^{+}_{v,i}) \qquad \text{(II.4)}$$

implies

$$\mathcal{R}(f) = -\frac{\partial}{\partial r_i}\left[f(V^-_{r,i}+V^+_{r,i})\right] - \frac{\partial}{\partial v_i}\left[f(V^-_{v,i}+V^+_{v,i})\right] \qquad (II.5)$$

and thus, in (I.3) and (I.4)

$$\begin{bmatrix} \underline{V}_r \\ \\ \underline{V}_v \end{bmatrix} = \begin{bmatrix} \underline{V}^-_r \\ \\ \underline{V}^-_v \end{bmatrix} + \begin{bmatrix} \underline{V}^+_r \\ \\ \underline{V}^+_v \end{bmatrix} \qquad (II.6)$$

The class of $\mathcal{R}^-$ that will be considered is defined as follows. Let us consider a particle represented by the position coordinate $\underline{r}$ and velocity $\underline{v}$ and moving according to the Newtonian law

$$\begin{aligned} \dot{\underline{r}} &= \underline{v} \\ \dot{\underline{v}} &= \underline{\mathcal{F}}(\underline{r},t) \end{aligned} \qquad (II.7)$$

where $\underline{\mathcal{F}}$ is a force and the particle has unit mass. The operators $\mathcal{R}^-$ considered are defined now as the right hand side of the Liouville equation (I.4) corresponding to (II.7), thus

$$\mathcal{R}^-(f) = -v_i\frac{\partial f}{\partial r_i} - \frac{\partial}{\partial v_i}\left(f\ \mathcal{F}_i(\underline{r},t)\right) . \qquad (II.8)$$

If $\underline{\mathcal{F}} = 0$, we recognize the familiar free flow term. A direct verification shows that the operator introduced in (II.8) has in fact no non-conservative part, in the sense of (II.2). In order to be able to consider also the Vlasov-type kinetic equations, we shall admit that the force $\underline{\mathcal{F}}$ can depend on $n(\underline{r},t)=\int d^3\underline{v}\ f(\underline{r},\underline{v},t)$. This generalization is very familiar in the context of the Vlasov equation. In this case, the Newtonian dynamics (II.7) are replaced by

$$\begin{aligned} \dot{\underline{r}} &= \underline{v} \\ \dot{\underline{v}} &= \underline{\mathcal{F}}(n;\underline{r},t) \end{aligned} \qquad (II.9)$$

and the right hand side of the Liouville equation (I.4) becomes

$$\mathcal{R}^{-}(f) = - v_i \frac{\partial f}{\partial r_i} - \frac{\partial}{\partial v_i} (f \ \mathcal{F}_i(n;\underline{r},t)) \quad . \tag{II.10}$$

The inverse Liouville problem for (I.1) where $\mathcal{R}$ is replaced by $\mathcal{R}^-$ introduced in (II.8) and (II.10) is of course trivial. The solutions are given by (II.7) and (II.9) respectively.

We proceed now to the specification of the class of the non-conservative operators $\mathcal{R}^+$ that we shall consider. We propose to consider the class of gain-loss operators describing phenomena without memory, i.e., such that the probability of transition between two points depends only upon these points and the corresponding times. Now, let $X \in \mathbb{R}^{6N}$ be a point in the dynamical space of the system considered, and $f_N(X,t)$ the corresponding density at time t. By introducing the probability density $P(X_2,t_2|X_1,t_1)$ of the transition from (X_1,t_1) to the neighborhood of (X_2,t_2), $t_1 < t_2$, one successively obtains

$$\frac{\partial}{\partial t} f_N(X,t) = \lim_{\Delta t \to 0} \frac{f_N(X,t_2) - f_N(X,t_1)}{\Delta t} \quad ; \qquad t_1 < t < t_2 \ , \quad \Delta t = t_2 - t_1$$

$$f_N(X,t_2) = \int dX' \ f_N(X',t_1) P(X,t_2|X',t_1)$$

$$f_N(X,t_1) = \int dX' \ f_N(X,t_1) P(X',t_2|X,t_1)$$

$$\frac{\partial}{\partial t} f_N(X,t) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{\mathbb{R}^{6N}} dX' [f_N(X',t_1)P(X,t_2|X',t_1) - f_N(X,t_1)P(X',t_2|X,t_1)] . \tag{II.11}$$

Let us now consider the case in which, for Δt sufficiently small, one may introduce the idea of a transition probability density per unit of time, w :

$$P(X,t_2|X',t_1) = (t_2-t_1) w(X;X') = \Delta t \ w(X;X') \tag{II.12}$$

The equation (II.11) then reduces to

$$\frac{\partial}{\partial t} f_N(X,t) = \int_{\mathbb{R}^{6N}} dX' \, [f_N(X',t)w(X;X') - f_N(X,t)w(X';X)] \qquad \text{(II.13)}$$

By putting $X=(\underline{r}_\ell,\underline{v}_\ell)$, $\ell=1,\dots,N$, and using the microreversibility relation

$$w(\underline{r}_\ell,\underline{v}_\ell\,;\underline{r}'_\ell,\underline{v}'_\ell) = w(\underline{r}_\ell,-\underline{v}_\ell\,;\underline{r}'_\ell,-\underline{v}'_\ell) \quad , \qquad \text{(II.14)}$$

one may verify that the integral operator present in (II.13) is of type $\mathcal{R}^+(f_N)$ in the sense of (II.2). Furthermore, we suppose that the so-called detailed balance condition

$$w(\underline{r}_\ell,\underline{v}_\ell\,;\underline{r}'_\ell,\underline{v}'_\ell)\; f_N^{eq}(\underline{r}'_\ell,\underline{v}'_\ell) = w(\underline{r}'_\ell,\underline{v}'_\ell\,;\underline{r}_\ell,\underline{v}_\ell)\; f_N^{eq}(\underline{r}_\ell,\underline{v}_\ell) \qquad \text{(II.15)}$$

is satisfied, where $f_N^{eq}(\underline{r}_\ell,\underline{v}_\ell) = f_N^{eq}(\underline{r}_\ell,-\underline{v}_\ell)$ is the unique time independent solution of (II.13).

In the following we shall obtain a general formulation giving a physically significant solution to the inverse Liouville problem for the kinetic equations of type (II.13), and even of type (II.11). However we are interested in solving the inverse Liouville problem for the kinetic equations which govern one-particle distribution functions $f_1(\underline{r}_1,\underline{v}_1,t)$,

$$f_1(\underline{r}_1,\underline{v}_1,t) = \int d^3\underline{r}_2\; d^3\underline{v}_2\; \dots\; f_N(\underline{r}_1,\underline{v}_1,\underline{r}_2,\underline{v}_2,\dots,t) \qquad \text{(II.16)}$$

and we shall consider explicitly the cases $N=1$ and $N=2$, for which the following notation will be used : $f_1(\underline{r}_1,\underline{v}_1,t) = f(\underline{r},\underline{v},t)$, $f_2(\underline{r}_1,\underline{v}_1,\underline{r}_2,\underline{v}_2,t) = f_2(\underline{r},\underline{v},\underline{\xi},\underline{\nu},t)$. Let us suppose then that there is no position diffusion, and that transition probability depends only upon velocity and is symmetrical :

$$N=1 \;\; : \;\; w = W(\underline{v};\underline{v}')\delta(\underline{r}-\underline{r}') \;\; ; \;\; W(\underline{v};\underline{v}') = W(\underline{v}';\underline{v})$$

$$N=2 \;\; : \;\; w = w^{*}(\underline{v},\underline{\nu};\underline{v}',\underline{\nu}')\delta(\underline{r}-\underline{r}')\delta(\underline{\xi}-\underline{\xi}')$$

$$w^{*}(\underline{v},\underline{\nu};\underline{v}',\underline{\nu}') = w^{*}(\underline{v}',\underline{\nu}';\underline{v},\underline{\nu}) \quad . \qquad \text{(II.17)}$$

For $N=1$, the relation (II.13) leads directly to the kinetic equation for the one-particle distribution function :

$$\frac{\partial}{\partial t} f(\underline{r},\underline{v},t) = \mathcal{R}^{+}(f) = \int d^{3}\underline{v}' \; W(\underline{v};\underline{v}') \; [f(\underline{r},\underline{v}',t) - f(\underline{r},\underline{v},t)] \; . \qquad \text{(II.18)}$$

For $N=2$, (II.13) leads first of all to

$$\frac{\partial}{\partial t} f_{2}(\underline{r},\underline{v},\underline{\xi},\underline{\nu},t) = \int d^{3}\underline{v}' \int d^{3}\underline{\nu}' w^{*}(\underline{v},\underline{\nu};\underline{v}',\underline{\nu}')[f_{2}(\underline{r},\underline{v}',\underline{\xi},\underline{\nu}',t)-f_{2}(\underline{r},\underline{v},\underline{\xi},\underline{\nu},t)]. \qquad \text{(II.19)}$$

The evolution of $f(\underline{r},\underline{v},t)$ is then obtained by summation with respect to $\underline{\xi}$ and $\underline{\nu}$. In fact, for given $\underline{r}$ and $\underline{v}$, the interaction vanishes outside a certain neighborhood of $\underline{r}$ called the volume of interaction $\mathcal{V}_{int}$. The integration with respect to $\underline{\xi}$ is then limited to this volume $\mathcal{V}_{int}$. By introducing the hypothesis of the Boltzmann chaos

$$f_{2}(\underline{r},\underline{v},\underline{\xi},\underline{\nu},t) = f(\underline{r},\underline{v},t)f(\underline{\xi},\underline{\nu},t)$$

and assuming that f is independent of position inside $\mathcal{V}_{int}$, (II.13) leads eventually, by putting $W = w^{*}\mathcal{V}_{int}$, to

$$\frac{\partial}{\partial t} f(\underline{r},\underline{v},t) = \mathcal{R}^{+}(f) = \int d^{3}\underline{\nu} \int d^{3}\underline{v}' \int d^{3}\underline{\nu}' W(\underline{v},\underline{\nu};\underline{v}',\underline{\nu}')[f(\underline{r},\underline{v}',t)f(\underline{r},\underline{\nu}',t) - f(\underline{r},\underline{v},t)f(\underline{r},\underline{\nu},t)]. \qquad \text{(II.20)}$$

Finally, let us recall that it follows from the $\mathcal{H}$-theorem that the only time independent solution of (II.20) is the one-particle distribution function f that satisfies

$$f(\underline{r},\underline{v}')f(\underline{r},\underline{v}') = f(\underline{r},\underline{v})f(\underline{r},\underline{v}) \qquad \text{(II.21)}$$

2°) <u>The principle of correspondence</u>.

We have now to solve the inverse Liouville problem for (I.1) where $\mathcal{R}$ is defined by (II.11), (II.13), (II.18) or (II.20). We shall observe first that the problem of writing a scalar function as a divergence of a vector function (the problem that is basically involved in the inverse Liouville problem) has an infinite number of solutions. There is however a natural requirement restricting the choice of possible solutions. Note first of all that, given

$$\frac{\partial f}{\partial t} = \mathcal{R}^+(f)$$

and a solution of the inverse Liouville problem, i.e., functions $\underline{V}_r^+(f;\underline{r},\underline{v},t)$ and $\underline{V}_v^+(f;\underline{r},\underline{v},t)$ such that

$$\dot{\underline{r}} = \underline{V}_r^+ \quad , \quad \dot{\underline{v}} = \underline{V}_v^+$$

$$\frac{\partial f}{\partial t} = \mathcal{R}^+(f) = -\frac{\partial}{\partial r_i}(f\,V^+_{r,i}) - \frac{\partial}{\partial v_i}(f\,V^+_{v,i}) \quad , \qquad \text{(II.22)}$$

it appears trivially that the conditions $\underline{V}_r^+ = 0$, $\underline{V}_v^+ = 0$ imply $\mathcal{R}^+(f) = 0$. The inverse however is not true in general. It seems nevertheless natural to require that the inverse should be true, i.e., to require that for all f that are solutions of $\mathcal{R}^+(f) = 0$ the functions $\underline{V}_r^+(f;\underline{r},\underline{v},t)$ and $\underline{V}_v^+(f;\underline{r},\underline{v},t)$ should vanish. Indeed, let us write the kinetic equation (from (I.1) and (II.1))

$$\frac{\partial f}{\partial t} = \mathcal{R}(f) = \mathcal{R}^-(f) + \mathcal{R}^+(f) \qquad \text{(II.23)}$$

and a quasi-particle dynamical evolution (from (I.3), (II.6) and (II.9)),

$$\dot{\underline{r}} = \underline{V}_r^- + \underline{V}_r^+ = \underline{v} + \underline{V}_r^+$$

$$\dot{\underline{v}} = \underline{V}_v^- + \underline{V}_v^+ = \underline{\mathcal{F}}(n;\underline{r},t) + \underline{V}_v^+ \qquad \text{(II.24)}$$

that is associated with (II.23) through the inverse Liouville problem. The dynamics defined by the vector field $(\underline{V}_r^-,\underline{V}_v^-)$ are classical dynamics in the sense that the force $\underline{\mathcal{F}}$ does not depend upon the velocity $\underline{v}$, and we note (from (II.10)) that they do correspond to the conservative part $\mathcal{R}^-(f)$ of the operator $\mathcal{R}(f)$. The preceding requirement $(\mathcal{R}^+(f) = 0 \Rightarrow (\underline{V}_r^+,\underline{V}_v^+) = 0)$ means physically that we associate a classical dynamical evolution $((\underline{V}_r^+,\underline{V}_v^+) = 0)$ to any conservative statistical evolution $(\mathcal{R}^+(f) = 0)$. The requirement will be referred to as the *principle of correspondence* between statistical mechanics and the associated dynamics in the inverse Liouville problem. Note, from (II.8) and (II.10), that $\mathcal{R}^-(f) = 0$ does not necessarily imply $(\underline{V}_r^-,\underline{V}_v^-) = 0$.

It may be useful to link up the principle of correspondence with the notion of thermodynamic equilibrium. According to (Grmela and Iscoe, 1978), a thermodynamic equilibrium state implied by (I.1) is a solution of $\mathcal{R}(f) = 0$ that is moreover invariant with respect to J defined in (II.3). As it follows directly from (II.1) and (II.2), the thermodynamic equilibrium states are thus solutions to $\mathcal{R}^-(f) = 0$, $\mathcal{R}^+(f) = 0$, that are invariant with respect to J. In the case of the Boltzmann equation this notion of thermodynamic equilibrium states is obviously equivalent to the notion of the equilibrium states introduced in Gibbs theory. With this definition of equilibrium, the principle of correspondence finally reduces to what appears, in the inverse Liouville problem, to be a natural property : in a state of thermodynamic equilibrium, the time evolution of the associated quasi-particle is governed by classical conservative dynamics.

Note finally that this correspondence principle has already been explicitly verified in the case of the Fokker-Planck equation (Tellez-Arenas, Fronteau and Combis, 1979).

3°) Solution of the inverse Liouville problem for $\mathcal{R}^+(f)$: the Irving-Kirkwood method.

We do not know as to whether the principle of correspondence singles out the solution of the inverse Liouville problem for $\mathcal{R}^+(f)$. One solution that satisfies this principle is however known to us from the Irving-Kirkwood method (Irving and Kirkwood, 1950 ; Noll, 1955) : given the quantity

$$\mathcal{R} = \int_{\mathbb{R}^{6N}} dX' \, [\phi(X',X) - \phi(X,X')] \tag{II.25}$$

where X, X' $\in \mathbb{R}^{6N}$, and where ϕ is a differentiable function $\mathbb{R}^{6N} \times \mathbb{R}^{6N} \rightarrow \mathbb{R}$, one has, for $\alpha = 1,\ldots,6N$

$$\mathcal{R} = - \frac{\partial}{\partial X_\alpha} K_\alpha(X)$$

$$K(X) = \int_{\mathbb{R}^{6N}} dX' \int_0^1 d\eta \; X' \, \phi[X(\eta),X'(\eta)] \tag{II.26}$$

$$X(\eta) = X - \eta X' \quad ; \quad X'(\eta) = X + (1-\eta)X' \ .$$

The proof follows immediately from three observations :

$$\int dX' \, [\phi(X',X) - \phi(X,X')] = \int dX' \, [\phi(X-X',X) - \phi(X,X+X')]$$

$$\phi(X-X',X) - \phi(X,X+X') = \int_0^1 d\eta \, \frac{d}{d\eta} \phi[X(\eta),X'(\eta)]$$

$$\frac{d}{d\eta} \phi[X(\eta),X'(\eta)] = - X'_\alpha \frac{\partial}{\partial X_\alpha} \phi[X-\eta X' \, , X+(1-\eta)X'] \ .$$

Note that it is possible to relax the condition of differentiability of ϕ by considering the derivatives in the weak sense. We can indeed use the Irving-Kirkwood method also in the case when ϕ involves Dirac delta functions.

The general class of operators $\mathcal{R}^+(f)$ defined by (II.13) is of type (II.25) and the Irving-Kirkwood method thus provides us with a solution to the inverse Liouville problem for this class of operators. We obtain, following (II.26),

$$\mathcal{R}^+(f_N(X,t)) = -\frac{\partial}{\partial X_\alpha}[f_N(X,t)V^+_\alpha(X,t)]$$

$$V^+(X,t) = \frac{1}{f_N(X,t)}\,K^+(f_N;X,t) = \frac{1}{f_N(X,t)}\int_{\mathbb{R}^{6N}} dX' \int_0^1 d\eta\, X'\, w[X'(\eta);X(\eta)]f_N(X(\eta),t). \qquad \text{(II.27)}$$

Note that the expression (II.27) of the current velocity satisfies the principle of correspondence. Indeed, according to the detailed balance condition (II.15), the only solution of $\mathcal{R}^+(f_N) = 0$ is $f_N^{eq}(X)$ such that $w(X;X')f_N^{eq}(X') = w(X';X)f_N^{eq}(X)$. If this relation is inserted into (II.27), one obtains $V^+(X,t) = 0$ after the change of variables $X' \to -X'$, $\eta \to 1-\eta$. The physical interpretation of (II.27) will be discussed in section III.

In the particular case where $N = 1$, i.e., for $X = (\underline{r},\underline{v})$, $w = W(\underline{v};\underline{v}')\delta(\underline{r}-\underline{r}')$ and $W(\underline{v};\underline{v}') = W(\underline{v}';\underline{v})$, the relation (II.18) leads to

$$\frac{\partial}{\partial t} f(\underline{r},\underline{v},t) = \int d^3\underline{v}'\; W(\underline{v};\underline{v}')[f(\underline{r},\underline{v}',t) - f(\underline{r},\underline{v},t)]$$

$$= -\frac{\partial}{\partial r_i}(f\,V^+_{r,i}) - \frac{\partial}{\partial v_i}(f\,V^+_{v,i}) \quad , \quad i = 1,2,3 \ . \qquad \text{(II.28)}$$

$$\underline{V}^+_r(f;\underline{r},\underline{v},t) = \frac{1}{f(\underline{r},\underline{v},t)}\int d^3\underline{r}' \int d^3\underline{v}' \int_0^1 d\eta\, \underline{r}'\; W(\underline{v}'(\eta);\underline{v}(\eta))\delta(\underline{r}')f(\underline{r}(\eta),\underline{v}(\eta),t) = 0\ . \qquad \text{(II.29)}$$

$$\underline{V}_v^+(f;\underline{r},\underline{v},t) = \frac{1}{f(\underline{r},\underline{v},t)}\int d^3\underline{r}'\int d^3\underline{v}'\int_0^1 d\eta\, \underline{v}'\, W(\underline{v}'(\eta);\underline{v}(\eta))\,\delta(\underline{r}')\,f(\underline{r}(\eta),\underline{v}(\eta),t)$$

$$= \frac{1}{f(\underline{r},\underline{v},t)}\int d^3\underline{v}'\int_0^1 d\eta\, \underline{v}'\, W(\underline{v}'(\eta);\underline{v}(\eta))\,f(\underline{r},\underline{v}(\eta),t) \qquad \text{(II.30)}$$

where

$$\underline{r}(\eta) = \underline{r} - \eta\underline{r}' \quad ; \quad \underline{r}'(\eta) = \underline{r} + (1-\eta)\underline{r}' \quad ; \quad \underline{v}(\eta) = \underline{v} - \eta\underline{v}' \quad ; \quad \underline{v}'(\eta) = \underline{v} + (1-\eta)\underline{v}' .$$

The case where $N = 2$ corresponds to the relation (II.20) which is not directly of type (II.25). It is thus preferable to return to equation (II.13) for which the solution to the inverse Liouville problem is given by (II.27). With $w = w^*(\underline{v},\underline{\nu};\underline{v}',\underline{\nu}')\delta(\underline{r}-\underline{r}')\delta(\underline{\xi}-\underline{\xi}')$ and $w^*(\underline{v},\underline{\nu};\underline{v}',\underline{\nu}') = w^*(\underline{v}',\underline{\nu}';\underline{v},\underline{\nu})$, one obtains first of all a result similar to (II.29,II.30), i.e.,

$$\frac{\partial}{\partial t} f_2(\underline{r},\underline{v},\underline{\xi},\underline{\nu},t) = -\frac{\partial}{\partial v_i} K^+_{v,i} - \frac{\partial}{\partial \nu_i} K^+_{\nu,i}$$

$$\underline{K}^+_r = 0 \quad ; \quad \underline{K}^+_\xi = 0$$

$$\underline{K}^+_v(f_2;\underline{r},\underline{v},\underline{\xi},\underline{\nu},t) = \int d^3\underline{v}'\int d^3\underline{\nu}'\int_0^1 d\eta\, \underline{v}'\, w^*(\underline{v}'(\eta),\underline{\nu}'(\eta);\underline{v}(\eta),\underline{\nu}(\eta)) \times$$

$$\times f_2(\underline{r},\underline{v}(\eta),\underline{\xi},\underline{\nu}(\eta),t) \qquad \text{(II.31)}$$

and an equivalent expression for $\underline{K}^+_\nu$. To deduce from this the solution to the inverse Liouville problem for (II.20), it is necessary to integrate the equation (II.31) with respect to $\underline{\xi}$ and $\underline{\nu}$. Realizing the fact that $\underline{K}^+_\nu$ vanishes for infinite $\underline{\nu}$, one obtains

$$\frac{\partial}{\partial t} f(\underline{r},\underline{v},t) = -\frac{\partial}{\partial v_i}\int d^3\underline{\xi}\int d^3\underline{\nu}\, K^+_{v,i} = -\frac{\partial}{\partial v_i}\left(f(\underline{r},\underline{v},t)\, V^+_{v,i}\right)$$

$$\underline{V}^+_v = \frac{1}{f(\underline{r},\underline{v},t)}\int d^3\underline{\xi}\int d^3\underline{\nu}\int d^3\underline{v}'\int d^3\underline{\nu}'\int_0^1 d\eta\, \underline{v}'\, w^*(\underline{v}'(\eta),\underline{\nu}'(\eta);\underline{v}(\eta),\underline{\nu}(\eta)) \times$$

$$\times f_2(\underline{r},\underline{v}(\eta),\underline{\xi},\underline{\nu}(\eta),t) . \qquad \text{(II.32)}$$

Using the same hypotheses as those leading from (II.19) to (II.20), one eventually obtains :

$$\underline{V}^{+}_{r} = 0$$

$$\underline{V}^{+}_{v} = \frac{1}{f(\underline{r},\underline{v},t)}\int d^3\underline{\nu}\int d^3\underline{v}'\int d^3\underline{\nu}'\int_0^1 d\eta\ \underline{v}'\ W(\underline{v}'(\eta),\underline{\nu}'(\eta);\underline{v}(\eta),\underline{\nu}(\eta))f(\underline{r},\underline{v}(\eta),t)\ \times$$
$$\times\ f(\underline{r},\underline{\nu}(\eta),t). \qquad \text{(II.33)}$$

Since the solutions of (II.21) are the only solutions of $\mathcal{R}^{+}(f) = 0$, we easily verify through the change of variables $(\underline{v}',\underline{\nu}') \rightarrow (-\underline{v}',-\underline{\nu}')$, $\eta \rightarrow 1-\eta$, that (II.33) satisfies the principle of correspondence.

To summarize, the Irving-Kirkwood method solves the inverse Liouville problem with the requirement of the principle of correspondence : solution (II.30) for $\mathcal{R}^{+}(f)$ defined in (II.18), solution (II.33) for $\mathcal{R}^{+}(f)$ defined in (II.20) and, in general, solution (II.27) for $\mathcal{R}^{+}(f_N)$ in (II.13,II.14).

III. PHYSICAL INTERPRETATION.

Following the method used, in the context of hydrodynamics, by Irving and Kirkwood in the appendix of (Irving and Kirkwood, 1950), we introduce in $\mathbb{R}^{6N}$ a mean velocity associated with a large class of statistical phenomena (those statistical phenomena with the absence of memory, i.e., for which transition probability depends only upon the two points involved in the transition and on the corresponding times). This mean velocity will be called the current velocity. Let X be a point of $\mathbb{R}^{6N}$, and $f_N(X,t)$ be the corresponding density at time t. We look for a definition of a "good" mean velocity V(X,t), and we consider therefore all the systems passing through a fixed X at time t. The simplest way to express that a system, which is at X_1 at time t_1 and at X_2 at time t_2 ($t_1 < t < t_2$; $t_2 - t_1 = \Delta t$ is arbitrarily small), is passing through X at time t is to introduce the following linear interpolation :

$$X = X_1 + \eta(X_2 - X_1) \quad , \qquad 0 \leqslant \eta \leqslant 1$$

and thus

$$X_1 = X - \eta Z \quad ; \quad X_2 = X + (1-\eta)Z \quad ; \quad Z = X_2 - X_1 \quad . \qquad \text{(III.1)}$$

It is therefore natural to define the current velocity at (X,t) as the limit, as $\Delta t \to 0$, of the average of $Z/\Delta t$ for all the systems passing through X at time t. We introduced the double-density $f_{2N}(X_1,t_1;X_2,t_2)$ for these systems, i.e., $f_{2N}(X-\eta Z,t_1;X+(1-\eta)Z,t_2)$. The double-density f_{2N} is related to the transition probability density P by

$$f_{2N}(X-\eta Z,t_1;X+(1-\eta)Z,t_2) = f_N(X-\eta Z,t_1)P(X+(1-\eta)Z,t_2|X-\eta Z,t_1) \ . \quad \text{(III.2)}$$

We obtain therefore for the current velocity

$$V(X,t) = \frac{\lim\limits_{\Delta t \to 0} \displaystyle\int_{\mathbb{R}^{6N}} dZ \int_0^1 d\eta \ \frac{Z}{\Delta t} \ f_N(X-\eta Z,t_1)P(X+(1-\eta)Z,t_2|X-\eta Z,t_1)}{\lim\limits_{\Delta t \to 0} \displaystyle\int_{\mathbb{R}^{6N}} dZ \int_0^1 d\eta \ f_N(X-\eta Z,t_1)P(X+(1-\eta)Z,t_2|X-\eta Z,t_1)} \ . \quad \text{(III.3)}$$

Since $\Delta t = t_2 - t_1 \to 0$ implies $P(X+(1-\eta)Z,t_2|X-\eta Z,t_1) \to \delta(Z)$, we note that the denominator in (III.3) is equal to $f_N(X,t)$. Finally, if the notation introduced previously is used, see (II.26,II.27), one obtains

$$V(X,t) = \frac{1}{f_N(X,t)} \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int_{\mathbb{R}^{6N}} dX' \int_0^1 d\eta \ X' \ f_N(X(\eta),t_1)P(X'(\eta),t_2|X(\eta),t_1) . \qquad \text{(III.4)}$$

In order to verify that $V(X,t)$ is the current velocity, i.e., that the Liouville equation

$$\frac{\partial}{\partial t} f_N(X,t) = - \frac{\partial}{\partial X_\alpha} [f_N(X,t) V_\alpha(X,t)]$$

is satisfied, we recall (II.11) which, by using (II.25,II.26), [putting $\phi(X',X) = f_N(X',t_1)P(X,t_2|X',t_1)$], becomes

$$\begin{aligned} \frac{\partial}{\partial t} f_N(X,t) &= - \frac{\partial}{\partial X_\alpha} \left[\lim_{\Delta t \to 0} \frac{1}{\Delta t} \; K_\alpha(X) \right] \\ &= - \frac{\partial}{\partial X_\alpha} \left[f_N(X,t) \frac{1}{f_N(X,t)} \; \lim_{\Delta t \to 0} \frac{1}{\Delta t} \; K_\alpha(X) \right] \\ &= - \frac{\partial}{\partial X_\alpha} [f_N(X,t) V_\alpha(X,t)] \; . \qquad \text{(III.5)} \end{aligned}$$

The physical considerations based on the notion of the current velocity therefore lead to a solution to the inverse Liouville problem for the class of kinetic equations (II.11) ; the solution is given by (III.4).

IV. PARTICULAR CASES OF THE FOKKER-PLANCK EQUATION AND OF THE B-G-K MODEL OF THE BOLTZMANN EQUATION.

In sections II and III, we applied the formalism of the inverse Liouville problem to the kinetic equation (II.13), the solution being given by (II.27), and to the kinetic equation (II.11), the solution being given by (III.4). We did not however explicitly specify the quantities w or P. In this section we shall discuss in more detail two special cases of (II.11) and (II.13), respectively the Fokker-Planck equation and the B-G-K model of the Boltzmann equation.

1°) Fokker-Planck equation.

Let us consider a stochastic process

$$dX(t) = D(X(t),t)dt + dW(t) \quad ; \quad X \in R^{6N}$$

in which D is a regular vector field and W(t) a Wiener process. The transition probability density $P(X'(\eta),t_2|X(\eta),t_1)$ that appears in (III.4) becomes, for small positive $\Delta t = t_2 - t_1$,

$$P(X'(\eta),t_2|X(\eta),t_1) = (2\pi\Delta t)^{-3N} \, (\det[\sigma^2])^{-1/2} \times \dots$$

$$\dots \times \exp\left\{-\frac{1}{2\Delta t}\,([\sigma^2]^{-1})_{\alpha\beta}\left[X'_\alpha - D_\alpha(X(\eta),t_1)\Delta t\right]\left[X'_\beta - D_\beta(X(\eta),t_1)\Delta t\right]\right\} \tag{IV.1}$$

where $\frac{1}{2}[\sigma^2]$ is the symmetric matrix of diffusion (the summation convention being used in (IV.1) : $\alpha,\beta = 1,\dots,6N$). This transition probability density is therefore of the form $p(X',X-\eta X',t_2,t_1)$ and, in the integral (III.4), the quantity $f_N P = f_N p$ can be extended in the neighborhood of X as follows :

$$\begin{aligned} f_N(X-\eta X',t_1)p(X',X-\eta X',t_2,t_1) &= f_N(X,t_1)p(X',X,t_2,t_1) \\ &- \eta\, X'_\alpha \frac{\partial}{\partial X_\alpha}\left[f_N(X,t_1)p(X',X,t_2,t_1)\right] \\ &+ \frac{\eta^2}{2} X'_\alpha \, X'_\beta \frac{\partial^2}{\partial X_\alpha \partial X_\beta}\left[f_N(X,t_1)p(X',X,t_2,t_1)\right] + O(X'_\alpha X'_\beta X'_\gamma) \; . \end{aligned} \tag{IV.2}$$

By inserting (IV.2) into $\int dX' \, X' \, f_N p$, one obtains

$$\begin{aligned} \int_{\mathbb{R}^{6N}} dX' \, X'_\gamma f_N p &= f_N(X,t_1) \int dX' \, X'_\gamma \, p - \eta \frac{\partial}{\partial X_\alpha} f_N(X,t_1) \int dX' \, X'_\gamma X'_\alpha p \\ &+ \frac{\eta^2}{2} \frac{\partial^2}{\partial X_\alpha \partial X_\beta} f_N(X,t_1) \int dX' \; X'_\gamma X'_\alpha X'_\beta \; p + \dots \end{aligned} \tag{IV.3}$$

Taking (IV.1) into account, one can calculate various moments arising in (IV.3) :

$$\int dX' \, X'_\gamma \, p = D_\gamma(X,t_1) \, \Delta t$$

$$\int dX' \, X'_\gamma X'_\alpha \, p = [\sigma^2]_{\gamma,\alpha} \, \Delta t + O(\Delta t)^2$$

$$\int dX' \, X'_\gamma X'_\alpha X'_\beta \, p = O(\Delta t)^2 \; .$$

By introducing these results into (IV.3), one obtains finally for (III.4)

$$V_\alpha(X,t) = D_\alpha(X,t) - \tfrac{1}{2}[\sigma^2]_{\alpha,\beta} \frac{\partial}{\partial X_\beta} \operatorname{Log} f_N(X,t) \quad . \qquad \text{(IV.4)}$$

The current velocity thus obtained is identical to the current velocity associated with Brownian motion. Note, however, that the present derivation of (IV.4) is different from that which is of current use in stochastic mechanics (Nelson, 1967). In the particular case $X = (\underline{r},\underline{v})$ and in the absence of any external field, the current velocity (IV.4) reduces to

$$V_{r,i} = V^-_{r,i} = v_i$$

$$V_{v,i} = V^+_{v,i} = -C\,v_i - A\frac{\partial}{\partial v_i} \operatorname{Log} f(\underline{r},\underline{v},t) \qquad \text{(IV.5)}$$

where C and A are the coefficients of dissipation and diffusion respectively. The corresponding Liouville equation (I.4) becomes identical to the Fokker-Planck equation

$$\frac{\partial}{\partial t} f(\underline{r},\underline{v},t) = \mathcal{R}^-(f) + \mathcal{R}^+(f)$$

$$\mathcal{R}^-(f) = -\,v_i \frac{\partial}{\partial r_i} f(\underline{r},\underline{v},t)$$

$$\mathcal{R}^+(f) = C\,\frac{\partial}{\partial v_i}\,[v_i\, f(\underline{r},\underline{v},t)] + A\,\frac{\partial}{\partial v_i}\frac{\partial}{\partial v_i} f(\underline{r},\underline{v},t) \qquad \text{(IV.6)}$$

The principle of correspondence introduced in section II is satisfied. In fact, at equilibrium, one has

$$f(\underline{r},\underline{v},t) = f^{eq}(\underline{v}) = G\, e^{-\frac{C}{2A}\underline{v}^2} \quad ; \quad G = \text{constant}$$

which implies simultaneously

$$\mathcal{R}^+(f) = 0 \quad \text{and} \quad \underline{V}_v^+ = 0 \quad . \qquad \text{(IV.7)}$$

In the case of the Fokker-Planck equation in $\mathbb{R}^{6N}$, and for a vector field D that is linear in X, it has been shown that the non-conservative part of the quasi-particle dynamics vanishes at equilibrium (Tellez-Arenas, Fronteau and Combis, 1979), which generalizes the result (IV.7).

The current $\underline{j} = f\,\underline{V}_v^+$ corresponding to (IV.5)

$$j_i = - C\, f\, v_i - A \frac{\partial}{\partial v_i} f$$

has already been used by other authors, notably* in (Chandrasekhar, 1943) and in (Trubnikov, 1965). However these authors did not consider the question from the angle of the inverse Liouville problem and furthermore did not envisage the purely dynamical aspect of it, that results from the explicit integration of the differential system. To our knowledge, the study of the statistical evolution in terms of non-conservative trajectories was considered only recently (Combis, Fronteau and Tellez-Arenas, 1979 ; Tellez-Arenas, Fronteau and Combis, 1979).

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*We thank N. Corngold for drawing to the attention of one of us (M.G.) these two references.

Finally, let us consider the simple case of the Fokker-Planck equation in the velocity space, which we will compare to the case of the B-G-K model in section IV.2. The condition leading to equilibrium at temperature T being satisfied, and Boltzmann's constant being taken as unity, the Fokker-Planck equation may be written, in one dimension, as follows :

$$\frac{\partial}{\partial t} f(v,t) = C \frac{\partial}{\partial v} [v f] + \frac{CT}{m} \frac{\partial^2}{\partial v^2} f \quad ; \quad C > 0 \quad . \tag{IV.8}$$

Let us choose, as the initial distribution f(v,0), the distribution corresponding to equilibrium at temperature $T_0 \neq T$:

$$f_0(v) = f(v,0) = \left(\frac{m}{2\pi T_0}\right)^{1/2} \exp\left[-\frac{mv^2}{2T_0}\right] \quad . \tag{IV.9}$$

The solution f(v,t) of the equation (IV.8) may then be written, for $t > 0$,

$$f(v,t) = \left(\frac{m}{2\pi[T + e^{-2Ct}(T_0 - T)]}\right)^{1/2} \exp\left[-\frac{mv^2}{2[T + e^{-2Ct}(T_0 - T)]}\right] \tag{IV.10}$$

and the following dynamics may be deduced from this and (IV.5) :

$$\dot{v} = - C v - \frac{CT}{m} \frac{\partial}{\partial v} \operatorname{Log} f(v,t) \tag{IV.11}$$

$$\dot{v} = - C v \left(1 - \frac{T}{T_0}\right) \frac{e^{-2Ct}}{e^{-2Ct}\left(1 - \frac{T}{T_0}\right) + \frac{T}{T_0}} \quad . \tag{IV.12}$$

It is verified that, in accordance with the principle of correspondence introduced in section II.2, $\dot{v}$ vanishes at thermodynamic equilibrium, either for $T_0 = T$, or for t tending towards infinity when $T_0 \neq T$.

2°) B-G-K model of the Boltzmann equation.

Let us consider the kinetic equation of the B-G-K model (Bhatnagar, Gross and Krook, 1954) in one dimension,

$$\frac{\partial}{\partial t} f(v,t) = \mu \int dv' \, [M(v)f(v',t) - M(v')f(v,t)] \tag{IV.13}$$

where M(v) is the equilibrium distribution at temperature T

$$M(v) = \left(\frac{m}{2\pi T}\right)^{1/2} \exp\left[-\frac{mv^2}{2T}\right] \tag{IV.14}$$

and μ the collision frequency. It is easily verified that the solution may be written*

$$f(v,t) = e^{-\mu t} \, [f_0(v) - M(v)] + M(v) \tag{IV.15}$$

where $f_0(v)$ is the initial distribution, which we choose to be of the form

$$f_0(v) = \left(\frac{m}{2\pi T_0}\right)^{1/2} \exp\left[-\frac{mv^2}{2T_0}\right] \quad . \tag{IV.16}$$

The general results obtained in section II.3 allow us to write the current velocity, in the velocity space, as follows :

$$\dot{v} = \mu \left\{e^{-\mu t}[f_0(v) - M(v)] + M(v)\right\}^{-1} \times$$
$$\times \int_{-\infty}^{+\infty} dv' \int_0^1 d\eta \, v' \, M(v'(\eta)) \left\{e^{-\mu t}[f_0(v(\eta)) - M(v(\eta))] + M(v(\eta))\right\} \tag{IV.17}$$

with $v(\eta) = v - \eta v'$ and $v'(\eta) = v + (1-\eta)v'$. The integral I,

$$I(v') = \int_0^1 d\eta \, M(v'(\eta)) \, f_0(v(\eta))$$

which may be written

$$I(v') = \frac{m}{2\pi(TT_0)^{1/2}} \int_0^1 d\eta \, \exp\left\{-\frac{m}{2}\,[(a\eta + b)^2 + c]\right\} \quad ,$$

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* We thank I. Iscoe for this observation.

$$a = v'\left(\frac{1}{T} + \frac{1}{T_0}\right)^{1/2} \quad , \quad c = \frac{v'^2}{T+T_0}$$

$$b = -\frac{v'}{T\left(\frac{1}{T}+\frac{1}{T_0}\right)^{1/2}} - v\left(\frac{1}{T}+\frac{1}{T_0}\right)^{1/2} \qquad \text{(IV.18)}$$

reduces to the following form :

$$I(v') = \frac{m}{2\pi(TT_0)^{1/2}v'} \exp\left[-\frac{mv'^2}{2(T+T_0)}\right] \int_{-\frac{v'\mathcal{T}}{T}}^{\frac{v'\mathcal{T}}{T_0}} du \exp\left[-\frac{m}{2\mathcal{T}}(u-v)^2\right]$$

$$\mathcal{T} = \frac{TT_0}{T+T_0} \quad . \qquad \text{(IV.19)}$$

In the expression of $v' I(v')$, the integration from $-\frac{v'\mathcal{T}}{T}$ to $\frac{v'\mathcal{T}}{T_0}$ may be accomplished in two domains : from $-\frac{v'\mathcal{T}}{T}$ to $\frac{v'\mathcal{T}}{T}$, and then from $\frac{v'\mathcal{T}}{T}$ to $\frac{v'\mathcal{T}}{T_0}$. The first term thus obtained is an odd function of v', whose contribution to the integral

$$\int_{-\infty}^{+\infty} dv'\, v'\, I(v')$$

is zero. One thus obtains

$$\int_{-\infty}^{+\infty} dv' \int_0^1 d\eta\, v'\, M(v'(\eta))\; f_0(v(\eta)) =$$

$$\frac{m}{2\pi(TT_0)^{1/2}} \int_{-\infty}^{+\infty} dv' \exp\left[-\frac{mv'^2}{2(T+T_0)}\right] \int_{\frac{v'\mathcal{T}}{T}}^{\frac{v'\mathcal{T}}{T_0}} du \exp\left[-\frac{m}{2\mathcal{T}}(u-v)^2\right] \qquad \text{(IV.20)}$$

Let us note that the above integral (IV.20) is zero for $T = T_0$, i.e., for $M = f_0$. Thus the expression (IV.17) of the current velocity $\dot{v}$ (in the velocity space) in fact reduces to the integral term containing the product $M f_0$, with $M \neq f_0$. By introducing the function F,

$$F(y,v) = \int_0^y du \, \exp\left[-\frac{m}{2\mathscr{C}}\,(u-v)^2\right] \quad , \tag{IV.21}$$

the expression (IV.17) may finally be written

$$\dot{v} = \mu\left\{e^{-\mu t}[f_0(v) - M(v)] + M(v)\right\}^{-1} \frac{m\,e^{-\mu t}}{2\pi(TT_0)^{1/2}} \times$$

$$\times \int_{-\infty}^{+\infty} dv' \left[F\left(\frac{v'\mathscr{C}}{T_0}, v\right) - F\left(\frac{v'\mathscr{C}}{T}, v\right)\right] \exp\left[-\frac{mv'^2}{2(T+T_0)}\right] \quad . \tag{IV.22}$$

When T is close to T_0, we may limit ourselves to the first terms of the expansion of the square bracket in (IV.22) :

$$F\left(\frac{v'\mathscr{C}}{T_0}, v\right) - F\left(\frac{v'\mathscr{C}}{T}, v\right) = \left[v'\mathscr{C}\left(\frac{1}{T_0} - \frac{1}{T}\right) - \frac{mv'^2}{2}\,\mathscr{C}\left(\frac{v'\mathscr{C}}{T} - v\right)\left(\frac{1}{T_0} - \frac{1}{T}\right)^2 + \dots\right] \times$$

$$\times \exp\left[-\frac{m}{2\mathscr{C}}\left(\frac{v'\mathscr{C}}{T} - v\right)^2\right] . \tag{IV.23}$$

By including these terms in (IV.22), one obtains for the term in v, in first order in $T-T_0$,

$$\dot{v} \simeq -\frac{\mu}{2}\, v\left(1 - \frac{T}{T_0}\right) \frac{e^{-\mu t}}{e^{-\mu t}\left[1 - \frac{M(v)}{f_0(v)}\right] + \frac{M(v)}{f_0(v)}} \quad . \tag{IV.24}$$

Note that the expression (IV.24) of the current velocity (in the velocity space), associated with the B-G-K model of the Boltzmann equation, has the same structure as the corresponding expression (IV.12) associated with the Fokker-Planck equation. This analogy may in fact be carried even further. Indeed, it is easily verified that the relation (IV.24) may identically be written in the form

$$\dot{v} \simeq -\frac{\mu}{2}\, v - \frac{\mu T}{2m} \frac{\partial}{\partial v} \operatorname{Log} f(v,t) \tag{IV.25}$$

which is the form (IV.11), with $C = \frac{\mu}{2}$.

V. CONCLUDING REMARKS.

We have succeeded in solving the inverse Liouville problem for a general class (II.11) of kinetic equations expressing a gain-loss balance. We have arrived at the same solution by, firstly, using the mathematical aspect of the Irving-Kirkwood method and, secondly, by following the physical intuition of a current velocity. We have used this general solution (III.4) in two different situations : on the one hand, by postulating the existence of a transition probability density per unit of time, which corresponds to the Boltzmann type equations*, and, on the other hand, by using the explicit form of the Wiener transition probability density, which corresponds to the Fokker-Planck type equations. One of the essential properties of the solution (III.4) is that it leads, in the cases studied, to quasi-particle dynamics which satisfy what we have called the principle of correspondence : when statistical equilibrium is reached, these dynamics become conservative.

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*The case of the Enskog equation is published separately by one of us in (Grmela, 1980).

On the other hand, the physical interpretation of V obtained in section III together with the intuition associated with particle dynamics might suggest an interesting new V and then, via the general Liouville equation (I.4), lead to new extended kinetic equations. We have not yet systematically investigated this possible use of the quasi-particle view of kinetic equations. Another possible use of (I.3), mentioned in section I, is to obtain solutions, or at least some qualitative properties of solutions, to (I.1). An obvious iteration method arises. We start with some $f^{(1)}(\underline{r},\underline{v},t)$ satisfying the given initial condition. By using $f^{(1)}$, we calculated V in (I.3). The equations (I.3) are now standard ordinary differential equations that can be solved, at least in principle. The solution has to be obtained for all initial values $(\underline{r}_0,\underline{v}_0)$. Supposing this step (in principle standard but, in practice, difficult) has been realized, we also have immediately (by the method of characteristics) a solution, that we denote $f^{(2)}$, to (I.4). Everything can now be repeated with $f^{(2)}$ replacing $f^{(1)}$. One can hope that this iterative process converges to a solution to (I.1).

Although only some of the consequences of the inverse Liouville problem (as presented here) have been developed, it seems to us that the results obtained may lead to progress in statistical physics, as much in the field of general ideas as in the field of calculation techniques.

APPENDIX

The expression "Liouville equation" is often used in the literature of Physics ; its meaning however varies from one author to another. In this appendix we intend to explain the meaning that we associate with the expression "Liouville equation" and recall its historical context.

Liouville in his paper (Liouville, 1838) proved the following theorem : given a system of ordinary differential equations

$$\frac{dX}{dt} = V(X,t) \quad ; \quad X = (X_1,X_2,\ldots,X_n) \in \mathbb{R}^n \qquad (A.1)$$

the Jacobian $J_t = D(X_t)/D(X_{t_0})$, [where by $X_t = X(t,X_{t_0})$ we denote that trajectory, passing through X_{t_0} at time t_0, which is determined by (A.1)], evolves in time according to[*]

$$\frac{d}{dt} \operatorname{Log}|J_t| = \frac{\partial}{\partial X_\alpha} V_\alpha \quad ; \quad \alpha = 1,\ldots,n \quad , \qquad (A.2)$$

the right hand side being evaluated at X_t. Liouville in his paper did not specify V (except by the obvious regularity conditions). Because of the prevalence of interest of physicists in conservative systems, the meaning of the "Liouville theorem" became associated only with a special case of the Liouville result, namely the case when $\frac{\partial}{\partial X_\alpha} V_\alpha = 0$ (i.e., for example, the case of Hamiltonian systems). Gibbs in his fundamental book (Gibbs, 1902) did not make any reference to Liouville's original paper. To our knowledge, the first reference to Liouville's paper in the context of statistical mechanics appears in (Tolman, 1938). Different

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[*] Liouville proved in fact a slightly more general result, since his theorem is related to the solution written in terms of integration constants and not in terms of initial conditions.

authors (Guiaşu, 1966 ; Gerlich, 1973) recently rederived the original Liouville result, and introduced it under the name "generalized Liouville theorem". In 1965, one of us (Fronteau, 1965), pointed out the true meaning of the theorem. In the mathematical literature however, this theorem was not completely forgotten (see, for example, Arnold, 1974, p.196).

By using the Liouville theorem, one can introduce the description of the time evolution generated by (A.1) in the context of statistical mechanics. We introduce a density f such that

$$f(X_t,t) \geqslant 0 \qquad (A.3)$$

$$f(X_t,t)\, dX_t = f(X_{t_0},t_0)\, dX_{t_0} \quad \text{, for all } t, \qquad (A.4)$$

where dX_t is an element of volume around a moving point X_t, and $f(X_t,t)$ is the density at that point. The relation (A.4), which expresses the absence of creation or annihilation of states (or equivalently the conservation of probability), can be also written

$$f(X_t,t)|J_t| = \text{constant}, \quad \text{for all } t \;. \qquad (A.5)$$

The equation (A.2) is therefore equivalent (if (A.5) is used) to

$$\frac{d}{dt} \operatorname{Log} f = - \frac{\partial}{\partial X_\alpha} V_\alpha \qquad (A.6)$$

$$\frac{\partial}{\partial t} f + \frac{\partial}{\partial X_\alpha} (f\, V_\alpha) = 0 \quad . \qquad (A.7)$$

In the particular case where $\frac{\partial}{\partial X_\alpha} V_\alpha = 0$, (A.7) reduces to the familiar form

$$\frac{\partial f}{\partial t} + V_\alpha \frac{\partial}{\partial X_\alpha} f = 0 \quad . \qquad (A.8)$$

Note that the relation (A.7), which is the evolution law for density, is referred to by several authors as the "continuity equation" or the "generalized

Liouville equation". In fact, as shown in this appendix, the term "generalized" is not appropriate. We propose to refer to (A.7) as the "general Liouville equation", or briefly "Liouville equation".

Independently of the Liouville theorem, another type of association between (A.1) and a partial differential equation of type (A.8) has been introduced in (Koopman, 1931 ; Carleman, 1932). Consider (A.1) as being autonomous (i.e., V independent of time). The flow generated by (A.1) is denoted $X_0 \to u_t X_0 = X_t$. Let φ be a real-valued function defined in $\mathbb{R}^n$. The flow u_t induces naturally a flow $\varphi_0 \to \varphi_t = U_t \varphi_0$, where φ_t is defined by

$$\varphi_t(X) = \varphi_0(u_{-t}(X)) \quad , \qquad \forall\, X \in \mathbb{R}^n \quad . \tag{A.9}$$

Note that $\varphi_t(X)$ has previously been written as $f(X,t)$. Now, if (A.9) is differentiated with respect to time, the equation (A.8) is recovered. Thus the equation obtained by Koopman and Carleman is identical to the Liouville equation corresponding to the case $\frac{\partial}{\partial X_\alpha} V_\alpha = 0$ (for instance, Hamiltonian systems). We note that (A.9) is the density conservation relation. However, if we want to use the more general condition, which states that there is neither creation nor annihilation, we must replace the density $\varphi(X_1,\dots,X_n)$ by the n-form

$$\varphi(X_1,\dots,X_n)\ dX_1\ \dots\ dX_n \quad .$$

Using the same type of induction introduced by Koopman and Carleman, the equation (A.7) is then recovered. This is the basis of a demonstration recently proposed by (Steeb, 1979).

It is well known that the Hamilton equations, which are a particular case of (A.1), and (A.8), constitute the framework of conservative statistical mechanics. The difficulties arising in attempts to understand the observed macroscopic time-irreversible evolution in this context are also well known. In order to contribute to this problem some authors have tried to change the framework by replacing the Hamilton equations by more general dynamical equations (A.1). To the Hamiltonian vector field was added firstly a traditional representation of friction (Chandrasekhar, 1943 ; Guiaşu, 1966 ; Fronteau, 1965 ; ....) and then a term representing diffusion (Chandrasekhar, 1943 ; Trubnikov, 1965 ; Fronteau, 1975 ; Salmon, 1975 ;....). The non-conservative dynamics, which are thus introduced, induce a new algebraic structure for statistical mechanics : the current Lie-structure, that is adapted to (A.8), becomes a Lie-admissible structure which is now adapted to (A.7). (Fronteau, Tellez-Arenas and Santilli, 1979).

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INVESTIGATION OF GENERALIZED LIOUVILLE EQUATION

G.A. Rudykh

The properties of a generalized Liouville operator and the propagator corresponding to it are studied in an appropriately chosen function space. The Hille–Yosida theorem is used to prove that the generalized Liouville operator is an infinitesimal generating operator of a strongly continuous, unique semigroup. The conditions under which this semigroup is contractive are considered.

Introduction

The paper is devoted to investigation of the generalized Liouville equation [1]

$$\frac{\partial f(q,p,t)}{\partial t} = L(t) f(q,p,t), \tag{1}$$

where

$$L(t)\cdot = (\mathscr{H}_n(t) - \mathscr{L}_n(t))\cdot = [H(q,p,t),\cdot] - \sum_{i=1} \frac{\partial}{\partial p_i}\{Q_i^*(q,p,t)\cdot\} \tag{2}$$

is the generalized Liouville operator, n is the number of degrees of freedom of the mechanical system, $q \overset{\Delta}{=} (q_1,\dots,q_n)$ is the vector of the generalized coordinates, $p \overset{\Delta}{=} (p_1,\dots,p_n)$ is the conjugate vector of the generalized momenta, $f(q,p,t)$ is the density distribution function, $H(q,p,t)$ is the Hamiltonian of the mechanical system, $[\cdot,\cdot]$ is the Poisson brackets, and $Q_i^*(q,p,t)$ are nonpotential forces.

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1. Choice of the Function Space

DEFINITION 1. The space Γ of a mechanical system with n degrees of freedom is an open, connected subset of $\mathcal{R}^{2n}$ equipped with a Lebesgue measure, $\mu(\Gamma) < \infty$, whose components are the n generalized coordinates and n conjugate momenta.

DEFINITION 2. The space Γ^t of a mechanical system with n degrees of freedom is an open, connected subset of $\mathcal{R}^{2n+1}$ equipped with a Lebesgue measure, $\mu(\Gamma^t) < \infty$, whose components are the n generalized coordinates, the conjugate momenta, and the time t. We shall denote a point in Γ and Γ^t by $x \overset{\Delta}{=} (q, p)$ and (x, t), respectively. If not stated otherwise, we shall assume that Γ and Γ^t are bounded subsets. The cylinder $G_{a,b} = \Gamma \times (a, b)$ is the set of points $(x, t) \in \Gamma^t, x \in \Gamma, t \in (a, b)$. Let $L_2(\Gamma)$ be a separable real Hilbert space. When investigating the differential evolution equation (1) it is convenient to consider two spaces: $L_2(a, b; L_2(\Gamma))$, which is a L_2 space over the Hilbert space $L_2(\Gamma)$, and the Sobelev space $W_2^1(G_{a,b})$. $L_2(a, b; L_2(\Gamma))$ is the space of classes of functions φ that are square summable on $[a, b]$, with values in $L_2(\Gamma)$. The scalar product and norm in this space are determined in accordance with

$$(\varphi, \psi)_{L_2(a, b; L_2(\Gamma))} = \int_a^b (\varphi, \psi)_{L_2(\Gamma)}\, dt, \quad \|\varphi\|_{L_2(a, b; L_2(\Gamma))} = \left(\int_a^b \|\varphi\|^2_{L_2(\Gamma)}\, dt\right)^{1/2} < \infty.$$

The space $L_2(a, b; L_2(\Gamma))$ is a complete separable Hilbert space. The space $W_2^1(G_{a,b})$, equipped with the norm

$$\|\varphi\|_{W_2^1(G_{a,b})} = \left(\int_{G_{a,b}} \varphi^2\, dx\, dt\right)^{1/2} + \left(\int_{G_{a,b}} \left[\left(\frac{\partial\varphi}{\partial t}\right)^2 - \sum_{i=1}^{2n} \left(\frac{\partial\varphi}{\partial x_i}\right)^2\right] dx\, dt\right)^{1/2},$$

is also a Hilbert space. Its elements are functions that belong to $L_2(a, b; L_2(\Gamma))$ and have partial derivatives of first order with respect to all the variables and time that also belong to $L_2(a, b; L_2(\Gamma))$.

We denote by $\{W_2^1, L_2\}$ the set of linear bounded operators mapping from $W_2^1(G_{a,b})$ to $L_2(a, b; L_2(\Gamma))$. Since $W_2^1(G_{a,b})$ and $L_2(a, b; L_2(\Gamma))$ are Banach spaces, $\{W_2^1, L_2\}$ is also a Banach space with the norm

$$\|S\|_{W_2^1 \to L_2} = \sup_{\substack{\varphi \in W_2^1(G_{a,b}) \\ \varphi \neq 0}} \frac{\|S\varphi\|_{L_2(a, b; L_2(\Gamma))}}{\|\varphi\|_{W_2^1(G_{a,b})}}.$$

By $C_0^\infty(a, b; L_2(\Gamma))$ we denote the space of functions that are infinitely differentiable on $[a, b]$ and take values in $L_2(\Gamma)$ with compact supports in Γ.

2. Theorem: The Class $C_0^\infty(a, b; L_2(\Gamma))$ Is Dense in the Space $L_2(a, b; L_2(\Gamma))$

The linear differential operator (2) is in the general case unbounded because there are differentiation operators in the Poisson brackets. Therefore, on the basis of the specific properties of Eq. (1), we shall regard the generalized Liouville operator as an operator mapping from the class $C_0^\infty(a, b; L_2(\Gamma))$ into the space $L_2(a, b; L_2(\Gamma))$. In what follows, we shall denote the class $C_0^\infty(a, b; L_2(\Gamma))$ and the space $L_2(a, b; L_2(\Gamma))$ by $C_0^\infty(\cdot)$ and $L_2(\cdot)$, respectively. The aim of the present section is to prove that the class $C_0^\infty(\cdot)$ is dense in the space $L_2(\cdot)$. We first prove the following proposition, which is a generalization of Lebesgue's lemma [2].

PROPOSITION 1. If the function $\varphi(x, t) \in L_2(\;)$, $-\infty < a < t < b < \infty$, then for every $\varepsilon > 0$ there exists $\delta > 0$ such that for $|h| < \delta$ the inequality $\|\varphi(x+h, t+h) - \varphi(x, t)\|_{L_2(\cdot)} < \varepsilon$ holds.

Proof. Without loss of generality, as in the proof in [2], we shall assume that a and b are finite, and the function $\varphi(x, t)$ is bounded. Then for every $\varepsilon_1 > 0$ there exists a step function $\psi(x, t)$ such that

$$\int_a^b \int_\Gamma |\varphi(x, t) - \psi(x, t)|^2\, d\Gamma\, dt < \varepsilon_1. \tag{2.1}$$

Applying the Minkowski inequality to the expression

$$\|\varphi(x+h, t+h) - \varphi(x, t)\|_{L_2(\cdot)} = \left(\int_a^b \int_\Gamma |\varphi(x+h, t+h) - \varphi(x, t)|^2\, d\Gamma\, dt\right)^{1/2},$$

we readily find that

$$\|\varphi(x+h,t+h)-\varphi(x,t)\|_{L_2(\cdot)}\leq\int_a^b\int_\Gamma|\psi(x+h,t+h)-\psi(x,t)|^2\,d\Gamma\,dt+\int_a^b\int_\Gamma|\varphi(x+h,t+h)-\psi(x+h,t+h)|^2\,d\Gamma\,dt+$$

$$\int_a^b\int_\Gamma|\varphi(x,t)-\psi(x,t)|^2\,d\Gamma\,dt, \tag{2.2}$$

and

$$\int_a^h\int_\Gamma|\psi(x+h,t+h)-\psi(x,t)|^2\,d\Gamma\,dt\to0 \text{ (as } h\to0),$$

$$\int_a^b\int_\Gamma|\varphi(x+h,t+h)-\psi(x+h,t+h)|^2\,d\Gamma\,dt<\varepsilon_1 \text{ (as } h\to0 \text{ and by virtue of (2.1))}$$

$$\int_a^b\int_\Gamma|\varphi(x,t)-\psi(x,t)|^2\,d\Gamma\,dt<\varepsilon_1.$$

Thus. the inequality (2.2) is transformed to $\|\varphi(x+h, t+h)-\varphi(x,t)\|_{L_2(\cdot)}<2\varepsilon_1=\varepsilon$, which proves the proposition.

THEOREM 1. The class $C_0^\infty(\cdot)$ is dense in the space $L_2(\cdot)$.

Proof. It is necessary to show that for arbitrary function $\varphi\in L_2(\cdot)$ there exists a sequence of functions $\{\psi_k\}_{k=1}^\infty\in C_0^\infty(\cdot)$ for which the strong convergence $\varphi=\operatorname{s-lim}_{k\to\infty}\psi_k$ holds in the norm in $L_2(\cdot)$. We consider the case when $a=-\infty$, $b=+\infty$, when $C_0^\infty(\cdot)$ is identical to $C_0^\infty(R_+^1;L_2(\Gamma))$, where by R_+^1 we denote the time space $(-\infty\leq t\leq\infty)$. Suppose the function $f(t)\in C_0^\infty(R_+^1)$ and $f(t)$ has the properties

$$f(t)\geq0;\quad\int_{R_+^1}f(t)\,dt=1;\quad\operatorname{supp}(f)\equiv\{t\in R_+^1;\ |t|<1\};\quad f(t)=0\quad\text{for }|t|\geq1. \tag{2.3}$$

We shall approximate the function $\varphi\in L_2(R_+^1;L_2(\Gamma))$ by Steklov-averaged functions of the form

$$f_h*\varphi=\varphi_h=\int_{R_+^1}f_h(t-s)\varphi(s)\,ds, \tag{2.4}$$

where $h>0$ is a parameter, and $f_h(t)=\frac{1}{h}f\left(\frac{t}{h}\right)$ is the kernel of the averaging. It is readily verified that $f_h(t)$ satisfies all the conditions (2.3) and at the same time is a function with compact support; further, the last equation holds for $|t|\geq h$. We consider the expression

$$\varphi_h-\varphi=\int_{|s|<h}f_h(s)\{\varphi(t-s)-\varphi(t)\}\,ds,$$

which. using (2.3) and the Hölder inequality, we can transform to

$$|\varphi_h-\varphi|^2\leq\left(\int_{|s|<h}f_h(s)|\varphi(t-s)-\varphi(t)|^2\,ds\right)^{1/2}\leq\int_{|s|<h}f_h(s)|\varphi(t-s)-\varphi(t)|^2\,ds. \tag{2.5}$$

We introduce

$$\rho(h)=\sup_{|s|<h}\int_{R_+^1}|\varphi(t+s)-\varphi(t)|^2\,dt, \tag{2.6}$$

which. as is readily shown (see Proposition 1), tends to zero as $h\to0$. Integrating (2.5) over R_+^1, applying Fubini's theorem, and using (2.6), we obtain

$$\|\varphi_h-\varphi\|^2_{L_2(R_+^1;L_2(\Gamma))}\leq\int_{|s|<h}f_h(s)\,ds\int_{R_+^1}|\varphi(t+s)-\varphi(t)|^2\,dt\leq\rho(h)\to0.$$

Thus. for the sequence of functions (2.4) the strong convergence $\varphi=\operatorname{s-lim}_{h\to0}\varphi_h$ in the norm holds in $L_2(R_+^1;L_2(\Gamma))$. On the other hand. each of the functions in this sequence is infinitely differentiable [3] and maps R_+^1 into $L_2(\Gamma)$. Finally, to prove the theorem, we consider the sequence of functions $\psi_k(t)=\psi(t/k)$, where $\psi\in C_0^\infty(R_+^1)$ and φ satisfies all the conditions (2.3). Since each of the functions (2.4) is infinitely differentiable and maps R_+^1 into $L_2(\Gamma)$, it is readily seen that $\{\psi_k\varphi_h\}_{k,h=1}^{\infty}\in C_0^\infty(R_+^1; L_2(\Gamma))$. Similarly, as above, it can be shown that

$$\lim_{\substack{k\to\infty\\ h\to\infty}}\|\psi_k\varphi_h-\varphi\|_{L_2(R_+^1;\, L_2(\Gamma))}=0,$$

which proves the theorem.

COROLLARY 1. The generalized Liouville operator $L: C_0^\infty(\cdot)\to L_2(\cdot)$ is densely defined.

3. Investigation of the Generalized Liouville Operator

We consider the Cauchy problem for the generalized Liouville equation (1),

$$\frac{\partial f(q,p,t)}{\partial t}=L(t)f(q,p,t),\quad f(q,p,t)|_{t=t_0}=f_0(q,p), \tag{3.1}$$

where $f_0(q,p)\in C_0^\infty(\Gamma)$; $f\in C_0^\infty(\cdot)$. As noted above, the operator (2) is in the general case unbounded. However, in appropriately chosen function spaces

PROPOSITION 2. The generalized Liouville operator L: $W_2^1(G_{a,b})\to L_2(\cdot)$ belongs to the set $\{W_2^1, L_2\}$.

Proof. If we can prove the validity of the inequality

$$\|Lf(q,p,t)\|^2_{L_2(\cdot)}\leqslant M^2\cdot\|f(q,p,t)\|^2_{W_2^1(G_{a,b})}, \tag{3.2}$$

in which M does not depend on the choice of the function $f(q,p,t)\in W_2^1(G_{a,b})$, then it will yield

$$\|Lf(q,p,t)\|_{L_2(\cdot)}\leqslant M\cdot\|f(q,p,t)\|_{W_2^1(G_{a,b})}. \tag{3.3}$$

Using (2), we obtain

$$\|Lf\|^2_{L_2(\cdot)}=\int_a^b\int_\Gamma (Lf)^2\,d\Gamma\,dt\leqslant\int_a^b\int_\Gamma\Big\{\Big|\sum_{i=1}^n\Big(\frac{\partial H}{\partial q_i}-Q_i^*\Big)\frac{\partial f}{\partial p_i}\Big|^2+\Big|\sum_{i=1}^n\frac{\partial H}{\partial p_i}\,\frac{\partial f}{\partial q_i}\Big|^2+$$

$$f^2\Big|\sum_{i=1}^n\frac{\partial Q_i^*}{\partial p_i}\Big|^2+2\Big|\sum_{i=1}^n\Big(\frac{\partial H}{\partial q_i}-Q_i^*\Big)\frac{\partial f}{\partial p_i}\Big|\,\Big|\sum_{i=1}^n\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i}\Big|+2\Big|\sum_{i=1}^n\Big(\frac{\partial H}{\partial q_i}-Q_i^*\Big)\frac{\partial f}{\partial p_i}\Big|\,\Big|f\sum_{i=1}^n\frac{\partial Q_i^*}{\partial p_i}\Big|+$$

$$2\Big|\sum_{i=1}^n\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i}\Big|\,\Big|f\sum_{i=1}^n\frac{\partial Q_i^*}{\partial p_i}\Big|\Big\}\,d\Gamma\,dt.$$

We introduce

$$A=\max_{(q,p,t)\in G_{a,b}}\Big\{\frac{\partial H}{\partial p_i};\ \Big(\frac{\partial H}{\partial q_i}-Q_i^*\Big);\ \sum_{i=1}\frac{\partial Q_i^*}{\partial p_i}\Big\}. \tag{3.4}$$

Using (3.4) and making some simple manipulations, we obtain

$$\|Lf\|^2_{L_2(\cdot)}\leqslant 7A^2\int_a^b\int_\Gamma\Big\{f^2+\sum_{i=1}^n\Big[\Big(\frac{\partial f}{\partial q_i}\Big)^2+\Big(\frac{\partial f}{\partial p_i}\Big)^2\Big]+\Big(\frac{\partial f}{\partial t}\Big)^2\Big\}d\Gamma\,dt\leqslant M^2\,\|f\|^2_{W_2^1(G_{a,b})}.$$

Thus, we have proved the validity of (3.2) and, therefore, (3.3) as well.

PROPOSITION 3. If the generalized Liouville operator (2) is defined on the subset $D(L)=C_0^\infty(\cdot)$ of the Hilbert space $L_2(\cdot)$ and maps into $L_2(\cdot)$, then:

1) the adjoint operator L^* has the form

$$L^*=-[H(q,p,t),\cdot\,]+\sum_{i=1}^n Q_i^*(q,p,t)\frac{\partial\,\cdot}{\partial p_i} \tag{3.5}$$

and is closed;

2) L admits closure (can be closed).

Proof. Since L is densely defined, there exists a unique operator L^* that is the adjoint of L; it is determined by the condition $(L\varphi,\psi)_{L_2(\cdot)}=(\varphi,L^*\psi)_{L_2(\cdot)}$, where $\varphi\in D(L)$; $\psi\in D(L^*)$. At the same time, $D(L^*)$ consists of all $\psi\in L_2(\cdot)$ for which the linear functional $\varphi\to(L\varphi,\psi)_{L_2(\cdot)}$ is continuous on D(L). Integrating the left-hand side of the last expression by parts and bearing in mind that the functions φ and ψ vanish outside the compact subset $K \subset \Gamma$, we obtain (3.5). On the other hand, because L is densely defined, it follows from [3] that the operator L^* is closed. Before we turn to the proof of 2), we show that $D(L^*)$ is dense. In accordance with Theorem II.4 of Riesz [4], the dual Hilbert space $L_2^*(\cdot)$ is isomorphic to $L_2(\cdot)$, and therefore, $D(L) \subset D(L^*)$ and $D(L^*)$ is dense, since $D(L)$ is. Thus, $D(L^*)$ is not empty. Suppose the sequence $\{x_k\}_{k=1}^{\infty} \in D(L)$ and $\operatorname{s-lim}\limits_{k\to\infty} x_k=0$, $\operatorname{s-lim}\limits_{k\to\infty} Lx_k=y$; then $\lim\limits_{k\to\infty}(Lx_k, \varphi)_{L_2(\cdot)}=\lim\limits_{k\to\infty}(x_k, L^*\varphi)_{L_2(\cdot)}$, for arbitrary element $\varphi \in D(L^*)$. On the one hand, we have $\lim\limits_{k\to\infty}(x_k, L^*\varphi)_{L_2(\cdot)}=0$, and on the other $\lim\limits_{k\to\infty}(Lx_k, \varphi)_{L_2(\cdot)}=(y, \varphi)_{L_2(\cdot)}$. Since φ is an arbitrary element in the domain of definition of the adjoint operator, combining the last two limiting relations we find that $y = 0$, which proves Proposition 2.

COROLLARY 2. The operator L^* is densely defined.

THEOREM 2. The generalized Liouville operator $L\colon C_0^\infty(\cdot)\to L_2(\cdot)$ is a closed operator.

Proof. Since $D(L^*)$ is dense, we can introduce the operator $L^{**} = (L^*)^*$, which is the only operator that is the adjoint of L^*. We find L^{**} from the relation $(L^*\varphi, \psi)_{L_2(\cdot)}=(\varphi, L^{**}\psi)_{L_2(\cdot)}$, where $\varphi\in D(L^*)$, $\psi\in D(L^{**})$. Using (3.5) and integrating the left-hand side of the preceding expression by parts, and noting also that the functions φ and ψ vanish outside the compact subset $K \subset \Gamma$, we conclude that $L^{**} = L$. But if an operator L satisfies $L = L^{**}$, then it is closed [3].

PROPOSITION 4. The operator L^*L with domain of definition $D(L^*L)=\{\varphi\in D(L)\colon L\varphi\in D(L^*)\}$ is self-adjoint and positive if and only if $\sigma(L^*L)\subset[0, \infty)$.

Proof. By Theorem 2, $(L^*L\varphi, \psi)_{L_2(\cdot)}=(L\varphi, L^{**}\psi)_{L_2(\cdot)}=(\varphi, L^*L\psi)_{L_2(\cdot)}$, i.e., $L^*L=(L^*L)^*$.

Necessity. We show that negative eigenvalues of the operator L^*L do not belong to its spectrum. Now the spectrum $\sigma(L^*L)$ of a self-adjoint operator lies on the real axis and if $-\lambda\notin\sigma(L^*L)$, is to hold it is necessary and sufficient that

$$\|(L^*L+\lambda I)\varphi\|_{L_2(\cdot)}\geqslant c\|\varphi\|_{L_2(\cdot)}, \tag{3.6}$$

where $c=\text{const}$; $\varphi\in D(L^*L)$. Suppose $(L^*L\varphi, \varphi)_{L_2(\cdot)}\geqslant 0$ and $\lambda > 0$; then, multiplying both sides of the equation $L^*L\varphi = \lambda\varphi$ scalarly by φ, we obtain $(\lambda\varphi, \varphi)_{L_2(\cdot)}=\lambda\|\varphi\|^2_{L_2(\cdot)}\leqslant(L^*L\varphi, \varphi)_{L_2(\cdot)}+(\lambda I\varphi, \varphi)_{L_2(\cdot)}=((L^*L+\lambda I)\varphi, \varphi)_{L_2(\cdot)}\leqslant \|(L^*L+\lambda I)\|_{L_2(\cdot)}\|\varphi\|_{L_2(\cdot)}$.

The relation (3.6) follows from the last expression, which proves the necessity.

Sufficiency. If $\sigma(L^*L)\subset[0, \infty)$, then the self-adjoint operator L^*L has the spectral resolution

$$(L^*L\varphi, \varphi)_{L_2(\cdot)}=\int\limits_{\sigma(L^*L)}\lambda\, dE_{\varphi,\varphi}, \tag{3.7}$$

where $E_{\varphi,\varphi}=(E_\lambda\varphi, \varphi)_{L_2(\cdot)}$; E_λ is an orthogonal projection operator which depends on the real parameter λ. Since each of the functions $E_{\varphi,\varphi}=(E_\lambda\varphi, \varphi)_{L_2(\cdot)}=(E_\lambda^2\varphi, \varphi)_{L_2(\cdot)}=(E_\lambda\varphi, E_\lambda^*\varphi)_{L_2(\cdot)}=\|(E_\lambda\varphi\|^2_{(L_2\cdot)}\geqslant 0$ and $\lambda > 0$, we conclude from (3.7) that $(L^*L\varphi, \varphi)_{L_2(\cdot)}\geqslant 0$.

COROLLARY 3. The generalized Liouville operator (2) has the polar decomposition $L=U\cdot(L^*L)^{1/2}=U\cdot|L|$, which follows from Theorem 2 and Proposition 4.

Here, $|L|$ is a positive self-adjoint operator, and U is partly isometric. Note that a polar representation of the generalized Liouville operator was used in [5] to find a formal solution of Eq. (1) by means of a Schmidt expansion. Consider the equation

$$L\varphi-\lambda\varphi=(L-\lambda I)\varphi=\psi, \tag{3.8}$$

where λ is a real parameter; $\varphi\in D(L)=C_0^\infty(\cdot)$; $\psi\in R(L)=L_2(\cdot)$. We have the mapping

$$L-\lambda I=L_\lambda\colon D(L)\to(L-\lambda I)D(L). \tag{3.9}$$

The values of the parameter λ for which the equation $(L - \lambda I)\varphi = 0$ has a solution (apart from the trivial $\varphi = 0$) are called the eigenvalues of the generalized Liouville operator. Suppose that for some λ the operator $L - \lambda I$ has an inverse,

$$(L-\lambda I)^{-1}=R_\lambda, \tag{3.10}$$

which is called the resolvent of L. If (3.9) is a one-to-one mapping, then the operator $L - \lambda I$ has the inverse (3.10), and

$$(L-\lambda I)^{-1}\colon (L-\lambda I)D(L)\to D(L). \tag{3.11}$$

The values of the parameter λ for which the operator (3.10) exists, is bounded, and defined everywhere on R(L) are called the resolvent values of the generalized Liouville operator.

PROPOSITION 5. If λ is not an eigenvalue of L, then (3.9) is a one-to-one mapping, an inverse operator $(L-\lambda I)^{-1}$, which acts in accordance with (3.11), exists, and it satisfies

$$\|(L-\lambda I)^{-1}\|_{L_2(\cdot)} \leqslant \alpha/(\lambda-\gamma), \quad \lambda>\gamma, \tag{3.12}$$

where α and γ are constants.

Proof. Since λ does not belong to the point spectrum of L, we can define for this last the inverse $(L-\lambda I)^{-1}$. Consider the expression $\|(L-\lambda I)\varphi\|^2_{L_2(\cdot)}$, which satisfies $\|(L-\lambda I)\varphi\|^2_{L_2(\cdot)} = \|L\varphi\|_{L_2(\cdot)} - \lambda\cdot(\varphi, (L^*+L)\varphi)_{L_2(\cdot)} + \lambda^2\|\varphi\|^2_{L_2(\cdot)}$. By virtue of (2) and Proposition 3,

$$\|(L-\lambda I)\varphi\|^2_{L_2(\cdot)} \geqslant \lambda^2\|\varphi\|^2_{L_2(\cdot)} + \lambda(\varphi, \varphi\chi)_{L_2(\cdot)}, \tag{3.13}$$

where

$$\chi(q,p,t) = \sum_{i=1}^{n} \frac{\partial Q_i^*(q,p,t)}{\partial p_i}. \tag{3.14}$$

We introduce the notation

$$\chi^* = \sup_{(q,p,t)\in\Gamma\times(a,b)} \chi(q,p,t), \quad \chi_* = \inf_{(q,p,t)\in\Gamma\times(a,b)} \chi(q,p,t), \tag{3.15}$$

where $0<a\leqslant t\leqslant b<\infty$, and consider three cases.

1. $\chi_* < 0$. Then it follows from (3.13) that $\|(L-\lambda I)\varphi\|^2_{L_2(\cdot)} \geqslant \lambda^2\|\varphi\|^2_{L_2(\cdot)} + \lambda B\|\varphi\|^2_{L_2(\cdot)}$, where $B=\chi_*<0$. It is readily seen that $\|(L-\lambda I)\varphi\|_{L_2(\cdot)} \geqslant (\lambda^2+\lambda B)\|\varphi\|^2_{L_2(\cdot)} \geqslant (\lambda+B)^2\|\varphi\|^2_{L_2(\cdot)}$. Finally,

$$\|(L-\lambda I)\varphi\|_{L_2(\cdot)} \geqslant (\lambda+B)\|\varphi\|_{L_2(\cdot)}, \quad \lambda+B>0. \tag{3.16}$$

2. The function $\chi(q, p, t) \geq 0$ everywhere in the region $\Gamma\times(a, b)$. In this case, it follows from (3.13) that

$$\|(L-\lambda I)\varphi\|_{L_2(\cdot)} \geqslant \lambda\|\varphi\|_{L_2(\cdot)}, \quad \lambda>0. \tag{3.17}$$

3. $\chi_* > 0$. On the basis of (3.13), we have $\|(L-\lambda I)\varphi\|^2_{L_2(\cdot)} \geqslant \lambda^2\|\varphi\|^2_{L_2(\cdot)} + \lambda\tilde{B}\|\varphi\|^2_{L_2(\cdot)}$, where $\tilde{B} = \chi_* > 0$. Using the inequality $(\lambda^2+\lambda\tilde{B})^{1/2} \geqslant (\lambda+\tilde{B})/\sqrt{2}$, which holds for $\lambda \geq \tilde{B}$, we find that

$$\|(L-\lambda I)\varphi\|_{L_2(\cdot)} \geqq \frac{\lambda+\tilde{B}}{\sqrt{2}}\|\varphi\|_{L_2(\cdot)}, \quad \lambda>0. \tag{3.18}$$

On the other hand, it follows from the obvious inequality $\|\varphi\|_{L_2(\cdot)} = \|(L-\lambda I)^{-1}(L-\lambda I)\varphi\|_{L_2(\cdot)} \leqslant \|(L-\lambda I)^{-1}\|_{L_2(\cdot)}\cdot \|(L-\lambda I)\varphi\|_{L_2(\cdot)}$ that

$$\|(L-\lambda I)\varphi\|_{L_2(\cdot)} \geqslant \|\varphi\|_{L_2(\cdot)}/\|(L-\lambda I)^{-1}\|_{L_2(\cdot)}.$$

Finally, comparing each of the estimates (3.16), (3.17), and (3.18) with the preceding inequality, we obtain:

in case 1,

$$\|(L-\lambda I)^{-1}\|_{L_2(\cdot)} \leqslant 1/(\lambda+B), \quad \lambda+B>0, \quad B<0; \tag{3.19}$$

in case 2,

$$\|(L-\lambda I)^{-1}\|_{L_2(\cdot)} \leqslant 1/\lambda, \quad \lambda>0; \tag{3.20}$$

in case 3,

$$\|(L-\lambda I)^{-1}\|_{L_2(\cdot)} \leqslant \sqrt{2}/(\lambda-(-\tilde{B})), \quad \lambda>0, \quad \tilde{B}>0. \tag{3.21}$$

We now show that the operator L_λ is closed in the norm in $L_2(\cdot)$. Suppose the sequence $\{\varphi_n\}_{n=1}^{\infty}\in D(L)$, $s\text{-}\lim_{n\to\infty}\varphi_n=\varphi_0$ and $s\text{-}\lim_{n\to\infty}(L-\lambda I)\varphi_n=u_0$. By the inequality (3.13), the sequence $\{\varphi_n\}_{n=1}^{\infty}$ is fundamental, and therefore $s\text{-}\lim_{n\to\infty}\varphi_n=\varphi_0\in L_2(\cdot)$. On the other hand, the sequence $\{L\varphi_n\}_{n=1}^{\infty}$ is also fundamental. Since the generalized Liouville operator L is closed, $\varphi_0\in D(L)$ and $s\text{-}\lim_{n\to\infty} L\varphi_n = L\varphi_0$. Thus, $(L-\lambda I)\varphi_0=u_0$. As in the proof of Theorem 1, it is easy to show that the domain of definition of the operator L_λ is a dense subset in the Hilbert space $L_2(\cdot)$, i.e., L_λ is densely defined. Using this and the fact that $L - \lambda I$ is closed, we conclude that the set $(L - \lambda I)D(L)$ coincides with $L_2(\cdot)$. If (3.9) is not a one-to-one mapping, then λ is an eigenvalue of L; for in this case there will exist functions $\varphi_1\neq\varphi_2\in D(L)$ for each of which Eq. (3.5) is satisfied: $L\varphi_1-\lambda\varphi_1=\psi$, $L\varphi_2-\lambda\varphi_2=\psi$. Subtracting the second from the first, we conclude that $L(\varphi_1-\varphi_2)-\lambda(\varphi_1-\varphi_2)=0$, i.e., λ is an eigenvalue of L. But by hypothesis λ is not an eigenvalue of L. This completes the proof.

We consider the formal solution to the Cauchy problem (3.1) in the form of the T product of operators

$$f(q,p,t)=\tilde{T}(t-t_0)f_0(q,p), \tag{3.22}$$

where $f_0(q,p)\in C^{\infty}(\Gamma)$; $f(q,p,t)\in C^{\infty}(\cdot)$;

$$\tilde{T}(t-t_0)=\exp\left\{\int_{t_0}^{t} L(\xi)d\xi\right\}$$

is the solving operator (propagator) of the problem (3.1).

PROPOSITION 6. If for each $-\infty < t < \infty$ the functions $H(q,p,t), f(q,p,t)\in C^{\infty}(\Gamma)$ and are integrable once with respect to t, then the propagator (3.23) forms a continuous one-parameter Lie group (phase flow).

The proof is analogous to the proof of Theorem 4 in [6].

COROLLARY 4. The infinitesimal operator of the one-parameter Lie group $\tilde{T}(t-t_0)$ has the form $d(\tilde{T}(t-t_0)f(q,p,t))/dt|_{t=t_0}=Lf(q,p,t)$ and is a closed operator (see Theorem 2).

THEOREM 3. For $0<a\leqslant t_0<t\leqslant b<\infty$ the generalized Liouville operator L defined by formula (2) with domain of definition $D(L)=C_0^{\infty}(\cdot)\subset L_2(\cdot)$ is the infinitesimal generating operator of a strongly continuous (for $t = t_0$) unique semigroup $\{\tilde{T}(t-t_0),\ 0\leqslant t_0<t<\infty\}$, which has the following properties:

1) $\tilde{T}(0)=I,\ \tilde{T}(t)\tilde{T}(\tau-t)=\tilde{T}(\tau),\ \tilde{T}(t)\tilde{T}(-t)=I,\ \tilde{T}(\tau_1)\tilde{T}(\tau_2)=\tilde{T}(\tau_1+\tau_2)$;
2) $\|\tilde{T}(t-t_0)\|_{L_2(\cdot)}\leqslant\alpha\exp\{\gamma(t-t_0)\}$, where α and γ are constants;
3) $\operatorname*{s-lim}_{t\to t_0}\tilde{T}(t-t_0)f(q,p,t)=f(q,p,t)$ in the norm in $L_2(\cdot)$.

Proof. The validity of $\tilde{T}(0) = I$ follows directly from (3.23). For $0 \le t \le \tau < \infty$,

$$\tilde{T}(t)\tilde{T}(\tau-t)=\left\{1+\int_0^t L(\xi)d\xi+\frac{1}{2!}\left(\int_0^t L(\xi)d\xi\right)^2+\ldots\right\}\left\{1+\int_t^\tau L(\xi)d\xi+\frac{1}{2!}\left(\int_t^\tau L(\xi)d\xi\right)^2+\ldots\right\}=$$

$$1+\int_0^t L(\xi)d\xi+\int_t^\tau L(\xi)d\xi+\frac{1}{2}\left(\int_0^t L(\xi)d\xi\right)^2+\frac{1}{2}\left(\int_t^\tau L(\xi)d\xi\right)^2+\int_0^t L(\xi)d\xi\int_t^\tau L(\xi)d\xi+\ldots=1+\int_0^\tau L(\xi)d\xi+$$

$$\frac{1}{2}\left\{\left(\int_0^t L(\xi)d\xi\right)^2+2\int_0^t L(\xi)d\xi\int_t^\tau L(\xi)d\xi+\left(\int_t^\tau L(\xi)d\xi\right)^2\right\}+\ldots=\exp\left\{\int_0^\tau L(\xi)d\xi\right\}=\tilde{T}(\tau).$$

Setting $\tau = 0$ in the preceding expression and noting that $\tilde{T}(0) = I$, we obtain $\tilde{T}(t)\tilde{T}(-t) = I$. Similarly, $\tilde{T}(\tau_1)\tilde{T}(\tau_2)=\tilde{T}(\tau_1+\tau_2)$. In this case, the propagator (3.23) satisfies

$$\|\tilde{T}(t-t_0)\|\leqslant\alpha\cdot\exp\{\gamma(t-t_0)\}. \tag{3.24}$$

From (3.22), (3.23), and (3.24), we obtain the following estimates:

in case 1,

$$\|f(q,p,t)\|_{L_2(\cdot)}\leqslant e^{-B(t-t_0)}\|f_0(q,p)\|_{L_2(\cdot)},\quad \|\tilde{T}(t-t_0)\|\leqslant e^{-B(t-t_0)}; \tag{3.25}$$

in case 2,

$$\|f(q,p,t)\|_{L_2(\cdot)}=\|f_0(q,p)\|_{L_2(\cdot)},\quad \|\tilde{T}(t-t_0)\|=1; \tag{3.26}$$

in case 3,

$$\|f(q,p,t)\|_{L_2(\cdot)}\leqslant\sqrt{2}e^{-\tilde{B}(t-t_0)}\|f_0(q,p)\|_{L_2(\cdot)},\quad \|\tilde{T}(t-t_0)\|\leqslant\sqrt{2}e^{-\tilde{B}(t-t_0)}, \tag{3.27}$$

where $B = \chi_* < 0$ and $\tilde{B} = \varkappa_* > 0$. Since L is closed (Theorem 2) and its domain of definition $D(L) = C_0^{\infty}(\cdot)$ is dense in $L_2(\cdot)$ (Theorem 1), and for $\lambda > \gamma$ its resolvent (3.12) is defined and satisfies the estimates (3.19), (3.20), and (3.21), all the conditions of the Hille–Yosida theorem [3] are satisfied, from which Property 3 follows and also the fact that L is an infinitesimal generating operator of a strongly continuous (for $t = t_0$) unique semigroup $\{\tilde{T}(t-t_0),\ 0\leqslant t_0<t<\infty\}$. Thus, if the inequality (3.26) or (3.27) holds, the generalized Liouville operator $L:C_0^{\infty}(\cdot)\to L_2(\cdot)$ is the infinitesimal generating operator of a strongly continuous (for $t = t_0$) unique contractive semigroup.

If the function $\varkappa(q, p, t)$ defined by (3.14) vanishes identically, then by a certain redefinition of the Hamiltonian of the mechanical system the generalized Liouville equation (3.1) can be reduced to the classical equation

$$\frac{\partial f(q,p,t)}{\partial t}=\mathscr{H}_{\kappa} f(q,p,t), \quad f(q,p,t)|_{t=t_0}=f_0(q,p), \tag{3.28}$$

where $\mathscr{H}_{\kappa}\cdot=[H(q,p,t),\ \cdot]$ is the classical Liouville operator. In accordance with (3.26), the propagator corresponding to the classical Liouville equation (3.28) is a unitary operator in the space $L_2(\cdot)$. It is this that is the L_2 version of the classical Liouville theorem.

In conclusion, we formulate the classical Liouville theorem in a form that enables one, given the instantaneous value of the function $f(q, p, t)$ of the Cauchy problem (3.28), to find the exact solution of the nonconservative Hamiltonian scheme of equations

$$\dot{q}_i=\frac{\partial H(q,p,t)}{\partial p_i},\quad \dot{p}_i=-\frac{\partial H(q,p,t)}{\partial q_i},\ q_i(t)|_{t=t_0}=q_i^0,\ p_i(t)|_{t=t_0}=p_i^0. \tag{3.29}$$

We shall say that the nonconservative Hamiltonian system of equations (3.29) satisfies Assumption A if the function $H(q,p,t)\in C^{(2,2,1)}_{qpt}(\Omega^1)$, and the solutions of the system can be continued to infinity and remain in the region Ω when they are continued both to the right and to the left with respect to t. Here, $\Omega\subseteq\Gamma$ is a bounded open subset of Γ; $\Omega^1=\Omega\times J$, $J=\{t: t_0\leqslant t<\infty\}$.

THEOREM 4. If Assumption A is satisfied in the region Ω^1 for the nonconservative Hamiltonian system of equations (3.29), and $f(q, p, t)$ is the instantaneous value of the probability density distribution function which satisfies the Cauchy problem (3.28), and at the initial time $t = t_0$ the function $f_0(q, p)$ has one unconditional extremum (a maximum) at the point (q^0, p^0), then at any fixed time $t = t^* \geq t_0$

$$\max_{(q,p)\in\Omega} f(q,p,t^*)=f(q(q^0,p^0,t_0,t^*),\ p(q^0,p^0,t_0,t^*),t^*). \tag{3.30}$$

Proof. Suppose that the conditions of the theorem are satisfied but (3.30) does not hold, i.e., $\max_{(q,p)\in\Omega} f(q,p,t^*)\gtrless f(q(q^0,p^0,t_0,t^*),\ p(q^0,p^0,t_0,t^*),t^*)$, $t^*\in J$. By Assumption A, a solution $q=q(q^0,p^0,t_0,t)$, $p=p(q^0,p^0,t_0,t)$ to the Cauchy problem (3.29) exists, is unique, depends continuously on the initial states in the region Ω^1, and for $t = t_0$ is equal to $q^0=q(q^0,p^0,t_0,t_0)$, $p^0=p(q^0,p^0,t_0,t_0)$; therefore, the foregoing inequality is also satisfied at the time $t^* = t_0$. In other words, $\max_{(q,p)\in\Omega} f(q,p,t_0)\gtrless f(q(q^0,p^0,t_0,t_0),\ p(q^0,p^0,t_0,t_0),t_0)$. On the other hand, by the conditions of the theorem, $\max_{(q,p)\in\Omega} f(q,p,t_0)=f(q(q^0,p^0,t_0,t_0),\ p(q^0,p^0,t_0,t_0),t_0)$. Thus, we have obtained a contradiction, which proves the theorem.

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SHORT–RANGE INTERACTIONS AND IRREVERSIBILITY IN STATISTICAL MECHANICS

A. Tellez–Arenas
Département de Physique
Université d'Orléans
F–45046 Orléans Cedex, France
and
The Institute for Basic Research
Harvard Grounds, 96 Prescott Street
Cambridge, Massachusetts 02138, USA

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Abstract

The text of this paper corresponds to the talk given at the First International Conference on Non–Potential Interactions and their Lie–admissible Treatment under the heading "Short–range Interactions and T–symmetry breaking in Statistical Mechanics". The aim of this talk was to show that the idea of overlapping associated with short–range interactions allows one very simply to introduce irreversibility into the reversible laws of evolution deduced from Hamiltonian mechanics and in a way that shows itself finally to be correct. In order to do this we adopted the principle which is the basis of the work of this Conference. This is that, although the description of a set of interacting particles by local potential theories is justified when these particles may be considered as points, i.e., when only long–range interactions occur, it is no longer possible to ignore the finite size and mutual overlap of the particles when short–range interactions take place, and in this latter case a description involving non–local non–potential terms is required. Thus, on one hand we recall that when a variation is observed in the individual state of a body in short–range interaction, the notion of overlapping expresses itself by the existence of a non–arbitrary small time interval, and, on the other hand, we show that this finite time interval brings out a non–locality in time that breaks the reversibility. Starting from the first equation in the reversible BBGKY sequence, we obtained in this way a new, irreversible equation, which seems to be well adapted to the description of evolution phenomena in Statistical Mechanics since it reduces to the Boltzmann Equation when the general conditions of validity of the latter are satisfied.

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INTERACTIONS A COURTE PORTEE
ET IRREVERSIBILITE EN MECANIQUE STATISTIQUE

1. INTRODUCTION.

Les molécules, les atomes, les noyaux, les particules fondamentales, ont une extension finie dans l'espace. Cela n'est mis en cause par personne, même si la structure interne de ces corps microscopiques, et en particulier celle des particules subatomiques, n'est pas encore bien connue. De même personne ne doute de l'existence et de l'importance, au niveau microscopique, d'interactions dont la portée ne s'étend guère au-delà de la "matière" elle-même et qui ne peuvent donc se manifester entre deux corps que si ces deux corps viennent au "contact" l'un de l'autre. Le terme "contact", étant donné la nature des corps, signifie en fait pénétration mutuelle, plus ou moins importante selon le type d'interaction mis en jeu. Cette notion de pénétration mutuelle est une propriété essentielle des interactions à courte portée, qui leur confère un caractère très particulier en comparaison des interactions à longue portée et qui, de ce fait, devrait les placer d'emblée dans un domaine de la physique peu étudié jusqu'à présent. En effet, c'est un des mérites du professeur R.M. Santilli que d'avoir rappelé, et formulé de manière précise[1], les deux propriétés suivantes : -lorsque ne se manifestent que des interactions à longue portée, l'approximation qui consiste à assimiler les corps réels à des points est acceptable et les théories utilisées peuvent être de nature potentielle ; -si l'évolution du système considéré est régie essentiellement par des interactions à courte portée, les phénomènes de recouvrement qui apparaissent nécessairement se traduisent par des effets non locaux qui ne peuvent pas être correctement analysés dans le cadre de théories purement potentielles.

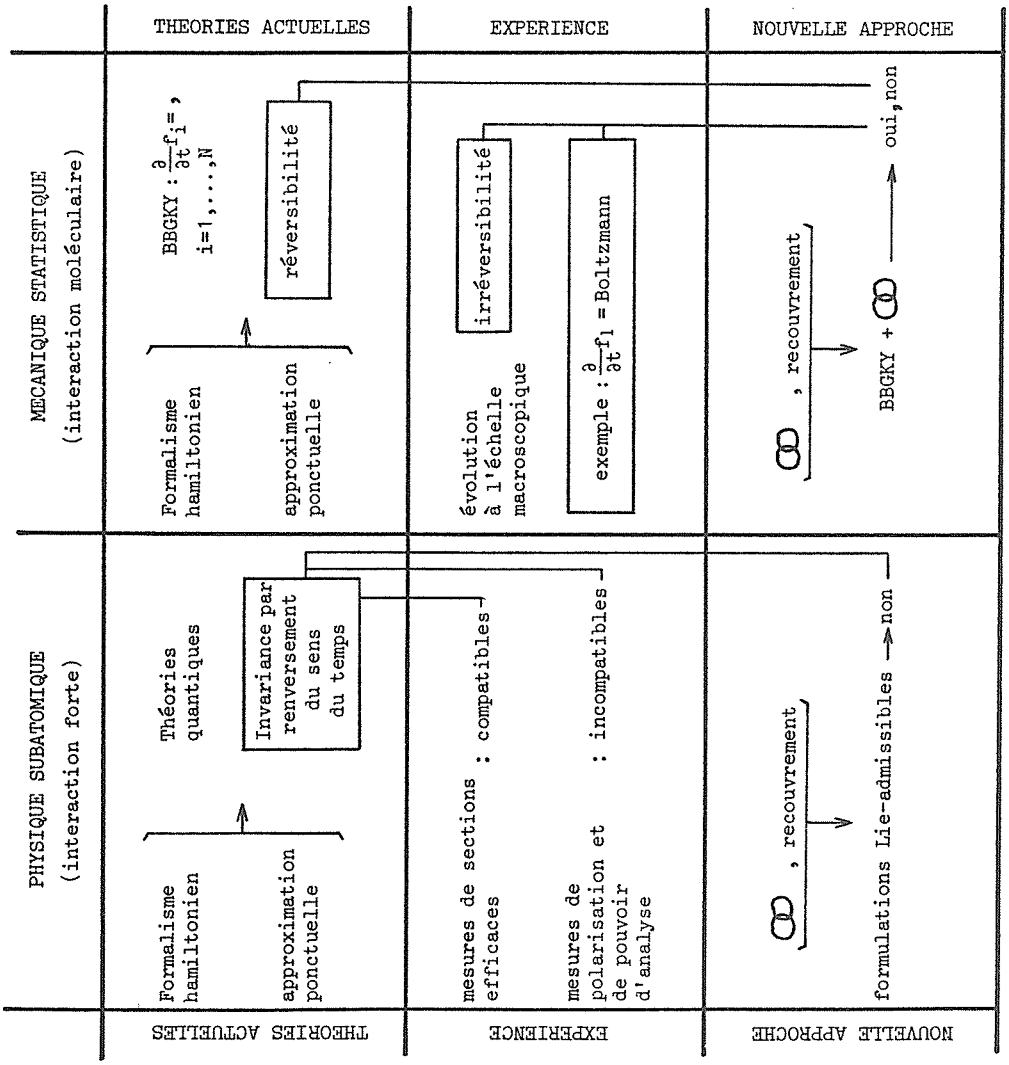
Les considérations générales rappelées ci-dessus représentent la base des travaux de physique théorique et expérimentale, ainsi que de mathématique, exposés lors de cette Conférence. Une part importante de ces travaux est constituée par l'étude des relations pouvant exister entre le caractère particulier des interactions à courte portée et l'altération plus ou moins prononcée des symétries exactes généralement associées aux théories actuelles, de nature potentielle. Dans ce cadre, nous allons nous intéresser à la notion de symétrie, ou de non symétrie, lors du renversement du sens du temps en mécanique statistique. Les exposés suivants aborderont le problème posé par ce type de symétrie à propos, cette fois, de l'interaction forte qui se manifeste en particulier dans les réactions nucléaires. Il me semble donc utile de rappeler très brièvement dans cette introduction les similitudes et les différences qui existent entre ces deux domaines — physique nucléaire et physique des particules (interaction forte) d'une part, et mécanique statistique des ensembles de molécules (interaction moléculaire) d'autre part — en ce qui concerne le renversement du sens du temps.

En physique subatomique, les théories actuelles sont des théories quantiques issues du formalisme hamiltonien, c'est-à-dire de la notion d'interaction potentielle, notion elle-même directement associée à l'image idéale de particules ponctuelles. Ces théories admettent l'invariance par renversement du temps de l'interaction forte. Les expériences faites sur ce sujet avaient donné jusqu'à présent des résultats qui semblaient compatibles avec cette invariance. Elles se limitaient toutefois à des mesures de sections efficaces, peu sensibles au phénomène étudié. Des expériences de polarisation, faites récemment[2] en collaboration par l'Université Laval au Québec (Canada) et le laboratoire Berkeley de l'Université de Californie (USA), montrent en fait, de manière très nette, que l'interaction forte ne serait pas invariante par renversement du temps. Ces nouvelles expériences, d'une très grande importance pour la physique nucléaire, seront présentées[3] dans cette Conférence par le professeur R.J. Slobodrian, de l'Université Laval. La nouvelle approche des phénomènes subatomiques, qui consiste à tenir compte de la notion de recouvrement nécessairement associée aux interactions à courte portée, se développe actuellement dans le cadre d'une formulation Lie-admissible. Le professeur R. Mignani, de l'Université de Rome, montrera comment cette formulation prédit en effet une non invariance par renversement du temps dans les réactions nucléaires[4].

En mécanique statistique classique, la théorie actuelle s'appuie comme précédemment sur l'approximation ponctuelle de la formulation hamiltonienne et elle se traduit, en particulier, par la séquence d'équations couplées BBGKY qui régit l'évolution dans le temps des densités de probabilité réduites. Du fait du formalisme dont elles sont issues, ces équations théoriques sont réversibles. Sur le plan expérimental, la situation en mécanique statistique est plus claire que celle qui existe en physique nucléaire : les lois phénoménologiques qui décrivent effectivement l'évolution des phénomènes sont irréversibles (exemple : l'équation de Boltzmann) et donc profondément différentes des équations réversibles BBGKY. Quant à la nouvelle approche des interactions à courte portée en mécanique statistique, elle peut se concevoir de la manière suivante : -admettre, comme première approximation, l'image idéale de particules ponctuelles obéissant à une dynamique hamiltonienne, et les équations BBGKY qui en résultent ; -trouver pour ces équations une formulation qui fasse apparaître explicitement la notion de variation de l'état d'un corps pendant un intervalle de temps donné, au cours d'une interaction à courte portée ; -introduire dans cette nouvelle formulation le concept d'intervalle de temps fini (non arbitrairement petit) correspondant à une variation significative de l'état d'un corps en interaction. C'est cette nouvelle approche qui est décrite dans le présent article. Elle introduit dans les équations d'évolution une non localité en temps qui brise la réversibilité, d'une manière semble-t-il satisfaisante puisque l'équation ainsi obtenue pour la densité de probabilité à un corps contient l'équation de Boltzmann.

Le tableau suivant résume la situation exposée ci-dessus, en ce qui concerne la notion d'invariance ou de non invariance par renversement du temps en physique subatomique et en mécanique statistique classique.

SYMETRIES LORS DU RENVERSEMENT DU SENS DU TEMPS
EN PHYSIQUE SUBATOMIQUE ET EN MECANIQUE STATISTIQUE CLASSIQUE



	THEORIES ACTUELLES	EXPERIENCE	NOUVELLE APPROCHE
MECANIQUE STATISTIQUE (interaction moléculaire)	Formalisme hamiltonien approximation ponctuelle ↑ BBGKY : $\frac{\partial}{\partial t} f_i =$, $i = 1, \ldots, N$ réversibilité	évolution à l'échelle macroscopique irréversibilité exemple : $\frac{\partial}{\partial t} f_1$ = Boltzmann	⚭ , recouvrement → BBGKY + ⚭ → oui, non
PHYSIQUE SUBATOMIQUE (interaction forte)	Formalisme hamiltonien approximation ponctuelle ↑ Théories quantiques Invariance par renversement du sens du temps	mesures de sections efficaces : compatibles mesures de polarisation et de pouvoir d'analyse : incompatibles	⚭ , recouvrement → formulations Lie-admissibles → non

THEORIES ACTUELLES | EXPERIENCE | NOUVELLE APPROCHE

2. NOUVELLE FORMULATION DE L'EQUATION BBGKY$_1$.

Soit un système constitué par un ensemble de N molécules identiques, repérée chacune par $z_i = (\underline{r}_i, \underline{v}_i)$, $i = 1,\dots,N$. La densité de probabilité $f_N(z_1,\dots,z_N,t)$ associée à ce système est telle que $f_N(z_1,\dots,z_N,t)dz_1\dots dz_N$ est la probabilité de le trouver dans l'élément de volume $dz_1\dots dz_N$ autour du point $z_1,\dots,z_N$ à l'instant t. La densité de probabilité réduite $f_i(z_1,\dots,z_i,t)$ est définie par la relation

$$f_i(z_1,\dots,z_i,t) = \int dz_{i+1}\dots dz_N \; f_N(z_1,\dots,z_N,t) \quad .$$

$f_1(z_1,t)dz_1$ est donc la probabilité de trouver la particule baptisée 1 dans l'élément de volume dz_1 autour de z_1 à l'instant t, indépendamment de l'état des autres particules du système. L'approximation qui consiste à assimiler les molécules à des points décrivant des trajectoires différentiables se traduit par le fait que le système considéré obéit à une dynamique locale de type hamiltonien, s'écrivant

$$\begin{aligned} \dot{\underline{r}}_i &= \underline{v}_i \\ \dot{\underline{v}}_i &= \sum_{j\neq i} \underline{\gamma}(z_i,z_j) \quad ; \quad i,j = 1,\dots,N \end{aligned} \tag{2.1}$$

où l'accélération $\underline{\gamma}$ dérive d'un potentiel. L'évolution de la densité de probabilité réduite $f_1(z_1,t)$ est alors régie par la première équation, notée BBGKY$_1$, de la séquence BBGKY :

$$\text{BBGKY}_1 \left\{ \begin{aligned} &\frac{\partial}{\partial t} f_1(z,t) = -\underline{v}.\underline{\text{grad}}_{\underline{r}} f_1(z,t) - (N-1)\text{div}_{\underline{v}}\left[f_1(z,t)\underline{\Gamma}(z,t)\right] && (2.2) \\ &\underline{\Gamma}(z,t) = \frac{1}{f_1(z,t)} \int dz' \; \underline{\gamma}(z,z')f_2(z,z',t) && (2.3) \end{aligned} \right.$$

où l'évolution de la densité de probabilité $f_2(z,z',t)$ est régie par BBGKY$_2$ qui dépend elle-même de $f_3(z,z',z'',t)$, etc... Les équations BBGKY sont réversibles au sens dynamique. Cela signifie que si $f_1(z,t) = f_1(\underline{r},\underline{v},t)$ est une solution de l'équation BBGKY$_1$, alors $f_1(\underline{r},-\underline{v},-t)$ en est aussi une. Cette réversibilité, qui est une conséquence directe de la dynamique hamiltonienne (2.1), implique la réversibilité des lois théoriques d'évolution macroscopique déduites de ce formalisme : si M(t) est une variable macroscopique et L[M(t)] une loi théorique d'évolution associée à cette variable, alors L[M(-t)] doit aussi être une loi d'évolution. Autrement dit, la réversibilité des équations (2.2) se traduit par le fait qu'il serait impossible de déterminer le sens d'écoulement du temps par une observation de la variable M(t). En fait la réalité physique des phénomènes macroscopiques est tout autre, l'une de leur caractéristique essentielle étant l'irréversibilité : si L[M(t)] est une loi d'évolution possible, L[M(-t)] n'en est généralement pas une.

L'objet de cet article est d'introduire l'irréversibilité dans l'équation réversible $BBGKY_1$ par l'intermédiaire de la notion de recouvrement, notion qui est nécessairement associée aux interactions à courte portée, et qui n'est cependant pas prise en compte par une dynamique du type (2.1). Une première méthode consisterait à tenter de modifier cette dynamique. En l'absence d'informations précises sur la nature des corps et sur la nature des interactions, il semble très difficile, sinon impossible, de procéder ainsi. Nous allons donc nous placer au niveau statistique et considérer l'expression (2.3), dont la signification physique permet aisément une généralisation susceptible de prendre en compte qualitativement la notion de recouvrement. En effet, l'expression (2.3) montre que $\underline{\Gamma}(z,t)$ est l'accélération moyenne d'une molécule donnée située en z à l'instant t dans l'ensemble N considéré, sous l'action d'une autre molécule de cet ensemble. Cette accélération moyenne peut s'écrire d'une autre manière, en faisant intervenir la notion de variation de la vitesse durant un certain intervalle de temps. Il suffit pour cela de considérer une paire de molécules subissant des diffusions du type

$$(z_0,z_0',t_0) \rightarrow (z,z',t) \rightarrow (z_1,z_1',t_1) \quad , \quad t_1 > t > t_0$$

pour z et t fixés. Les molécules de l'ensemble N étant assimilées à des points décrivant les trajectoires différentiables de la dynamique (2.1), $\underline{\Gamma}(z,t)$ peut s'écrire sous la forme suivante :

$$\underline{\Gamma}(z,t) = \lim_{t_1-t_0\to 0} \left[f_1(z,t)\right]^{-1} \int dz' \int_{C(z,z',t)} dz_0dz_0'dz_1dz_1' \, \frac{\underline{v}_1-\underline{v}_0}{t_1-t_0} \left[f_2\, P\right]_{\substack{z_0,z_0'\\ z_1,z_1'\\ t_0,t_1}} \qquad (2.4)$$

$$\left[f_2\, P\right]_{\substack{z_0,z_0'\\ z_1,z_1'\\ t_0,t_1}} = f_2(z_0,z_0',t_0)P(z_1,z_1',t_1;z_0,z_0',t_0)$$

$f_2(z_0,z_0',t_0)dz_0dz_0'$ est la probabilité de trouver la paire considérée au point (z_0,z_0') à l'instant t_0. $P(z_1,z_1',t_1;z_0,z_0',t_0)dz_1dz_1'$ est la probabilité de transition correspondant au passage de cette paire du point (z_0,z_0') à l'instant t_0 au point (z_1,z_1') à l'instant t_1 (on se limite à des phénomènes sans mémoire). Remarquons que P est une densité de probabilité de transition dans l'ensemble N et qu'elle doit donc prendre en compte d'éventuelles interactions entre la paire considérée et d'autres molécules de l'ensemble. La notation $C(z,z',t)$ rappelle que les variables $z_0,z_0',t_0,z,z',t,z_1,z_1',t_1$ ne sont pas indépendantes : l'intégration par rapport à z_0,z_0',z_1,z_1' est limitée aux paires (z_0,z_0',t_0) et (z_1,z_1',t_1) qui se correspondent par une diffusion engendrant la paire (z,z',t), de manière compatible avec la dynamique (2.1). En fait, à la limite $t_1-t_0\to 0$, la qualité différentiable des trajectoires permet aisément de tenir compte de la contrainte $C(z,z',t)$, indépendamment de la dynamique (2.1), en utilisant les relations de définition de la vitesse et de l'accélération et en introduisant de nouvelles variables :

$$t_1-t_0\to 0 \quad \left\{ \begin{array}{l} \underline{v} = \dfrac{\underline{r}-\underline{r}_0}{t-t_0} = \dfrac{\underline{r}_1-\underline{r}}{t_1-t} \quad ; \quad \underline{\gamma} = \dfrac{\underline{v}-\underline{v}_0}{t-t_0} = \dfrac{\underline{v}_1-\underline{v}}{t_1-t} \\ \underline{q} = \underline{r}_1-\underline{r}_0 \quad ; \quad \underline{u} = \underline{v}_1-\underline{v}_0 \quad ; \quad a = (\underline{q},\underline{u}) \\ \underline{q}' = \underline{r}_1'-\underline{r}_0' \quad ; \quad \underline{u}' = \underline{v}_1'-\underline{v}_0' \quad ; \quad a' = (\underline{q}',\underline{u}') \\ \Delta t = t_1-t_0 \quad ; \quad \eta = \dfrac{t-t_0}{\Delta t} \\ z_{0\eta} = z-\eta a \; ; \quad z_{1\eta} = z+(1-\eta)a \\ z_{0\eta}' = z'-\eta a' \quad ; \quad z_{1\eta}' = z'+(1-\eta)a' \\ t_{0\eta} = t-\eta\Delta t \quad ; \quad t_{1\eta} = t+(1-\eta)\Delta t \end{array} \right\} \qquad (2.5)$$

Avec ces nouvelles variables, l'expression (2.4) s'écrit

$$\underline{\Gamma}(z,t) = \lim_{\Delta t \to 0} \left[f_1(z,t)\right]^{-1} \int dz'dada' \int_0^1 d\eta \, \frac{\underline{u}}{\Delta t} \left[f_2 \, P\right]_{\substack{z_{0\eta}, z'_{0\eta} \\ z_{1\eta}, z'_{1\eta} \\ t_{0\eta}, t_{1\eta}}} , \qquad (2.6)$$

où l'intégration en η correspond à une distribution uniforme de l'intervalle Δt autour du temps t donné.

On vérifie aisément qu'à la limite $\Delta t \to 0$ cette dernière expression est équivalente à l'expression initiale (2.3), en utilisant la propriété

$$\lim_{\Delta t \to 0} P(z_{1\eta}, z'_{1\eta}, t_{1\eta} \,;\, z_{0\eta}, z'_{0\eta}, t_{0\eta}) = \delta(a)\delta(a')$$

Nous avons donc obtenu, par l'intermédiaire de l'expression (2.6), une nouvelle formulation de l'équation $BBGKY_1$, formulation qui présente les deux propriétés suivantes :

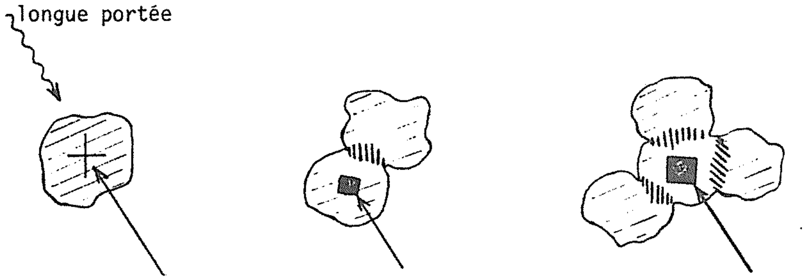
a) à la limite $\Delta t \to 0$, elle est équivalente à la formulation habituelle (2.2,3) associée à la dynamique hamiltonienne (2.1) ;

b) elle se prête immédiatement à une extension capable de modifier profondément la nature de l'équation $BBGKY_1$. Cette extension consiste en la *suppression du passage à la limite* $\Delta t \to 0$, *l'intervalle* Δt *associé à la variation de l'état d'un corps en interaction à courte portée étant considéré comme fini, c'est-à-dire non arbitrairement petit.*

Nous allons voir que l'extension $(\Delta t \to 0) \to (\Delta t = \tau \text{ fini})$, qui introduit l'irréversibilité dans les lois d'évolution, est physiquement justifiable par les phénomènes de recouvrement qui apparaissent lors des interactions à courte portée.

3. RECOUVREMENT DANS LES INTERACTIONS A COURTE PORTEE ET IRREVERSIBILITE.

Dans l'approximation ponctuelle représentée par la dynamique (2.1) et l'équation (2.2), la notion de variation de la position ou de la vitesse d'une particule durant un intervalle de temps donné reste significative quelle que soit la longueur de cet intervalle et quel que soit le type d'interaction (potentielle) subi par la particule. Cette caractéristique permet de concevoir physiquement une variation de vitesse $\underline{u}$ durant un intervalle Δt arbitrairement petit, ce qui signifie mathématiquement que dans l'expression (2.6) la limite $\Delta t \rightarrow 0$ est effectivement atteinte. Par contre, lorsqu'on admet la notion de recouvrement, de pénétration mutuelle, de deux corps d'extension finie en interaction à courte portée, l'intervalle de temps minimum correspondant à une variation significative de l'état d'un des deux corps en interaction est certainement fini. Cet intervalle de temps minimum, τ, dépend du volume moyen de la zone de recouvrement, et donc de la nature de l'interaction et des énergies mises en jeu. Cela se conçoit aisément de façon qualitative. Imaginons une particule sous la forme d'une boule de gélatine translucide aux contours irréguliers et de structure interne non uniforme. Si cette particule est isolée, ou soumise à des interactions à longue portée, il est possible à chaque instant de déterminer avec précision son centre de masse, par exemple par une série de clichés pris de directions différentes. On peut alors, en première approximation, représenter cette particule par son centre de masse et décrire son mouvement par une dynamique hamiltonienne. Par contre, s'il y a pénétration mutuelle au cours d'une interaction à courte portée (et que dans la zone de recouvrement rien ne permette de distinguer la matière appartenant à l'un des corps de celle appartenant à l'autre), et bien que le centre de masse du système global formé par les corps en interaction puisse encore être déterminé avec précision, il y a nécessairement une indétermination sur la position du centre de masse d'un corps déterminé. Cette indétermination est généralement d'autant plus grande que le volume de la zone de recouvrement et la masse qu'il contient sont importants. Dans ces conditions, la notion de variation de la position ou de la vitesse d'un corps doit correspondre, pour être significative, à une variation au moins égale aux incertitudes dues au phénomène de recouvrement. Cette variation minimale non arbitrairement petite n'est concevable que pour un intervalle de temps τ lui-même non arbitrairement petit. Le schéma suivant, dans lequel $\delta^3\underline{r}$ représente l'incertitude sur la position du centre de masse d'un corps, résume le point de vue précédent.



Finalement le passage de l'approximation ponctuelle à la notion de pénétration mutuelle se traduit par l'extension ($\Delta t \to 0$) → ($\Delta t = \tau$ fini). Cette extension modifie profondément la nature de l'expression (2.6) de l'accélération moyenne $\underline{\Gamma}(z,t)$ de l'approximation ponctuelle et fournit une nouvelle expression $\underline{X}_\tau(z,t)$ adaptée à la notion de pénétration mutuelle :

$$\underline{X}_\tau(z,t) = \left[f_1(z,t)\right]^{-1} \int dz'\,da\,da' \int_0^1 d\eta \, \frac{\underline{u}}{\tau} \left[f_2\, P\right]_{\substack{z_{0\eta},z'_{0\eta} \\ z_{1\eta},z'_{1\eta} \\ t_{0\eta},t_{1\eta}}} \qquad (3.1)$$

où maintenant $\eta = \frac{t-t_0}{\tau}$, $t_{0\eta} = t-\eta\tau$ et $t_{1\eta} = t+(1-\eta)\tau$. Cette expression (3.1) de $\underline{X}_\tau(z,t)$ peut aussi s'écrire explicitement en fonction du temps :

$$\underline{X}_\tau(z,t) = \left[f_1(z,t)\right]^{-1} \int dz'\,da\,da' \, \frac{1}{\tau} \int_{t-\tau}^{t} dt' \, \frac{\underline{u}}{\tau} \left[f_2\, P\right]_{\substack{z_{0t'},z'_{0t'} \\ z_{1t'},z'_{1t'} \\ t',t'+\tau}} \qquad (3.2)$$

avec

$$z_{0t'} = z - \frac{t-t'}{\tau} a \quad ; \quad z'_{0t'} = z' - \frac{t-t'}{\tau} a'$$

$$z_{1t'} = z + \left(1 - \frac{t-t'}{\tau}\right) a \quad ; \quad z'_{1t'} = 1 + \left(1 - \frac{t-t'}{\tau}\right) a'$$

On voit que l'introduction de l'intervalle de temps minimum τ se traduit par une non localité en temps sous la forme d'une valeur moyenne calculée sur cet intervalle. La nouvelle équation d'évolution ainsi obtenue pour $f_1(z,t)$ s'écrit

$$\text{BBGKY}_1\infty \quad : \quad \frac{\partial}{\partial t} f_1(z,t) = - \underline{v} . \underline{\text{grad}}_{\underline{r}} f_1(z,t) + R[f_1] \qquad (3.3)$$

$$R[f_1] = - (N-1) \text{div}_{\underline{v}} [f_1(z,t) \underline{X}_\tau(z,t)]$$

L'expression (3.2) de $\underline{X}_\tau(z,t)$ montre que cette nouvelle équation est irréversible.

Il reste maintenant à vérifier que l'équation irréversible (3.3) est susceptible de décrire correctement l'évolution des phénomènes expérimentaux. Pour cela, nous allons montrer qu'elle se réduit à l'équation de Boltzmann lorsque les conditions habituelles de validité de cette dernière sont satisfaites. Rappelons ces conditions :

a) l'évolution est essentiellement déterminée par les interactions à courte portée, c'est-à-dire qu'en première approximation la vitesse d'une molécule ne varie pas en dehors d'une zone de collision ;

b) dans une zone de collision, les densités de probabilité de transition $P(z_1,z'_1,t_1;z_0,z'_0,t_0)$ dépendent uniquement des vitesses et de l'intervalle t_1-t_0 ;

c) la dépendance explicite des densités de probabilité en position et en temps est suffisamment faible pour qu'elle puisse être négligée à l'intérieur du volume moyen V_{col} d'une zone de collision et durant un intervalle de temps du même ordre de grandeur que la durée moyenne d'une collision.

Remarquons d'autre part que, de façon générale, l'intégration sur les variables $\underline{q}$ et $\underline{q}'$ dans l'expression (3.1) est en fait limitée aux volumes d'incertitudes $\delta^3\underline{r}$

et $\delta^3\underline{r}' = \delta^3\underline{r}$ associés aux centres de masse de chacun des deux corps en interaction. En effet la densité de probabilité de transition P qui figure dans cette expression (3.1) correspond à une transition de durée τ au cours de laquelle les variations $\underline{q}$ et $\underline{q}'$ sur les positions sont du même ordre de grandeur que les incertitudes $\delta\underline{r}$ sur les centres de masse. Cette remarque et les conditions a), b) et c) réduisent l'expression (3.1) à une forme beaucoup plus simple :

$$\underline{X}_\tau(z,t) = \left[f_1(z,t)\right]^{-1} \int_{\substack{\underline{r}' \in V_{col} \\ \underline{q},\underline{q}' \in \delta^3\underline{r}}} d\underline{r}'d\underline{v}'d\underline{q}d\underline{u}d\underline{q}'d\underline{u}' \int_0^1 d\eta \frac{\underline{u}}{\tau} f_2(r,v_{0\eta},r,v'_{0\eta},t)P_\tau(v_{1\eta},v'_{1\eta};v_{0\eta},v'_{0\eta})$$

$$\underline{X}_\tau(z,t) = \left[f_1(z,t)\right]^{-1} \int d\underline{v}'d\underline{u}d\underline{u}' \int_0^1 d\eta \frac{\underline{u}}{\tau}\, \phi \tag{3.4}$$

$$\phi = f_2(r,v_{0\eta},r,v'_{0\eta},t)V_{col}\; W_\tau(v_{1\eta},v'_{1\eta};v_{0\eta},v'_{0\eta})$$

où $W_\tau = (\delta^3\underline{r})^2 P_\tau$ est une densité de probabilité de transition dans l'espace des vitesses. On peut maintenant trouver la forme du terme de collision $R[f_1]$ de l'équation $\mathrm{BBGKY}_1\infty$ (3.3), en utilisant une méthode introduite[5] par Irving et Kirkwood. On obtient ainsi

$$R[f_1] = -\,(N-1)\mathrm{div}_{\underline{v}}[f_1(z,t)\underline{X}_\tau(z,t)] = -\,(N-1) \int d\underline{v}'d\underline{u}d\underline{u}' \int_0^1 d\eta \frac{\underline{u}}{\tau} \cdot \underline{\mathrm{grad}}_{\underline{v}}\phi$$

$$-\,\underline{u} \cdot \underline{\mathrm{grad}}_{\underline{v}}\phi = \frac{d\phi}{d\eta} + \mathrm{div}_{\underline{v}'}(\underline{u}'\phi)$$

$$R[f_1] = (N-1) \int d\underline{v}'d\underline{u}d\underline{u}'\; \frac{1}{\tau}\, [\phi(\eta=1) - \phi(\eta=0)]$$

la contribution du terme $\mathrm{div}_{\underline{v}'}(\underline{u}'\phi)$ dans l'intégrale $\int d\underline{v}'$ étant considérée comme nulle.

Finalement le terme de collision de l'équation $\mathrm{BBGKY}_1\infty$ s'écrit

$$R[f_1] = (N-1) \int d\underline{v}'d\underline{\nu}d\underline{\nu}'\; V_{col.}\, \frac{1}{\tau}\, \Big[f_2(\underline{r},\underline{\nu},\underline{r},\underline{\nu}',t)W_\tau(\underline{v},\underline{v}';\underline{\nu},\underline{\nu}') - f_2(\underline{r},\underline{v},\underline{r},\underline{v}',t)W_\tau(\underline{\nu},\underline{\nu}';\underline{v},\underline{v}')\Big] \tag{3.5}$$

C'est bien une expression de ce type qui est à la base de l'équation de Boltzmann. Pour obtenir la forme habituelle de cette équation, il suffit maintenant d'introduire la notion de densité de probabilité de transition par unité de temps, $W^* = \frac{1}{\tau} W_\tau$, directement liée à la section efficace différentielle de collision dans le cas où les collisions à trois corps ou plus sont négligées. Pour des collisions du type $(\underline{v},\underline{v}') \rightarrow (\underline{\nu},\underline{\nu}')$ et des angles de diffusions (θ,φ) dans le système du centre de masse, on obtient

$$W^*(\underline{\nu},\underline{\nu}';\underline{v},\underline{v}')V_{\mathrm{col}}\, d\underline{\nu}d\underline{\nu}' = |\underline{v}-\underline{v}'|\,\frac{d\sigma}{d\Omega}\sin\theta\, d\theta d\varphi \qquad (3.6)$$

Dans le cas de collisions élastiques entre corps identiques, et en admettant l'invariance des interactions pour une réaction et la réaction inverse, on a d'autre part

$$W^*(\underline{v},\underline{v}';\underline{\nu},\underline{\nu}') = W^*(\underline{\nu},\underline{\nu}';\underline{v},\underline{v}') \qquad (3.7)$$

Les relations (3.6) et (3.7) transforment l'expression (3.5) en la forme habituelle du terme de collision de l'équation de Boltzmann. La méthode que nous avons utilisée pour tenir compte des phénomènes de recouvrement lors des interactions à courte portée introduit donc l'irréversibilité d'une manière qui semble satisfaisante d'un point de vue phénoménologique.

4. RETOUR A LA NOTION DE DYNAMIQUE.

En associant à la dynamique hamiltonienne idéale (2.1) la notion d'intervalle de temps fini τ, correspondant à une variation significative de l'état d'un corps en interaction à courte portée, nous avons obtenu l'équation irréversible $\mathrm{BBGKY}_1\infty$ (3.3), qui "contient" l'équation de Boltzmann et qui a donc quelque chance d'être bien adaptée à la description des phénomènes expérimentaux. On peut maintenant envisager d'associer au système des N molécules en interaction une dynamique généralisée A, non potentielle, qui engendrerait directement l'équation $\mathrm{BBGKY}_1\infty$. On peut aussi envisager de faire correspondre à cette équation un ensemble de N quasi-particules statistiques indépendantes se déplaçant dans un champ moyen de nature non potentielle[6,7,8]. La dynamique B de ces quasi-particules statistiques serait telle que les propriétés du système réel qui ne dépendent que de la densité f_1 seraient reproduites. Ces considérations se résument de la façon suivante :

approximation ponctuelle, interactions potentielles,
+
intervalle de temps fini τ

$$\Downarrow$$

$$\mathrm{BBGKY}_1 \infty \rightarrow \text{Boltzmann}$$

$$\Uparrow$$

approximation ponctuelle, interactions non-potentielles,

$$A : \begin{cases} \dot{\underline{r}}_i = \underline{v}_i \quad ; \quad i = 1,\dots,N \\ \dot{\underline{v}}_i = \sum\limits_{i \neq j} \underline{\gamma}_{NP}(z_i, z_j, t, \tau) \end{cases} \qquad (4.1)$$

$$B : \begin{cases} \dot{\underline{r}}_i = \underline{v}_i \quad ; \quad i = 1,\dots,N \\ \dot{\underline{v}}_i = \underline{\Gamma}_{NP}(z_i, t, \tau) \end{cases} \qquad (4.2)$$

Les dynamiques généralisées A et B engendrent respectivement (problème de Liouville directe [9]) les équations d'évolution suivantes :

$$A : \frac{\partial}{\partial t} f_1(z,t) = -\underline{v} \cdot \underline{\mathrm{grad}}_{\underline{r}} f_1(z,t) - (N-1)\,\mathrm{div}_{\underline{v}} \int dz' \, \underline{\gamma}_{NP}(z,z',t,\tau) f_2(z,z',t) \qquad (4.3)$$

$$B : \frac{\partial}{\partial t} f_1(z,t) = -\underline{v} \cdot \underline{\mathrm{grad}}_{\underline{r}} f_1(z,t) - \mathrm{div}_{\underline{v}} \left[f_1 \underline{\Gamma}_{NP}(z,t,\tau) \right] \qquad (4.4)$$

On peut donc immédiatement obtenir une solution possible pour $\underline{\gamma}_{NP}(z_i,z_j,t,\tau)$ et $\underline{\Gamma}_{NP}(z_i,t,\tau)$, par identification avec l'équation (3.3). En choisissant l'expression (3.2) de $\underline{X}_\tau(z,t)$, on trouve ainsi

$$\underline{\gamma}_{NP}(z_i,z_j,t,\tau) = \left[f_2(z_i,z_j,t)\right]^{-1} \int da_i da_j \, \frac{1}{\tau} \int_{t-\tau}^{t} dt' \, \frac{\underline{u}_i}{\tau} \left[f_2 \, P\right]_{\substack{z_{0it'},z_{0jt'} \\ z_{1it'},z_{1jt'} \\ t',t'+\tau}} \tag{4.5}$$

$$\underline{\Gamma}_{NP}(z_i,t,\tau) = (N-1)\left[f_1(z_i,t)\right]^{-1} \int dz_j \, \underline{\gamma}_{NP}(z_i,z_j,t,\tau) f_2(z_i,z_j,t) \tag{4.6}$$

avec

$$z_{0it'} = z_i - \frac{t-t'}{\tau} a_i \quad ; \quad z_{0jt'} = z_j - \frac{t-t'}{\tau} a_j$$

$$z_{1it'} = z_i + \left(1 - \frac{t-t'}{\tau}\right) a_i \quad ; \quad z_{1jt'} = z_j + \left(1 - \frac{t-t'}{\tau}\right) a_j$$

Les dynamiques non potentielles A et B qui, dans l'approximation ponctuelle, peuvent engendrer directement l'équation irréversible $BBGKY_1\infty$, sont donc très particulières. Elles sont en effet non locales en position, vitesse et temps, par l'intermédiaire de la densité de probabilité f_2. L'étude détaillée de telles dynamiques est sans doute irréalisable dans le cas général. Cela n'est pas surprenant puisqu'elles décrivent, au moins au niveau statistique, le mouvement de corps qui sont susceptibles de se pénétrer mutuellement. Nous pouvons cependant poser cette question : sachant que, pour un système régi par des interactions à courte portée, la dynamique potentielle idéale (2.1) et la dynamique généralisée non potentielle (4.1,4.5) ne sont que des représentations approximatives de la réalité physique, laquelle de ces deux représentations est la plus proche de cette réalité ? Il semble naturel de répondre que c'est la représentation généralisée (4.1,4.5), puisqu'elle est compatible avec la nature irréversible des lois d'évolution observées au niveau macroscopique. Remarquons toutefois que cette représentation généralisée des interactions internes du système N doit être complétée par les contraintes résultant des lois générales de conservation associées à tout système fermé[10,11]. Remarquons enfin que la nature non locale des dynamiques (4.1) et (4.2) implique un traitement Lie-admissible au sens le plus général[12].

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LETTER TO THE EDITOR

An algebraic approach to irreversible dynamical descriptions

J P Constantopoulos and C N Ktorides
Physics Department, University of Athens, Athens, Greece

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Abstract. We establish a connection between the non-unitary transformation scheme which breaks the time reversibility at the microscopical level and an algebraic deformation scheme which generalises the Lie product. This formal approach is further supported by an explicit construction of the various operators involved. The compatibility conditions are considered for this case and are found to be automatically satisfied by the algebraic deformation scheme in the particular case of the Fokker–Planck equation. In this way, a particular model of the non-unitary transformation scheme is given constructively.

In this note we present a construction of the Φ operator, which results formally in the Λ-transformation scheme of Prigogine and coworkers (Misra and Prigogine 1983, Prigogine 1979, 1981, Prigogine *et al* 1973), through an algebraic deformation approach (Fronteau *et al* 1979). Furthermore we shall demonstrate the intimate connection between the two aforementioned approaches and in particular, how the algebraic deformation scheme can be regarded as the case of what Prigogine *et al* call intrinsically random systems. We recall that the physically relevant distribution function ρ is defined in Prigogine (1981) by $\tilde{\rho} = \Lambda^{-1}\rho$, where Λ is a non-unitary transformation, and satisfies the modified Liouville equation

$$\mathrm{i}\partial_t\tilde{\rho} = \Phi\tilde{\rho} \tag{1}$$

where $\Phi(L) = \Lambda^{-1}L\Lambda$. Here L denotes the formal Liouville operator for a Hamiltonian system which is Hermitian and which can be easily adapted either to the classical (Poisson brackets) or to the quantum mechanical (commutator) case (Prigogine *et al* 1973). Now the requirement for the existence of a Lyapounov function implies the *star Hermiticity condition* on Φ, namely

$$\mathrm{i}\Phi(L) = [\mathrm{i}\Phi(L)]^* \tag{2}$$

where by definition

$$\Phi^*(L) = \Phi(-L)^\dagger \tag{2a}$$

and where the dagger denotes Hermitian conjugation. The above condition is a necessary ingredient for establishing an H-theorem (Prigogine 1981). In addition the star Hermiticity condition guarantees that in general the operator Φ can be divided into an even and an odd part. In other words instead of (1) we may write

$$\mathrm{i}\partial_t\tilde{\rho} = (\Phi^{\mathrm{odd}} + \Phi^{\mathrm{ev}})\tilde{\rho} \tag{1a}$$

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having so transformed the macroscopic thermodynamics distinction between reversible ($\Phi^{\rm ev}$) and irreversible ($\Phi^{\rm odd}$) processes into the microscopic description.

At this point, it is worth noticing that Grmela and Iscoe (1978) have also considered a *unique* decomposition of the general kinetic equation by writing

$$\partial_t\tilde{\rho}=R_-(\tilde{\rho})+R_+(\tilde{\rho}) \tag{3}$$

where $R_-(\tilde{\rho})$ stands for the time reversible part of the right-hand side and $R_+(\tilde{\rho})$ incorporates the irreversible behaviour which according to the previous considerations may be thought of as brought about by the non-unitary mapping Λ.

It is important to notice the difference between (1*a*) and (3). As noted already, (1*a*) is a 'generalised' Liouville equation which transcribes to the microscopic domain the thermodynamical distinction between reversible and irreversible processes. Equation (3), on the other hand, is a genuine macroscopic equation. Attributing the latter equation to the microscopic domain, Fronteau (1981 and references therein) has reached an interesting new interpretation. According to Fronteau (1981) the non-equilibrium statistical mechanical equation (3) leads to a quasiparticle concept. This new concept corresponds to a 'total' picture emerging for a particle when the interaction with all other particles is taken into account. Here, there occurs an interesting analogy with quantum field theory where one considers a bare and dressed particle, the latter being conceived of as a 'final' entity emerging once microscopic interactions have been taken into account.

The question arises whether (3) can be cast in the operator form of (1*a*) and *vice versa*. We shall show that this can be naturally achieved within the Lie admissible deformation scheme which generalises the Lie algebraic structure of the Poisson bracket. We recall that according to Fronteau *et al* (1979) the classical Liouville equation can be generalised by replacing the Poisson bracket with a new one, namely

$$\partial_t\tilde{\rho}=(H,\tilde{\rho}) \tag{4}$$

where

$$(H,\tilde{\rho})=HR\tilde{\rho}+\tilde{\rho}TH. \tag{4a}$$

In the above equations H is a 'Hamiltonian function' which describes only a part of the system. R and T are operators which in certain special cases reduce to functions on the phase space. We stress that (4) refers to the evolution of the physically relevant distribution function in phase space. It is for this reason that we have denoted the density in (4) by $\tilde{\rho}$.

Operators R and T describe the deformation content of the theory. According to our point of view these operators are capable of incorporating the dynamical content which leads to the quasiparticle picture.

We are now in position to relate, at least formally, the non-unitary transformation $\rho\rightarrow\tilde{\rho}=\Lambda^{-1}\rho$ with the aforementioned deformation scheme. In particular, if we start with the full Liouville equation and act by Λ^{-1} from the left we get

$$\mathrm{i}\partial_t\tilde{\rho}=\Lambda^{-1}H\Lambda\tilde{\rho}-\tilde{\rho}H. \tag{5}$$

Comparing with (4) and (4*a*) we notice that the operation by Λ^{-1} amounts to the identification

$$\Lambda^{-1}H\Lambda=HR, \qquad T=-I, \tag{6a, b}$$

where I is the identity operator.

Clearly, equations (6*a*) and (6*b*) relate (formally) the two aforementioned schemes. In particular, they provide a prescription for the specification of the non-unitary operator Λ provided that the deformation operator R is known. Conversely, if Λ is known a corresponding deformation operator can, in principle, be introduced via (6*a*).

In the bridging equations (6) appears only the Hamiltonian H and not the operator Φ. To proceed in this direction we construct the formal Liouville operator via the identification

$$L = \mathrm{i}\mathscr{H} \tag{7}$$

where

$$\mathscr{H} = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \right)$$

when the Hamiltonian H is known. In exactly the same way we may explicitly construct the operator Φ directly from (4) by taking into account the form of the generalised product (,) in the classical case (Fronteau *et al* 1979), namely

$$\Phi = \mathrm{i}\tilde{\mathscr{H}} \tag{8}$$

where

$$\tilde{\mathscr{H}} = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \right) + \sum_{i,j=1}^{n} \frac{\partial H}{\partial p_i} s_{ij} \frac{\partial}{\partial p_j}. \tag{8a}$$

Here s_{ij} is a well defined $n \times n$ matrix which expresses the content of the algebraic deformation in a precise form. We stress that the term $(\partial H/\partial p_i) s_{ij} \partial/\partial p_j$ should not be interpreted strictly as a friction term. This less interesting instance is also included in the formalism, but we are mostly interested in the case when s_{ij} includes the effective interaction of the whole with the individual. This is the case which leads to the quasiparticle concept.

Equations (7) and (8) split naturally in two parts. In particular we may write

$$\tilde{\mathscr{H}}^1 = \mathscr{H}^1 + \mathscr{S}, \qquad \tilde{\mathscr{H}}^2 = \mathscr{H}^2, \tag{9a, b}$$

where

$$\mathscr{H}^1 \equiv \sum_{i=1}^{n} \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i}, \qquad \mathscr{H}^2 \equiv -\sum_{i=1}^{n} \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i}, \qquad \mathscr{S} = \sum_{i,j=1}^{n} \frac{\partial H}{\partial p_i} s_{ij} \frac{\partial}{\partial p_j}.$$

Thus, given the Hamiltonian of the system and the algebraic deformation matrix s_{ij}, the formal operator Φ can be explicitly constructed through (9*a*), (9*b*) and (8). Clearly this is not enough. The star Hermiticity condition of Φ, or its counterpart on $\mathscr{S}$, has to be checked. In fact we have

$$\Phi(L) = \mathrm{i}\tilde{\mathscr{H}} = \mathrm{i}(-\mathrm{i}L + \mathscr{S}) = L + \mathrm{i}\mathscr{S}. \tag{10}$$

Now the star Hermiticity condition (2) imposed on (10) gives

$$-\tilde{\mathscr{H}} = (-\tilde{\mathscr{H}}(-L))^{\dagger} = -(\mathrm{i}L + \mathscr{S})^{\dagger} = \mathrm{i}L - \mathscr{S}^{\dagger} \tag{11}$$

which implies

$$\mathscr{S} = \mathscr{S}^{\dagger} \tag{12}$$

which means that the operator $\mathscr{S}$ is necessarily Hermitian.

As a particular example of the above analysis we consider the Fokker–Planck equation for one particle in three dimensions. In this case we have the decomposition (Grmela *et al* 1980)

$$\Phi^{\mathrm{ev}}\tilde{\rho} = \mathrm{i}R - \tilde{\rho} = \sum_{i=1}^{3} v_i \frac{\partial}{\partial r_i}\tilde{\rho}(r, v, t), \tag{13a}$$

$$\Phi^{\mathrm{odd}}\tilde{\rho} \equiv \mathrm{i}R + \tilde{\rho} = \sum_{i=1}^{3}\left(C\frac{\partial}{\partial v_i}(v_i\tilde{\rho}(r, v, t)) + A\frac{\partial}{\partial v_i}\frac{\partial}{\partial v_i}\tilde{\rho}(r, v, t)\right) \tag{13b}$$

where C and A are the coefficients of dissipation and diffusion.

From (13a) the relevant Hamiltonian can be identified as $H = \frac{1}{2}mv_i^2$. On the other hand, from (13b) we have

$$\mathscr{S} = \sum_{i,j=1}^{3} \frac{\partial H}{\partial v_i} s_{ij} \frac{\partial}{\partial v_j} = C + \sum_{i=1}^{3} Cv_i \frac{\partial}{\partial v_i} + \sum_{i=1}^{3} A \frac{\partial}{\partial v_i}\frac{\partial}{\partial v_i} = \sum_{i,j=1}^{3} v_i s_{ij} \frac{\partial}{\partial p_j}. \tag{14}$$

Condition (12) is automatically fulfilled for $\mathscr{S}$ by construction. The above is a particular instance of a more general situation. In fact, whenever the algebraic deformation scheme yields real and symmetric matrices s_{ij}, (12) will be automatically guaranteed by construction.

Concluding this note it is worth noticing that the alternative procedure for breaking time reversibility, namely via a projection operator P which acting on ρ eliminates unphysical effects, does not seem to have a deformation counterpart, in general. In order to study this situation, first we notice that P cannot commute with the Hamiltonian entering the Liouville equation (1).

In fact if it did we would have

$$\tilde{\rho} = P\rho = P\mathrm{e}^{-\mathrm{i}Ht}\rho(0)\mathrm{e}^{\mathrm{i}Ht} = \mathrm{e}^{-\mathrm{i}Ht}\tilde{\rho}(0)\mathrm{e}^{\mathrm{i}Ht}, \tag{15}$$

i.e. the evolution of $\tilde{\rho}$ would be determined by the original Hamiltonian which is undesirable.

Given that the commutator $[P, H]$ does not vanish we notice that the algebraic deformation scheme becomes effective only under special conditions. Specifically one must show the existence of an operator S which satisfies the relation

$$[P, H] = HSP. \tag{16}$$

If this happens to be the case we find

$$\mathrm{i}\partial_t\tilde{\rho} = PH\rho - \tilde{\rho}H = H(I+S)\tilde{\rho} - \tilde{\rho}H \tag{17}$$

where the natural identifications follow

$$R = I + S, \qquad T = -I. \tag{17a}$$

Clearly the conditions for the existence of an operator S satisfying (16) constitute an open question even in the formal case.

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THERMODYNAMIC ANALYSES OF LASER INSTABILITY AND SUPERRADIANCE

H. Hasegawa, S. Sawada and M. Mabuchi

Kyoto University, Kyoto, Japan

1. INTRODUCTION

The instability phenomena in nonlinear optics, laser and superradiance, have received the interest of theoretical investigation from a macroscopic point of view. In the Third Rochester Conference, Graham discussed[1] the problem of unifying the laser theory and the non-equilibrium thermodynamic theory of Glansdorff and Prigogine,[2] based on the entropy expression for the steady non-equilibrium state, S = lnP, where P is the well-established steady-state solution of the laser Fokker-Planck equation.

The difficulty, which led Graham to say[1] that "the relation of the quantity lnP to the non-equilibrium thermodynamics remained still unclear" so that "a unified treatment of thermodynamics and fluctuations far from equilibrium is still missing", is concerned with the fact that the central role played as a thermodynamic potential in the Glansdorff-Prigogine theory is the entropy production rather than the entropy itself. Here we find a better answer to the problem by focusing our consideration on a rudimentary point of contact between the thermodynamic and fluctuation theories, on the basis of which results of our numerical analyses will be presented.

Our standpoint is that the thermodynamic framework can be statistically reformulated by an explicit use of generally time-dependent solutions of the Fokker-Planck equation, which removes the "local equilibrium" assumption in the thermodynamics and which also enables us to extend the framework so that it may apply to transient phenomena as well. This has been discussed fully in a series of papers by one of the authors.[3]

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2. STATISTICAL DESCRIPTION OF THE THERMODYNAMICS OF A SYSTEM UNDER THE FOKKER-PLANCK EVOLUTION LAW

It is not an easy task to recapitulate the Glansdorff-Prigogine theory, but the following interpretative summary by means of the quantity $\mathcal{P}$, named entropy production, may be of assistance: (a) $\mathcal{P}$ is a non-negative quantity as a function of several variables, $\{x_\nu\}$ (state variables which characterize a thermodynamic state of the system evolving in time as $x_\nu(t)$), as well as of other time-independent parameters $\{\lambda_i\}$. (b) $\mathcal{P}$ attains its minimum value at the equilibrium (or, the steady non-equilibrium) state x^0_ν towards which every state temporally approaches. (c) Evolution criterion $(d/dt)\mathcal{P} \leq 0$; stability against fluctuations $\delta^2\mathcal{P} > 0$, where $\delta^2\mathcal{P}$ implies the second increment of the functional $\mathcal{P}(x(t))$ with respect to the variation $\delta x_\nu(t)$ from the realizable time evolution of the system. (d) The macroscopic course $x_\nu(t)$ that is realized must be always accompanied with fluctuations. In the vicinity of the equilibrium state x^0_ν the probability of occurrence of such fluctuations $\delta x_\nu(t)$, may be expressed in terms of the corresponding change in $\mathcal{P}$ through the Einstein formula $P \propto e^{\frac{1}{2}\delta^2 S}$ ($\delta^2\mathcal{P} = d/dt\,\delta^2 S$: the "excess entropy production").

The above aspects have been reviewed more fully by Nicolis,[4] who discussed the fluctuation property (d) to an extent by considering the Markoffian evolution law. Our view on this problem is that it is possible to complete Nicolis' argument so that essentially the entire aspect can be formulated on the Markoffian basis, in particular, on the Fokker-Planck evolution law.[3] We designate the space of the state variable $\{x_\nu\}$ (assumed to form a Cartesian coordinate system) as the "phase space", over which the probability distribution at time t, $\psi(x\ t)$, is defined. Let us take the form of equation satisfied by ψ as

$$\frac{\partial\psi}{\partial t} = -\frac{\partial}{\partial x_\mu}(K_\mu\psi) + \frac{1}{2}\frac{\partial^2}{\partial x_\mu \partial x_\nu}(K_{\mu\nu}\psi) \quad , \tag{1}$$

where, for simplicity the positive symmetric diffusion tensor $K_{\mu\nu}$ is assumed as constant and the drift velocity $K_\mu(x)$ (generally, a nonlinear function of x_ν's) is assumed to satisfy the potential condition, $\partial K_\mu/\partial x_\nu = \partial K_\nu/\partial x_\mu$. Then the steady-state solution $\psi_0(x)$ of Eq.(1) is obtainable from a direct integration

$$\psi_0(x) = \text{const.}\times\text{exp.}\left[\int_{x0}^{x} 2K^{-1}_{\mu\nu}\, K_\nu\, (x')\, dx'_\mu\right] \tag{2}$$

which is identical with Graham's P mentioned in the Introduction.

Our plan to unify the Fokker-Planck and the Glansdorff-Prigogine theories begins with a firm variational principle which is equivalent to solving Eq.(1), because historically the thermodynamic theory was initiated in connection with the variational principle by Onsager[5] and expounded by Prigogine's school.[6] Two forms of such principle are available:[3]

Onsager's variational principle

$$\int \mathcal{S}\frac{\partial\psi}{\partial t}\,dx - \frac{1}{2}\,\mathcal{P}\{\mathcal{S},\psi\} = \max.(\mathcal{S}) \quad , \tag{3}$$

where

$$\mathcal{P}\{\mathcal{S},\psi\} = \int \frac{1}{2}\,K_{\mu\nu}\,\frac{\partial\mathcal{S}}{\partial x_\mu}\,\frac{\partial\mathcal{S}}{\partial x_\nu}\,\psi\,dx \tag{3a}$$

with post-variation condition

$$\mathcal{S} = -\log(\psi/\psi_0) \qquad (\psi_0 \text{ defined by } (2)). \tag{3b}$$

Prigogine's variational principle (the local potential method)

$$\int \log\psi\,\left(\frac{\partial\psi_0}{\partial t} + \frac{\partial}{\partial x_\mu}(v_\mu\psi_0)\right)dx + \frac{1}{2}\,\mathcal{P}\{\log\psi,\psi_0\} = \min.(\log\psi) \quad , \tag{4}$$

where

$$\mathcal{P}\{\log\psi,\psi_0\} = \int \frac{1}{2}\,K_{\mu\nu}\,\frac{\partial\log\psi}{\partial x_\mu}\,\frac{\partial\log\psi}{\partial x_\nu}\,\psi_0\,dx \tag{4a}$$

with post-variation condition

$$\psi = \psi_0 \quad . \tag{4b}$$

Here ψ_0 is generally a time-dependent solution of Eq.(1) resulting from the variational principle. The reason why the maximum principle (3) is attributed to Onsager is clearly that it is analogous to the form:[5] [entropy production] - [dissipation function] = max. by the association

$$\int \mathcal{S}\frac{\partial\psi}{\partial t}\,dx \longrightarrow \text{[entropy production]}$$

$$\mathcal{P}\{\mathcal{S},\psi\} \longrightarrow 2\times\text{[dissipation function]} \ .$$

It can be shown[3] that by the satisfaction of the variational principle (3) together with (3a,b) (hence for a solution ψ of Eq.(1)), the following relations hold:

$$\int \mathcal{S}\,\frac{\partial\psi}{\partial t}\,dx = \mathcal{P}\{\mathcal{S},\psi\} = \frac{d}{dt}\int(\log(\psi_0/\psi))\psi\,dx \quad . \tag{5}$$

Therefore, the quantity $\mathcal{P}\{\mathcal{S},\psi\}$ (twice the "dissipation functional may be identified, under the Fokker-Planck evolution law resulting from Onsager's variational principle, with the "entropy production" - the total time derivative of a scalar quantity to be designated as entropy (incidentally, as the very information entropy).

With the above understanding of the entropy production, it can be seen intuitively that (b) $\mathcal{P}\{\mathcal{S},\psi\}$ tends to its minimum value 0 as ψ tends to the steady-state distribution ψ_0 (when the time goes to infinity), in the vicinity of which

(c) the evolution criterion $\frac{d}{dt}\mathcal{P} \leq 0$, (6)

and

the stability against $\delta\mathcal{S}$ $\delta^2\mathcal{P} > 0$ (7)

hold. Furthermore, it can be shown that the stability condition (7) is actually not restricted to the vicinity of the steady-state but extends over all the time regions as far as the solution $\psi(x\ t)$ exists. As to the Einstein fluctuation formula for the non-equilibrium steady-state, we have

(d) $P(zt_2/yt_1) = \text{const.}\times\exp.[-\frac{1}{2}\int_{t_1}^{t_2} K^{-1}_{\mu\nu}\ \delta\dot{x}_\mu(t)\ \delta\dot{x}_\nu(t)\ dt]$ (8)

which can be derived from the general Onsager-Machlup formula[3] based on a most-probable-path argument.

It is an interesting but difficult question whether the validity of the evolution criterion (6) holds unrestricted in the vicinity of the steady-state or not. In order to see the point of question in connection with Graham's argument,[1] let us reconsider the evolution criterion in the ordinary framework with the entropy function $S(x) = \log\psi_0(x)(=\ln P(x))$ for which

$$\mathcal{P}(x(t)) \equiv \frac{dS}{dt} = \frac{\partial S}{\partial x_\mu}\dot{x}_\mu = 2K^{-1}_{\mu\nu}K_\mu K_\nu \quad . \tag{9}$$

(We have used the potential condition and hence the expression (2) and also the macroscopic evolution law, $\dot{x}_\mu = K_\mu$.)

$$\frac{d}{dt}\mathcal{P} = 4K^{-1}_{\mu\nu}\dot{K}_\mu K_\nu = 4K^{-1}_{\mu\nu}\frac{\partial K_\mu}{\partial x_\lambda}K_\lambda K_\nu = 2\frac{\partial^2 S}{\partial x_\lambda \partial x_\nu}K_\lambda K_\nu \quad . \tag{10}$$

Therefore, the region of the phase space where the evolution criterion holds can be well identified with the one in which the curvature tensor $\partial^2 S/\partial x_\mu \partial x_\nu$ is non-positive. This is certainly violated in the vicinity of an unstable point (e.g., the unstable 0-photon state above threshold of the laser action), as it should. Let us now go over to the present new framework, for which we have derived the formula[3]

$$\frac{d}{dt}\mathcal{P}\{\mathscr{S},\psi\} = \int 2\,\frac{\partial^2 S}{\partial x_\mu \partial x_\nu}\,K_\mu K_\nu\,\psi\,dx - \int \frac{1}{2}K_{\mu\lambda}K_{\nu\sigma}\,\frac{\partial X_\lambda}{\partial x_\nu}\,\frac{\partial X_\sigma}{\partial x_\mu}\,\psi\,dx\ , \tag{11}$$

where $\mathscr{S}$ is given by (3b) and

$$X_\lambda \equiv \frac{\partial}{\partial x_\lambda}\log(\psi_0/\psi)\quad . \tag{11a}$$

The first term on the r.h.s. of (11) is the same contribution as in (10) averaged over the distribution ψ, to which the second term is added. This additional contribution is always negative and is originated as an effect of fluctuations. Thus, one can say qualitatively that the effect of fluctuations associated with the macroscopic drift motion is such that they tend to make its unstable behavior mild so that the validity of the evolution criterion (6) may be widened much from the prediction (10). This will be subject to a direct quantitative test in Section 4.

3. SOLUTIONS OF THE LASER AND SUPERRADIANCE FOKKER-PLANCK EQUATIONS BY THE VARIATIONAL METHOD

The single-mode laser action, described by the Langevin equation for a complex Van der Pol oscillator corresponding to the active-mode amplitude, i.e.,

$$\dot{b} - \beta(d-b^*b)b = \Gamma(t),\ \langle\Gamma(t)\Gamma^*(t')\rangle = Q\delta(t-t')\quad \text{etc.},$$

may have a counter description in terms of a probability distribution subject to the Fokker-Planck equation

$$\frac{\partial\psi}{\partial t} = -\beta\,\frac{\partial}{\partial b}\,((d-|b|^2)b\psi) + 4Q\,\frac{\partial^2\psi}{\partial b\partial b^*}\quad . \tag{12}$$

We restrict ourselves to the "uniform phase" case, and simplify (12) to

$$\frac{\partial\psi}{\partial t} = -2\,\frac{\partial}{\partial I}\,((a-I)I\psi) + 4\,\frac{\partial}{\partial I}\,(I\,\frac{\partial\psi}{\partial I})\quad , \tag{12'}$$

changing the variable to $I \propto b^*b$ (photon number, i.e., the intensity of the active mode) and following Risken's scaling procedure.[7] Let us now apply the Onsager's variational principle (3)-(3a,b) to solve Eq.(12'), which may be rewritten as follows:

$$\int_0^\infty \mathscr{S}\,\frac{\partial\log\psi}{t}\,\psi\,dI - \int_0^\infty 2I\left(\frac{\partial\mathscr{S}}{\partial I}\right)^2\psi\,dI = \max. \tag{13}$$

with post-variation setting

$$\mathcal{S} = \log(\psi_0/\psi) \quad . \tag{13a}$$

A detail of the variational procedure has been described elsewhere[3] but may be summarized in a word by the Rayleigh-Ritz method, viz.

$$\text{ansatz:} \quad \psi(I,t) = \exp.\times[u_0 + \frac{u_1}{2}I - \frac{u_2}{4}I^2 - \frac{u_3}{6}I^3 \text{----}] \ , \qquad (u_n = u_n(t)) \tag{14}$$

for which the coefficients $u_n (n \geq 1)$ can be determined from the variational principle, while u_0 can be determined from the normalization, $\int \psi \, dx = 1$. This condition may be re-expressed as

$$\int_0^\infty \frac{\partial \log\psi}{\partial t} \psi \, dI = \dot{u}_0 + \frac{<I>}{2}\dot{u}_1 - \frac{<I^2>}{4}\dot{u}_2 \text{---}$$

$$= 0 \quad , \tag{15}$$

with

$$<I^n> \equiv \int_0^\infty I^n \psi \, dI \qquad \text{(instantaneous moments)}, \tag{16}$$

which eliminates $\dot{u}_0$ by means of other $\dot{u}_n$'s and the moments.

Truncating the power series in the exponent of ψ up to I^3, we have derived a set of ordinary differential equations for u_n's. In virtue of the known steady-state solution ψ_0 for which u_1=a (the pump parameter), u_2=1 and $u_n(n \geq 3)$=0, the equation may have the form

$$\frac{d}{dt}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = M_1^{-1} \cdot M_2 \begin{pmatrix} u_1 - a \\ u_2 - 1 \\ u_3 \end{pmatrix} \quad , \tag{17}$$

where the two 3×3 matrices M_1 and M_2 are both symmetric given by

$$M_1 = \begin{bmatrix} \frac{-1}{4}<(I-<I>)^2> & \frac{1}{8}<(I-<I>)(I^2-<I^2>)> & \frac{1}{12}<(I-<I>)(I^3-<I^3>)> \\ & \frac{-1}{16}<(I^2-<I^2>)^2> & \frac{-1}{24}<(I^2-<I^2>)(I^3-<I^3>)> \\ * & & \frac{-1}{36}<(I^3-<I^3>)^2> \end{bmatrix}$$

$$M_2 = \begin{bmatrix} \langle I\rangle & -\ \langle I^2\rangle & -\ \langle I^3\rangle \\ & \langle I^3\rangle & \langle I^4\rangle \\ * & & \langle I^5\rangle \end{bmatrix} \tag{18}$$

A transient laser action can be simulated by the solution of Eq.(17) having the initial values

$$u_1 = -\infty\ ,\quad u_2 = u_3 = \text{---} = 0\quad ,\quad t=0 \tag{19}$$

and evolving in time such that $u_1 \to a$, $u_2 \to 1$ and $u_n (n \geq 3) \to 0$, as t tends to infinity.

We have carried out the above task with computer, using the Runge-Kutta method (i.e., replacing the differential equation by successive difference equations), where the initial values of u_1 are chosen, which are negatively large. The results of the integration of u_n's for three values of the pump parameter, a=0, 4 and 8, are shown in Fig. 1. It has been assured that a different choice of the initial u_1-values yields a difference in the results that is insignificant after a first passage of duration (i.e., after the passage of t_0 at which a kink occurs for every u_2-curve in Fig. 1). Clearly, this duration corresponds to the period in which the system "falls" rapidly from the unstable equilibrium point. The strange behavior of the u_2-curve after this duration indicates that tremendous fluctuations are produced accompanying this sharp fall and then are reduced; this is more conspicuous for the larger pumping. An advantage of the present method is that various lower-order moments and cumulants are obtained simultaneously in the course of the Runge-Kutta integration process in a self-consistent manner with the distribution function. The simplest ones, viz. $\langle I\rangle$ (intensity) and $\langle (I-\langle I\rangle)^2\rangle$ (intensity variance), are presented in Fig. 2. A remark should be made about the convergence problem, that is, the accuracy of the truncation up to n=3. An inquiry of this can be made by comparing the results with n=2 truncation and those with n=3, showing a fair result about u_n's and a satisfactory result about $\langle I\rangle$ and $\langle (I-\langle I\rangle)^2\rangle$.

Let us consider, as a second example, the original simple model of superradiance (superfluorescence) due to Bonifacio et al.[8] expressed in the operator master equation

$$\frac{\partial W}{\partial t} = \frac{1}{2} I_1 \left([R_-, WR_+] + [R_- W, R_+]\right).$$

The R_z-diagonal representation of this equation may be approximated by a Fokker-Planck equation, in accordance with the system-size

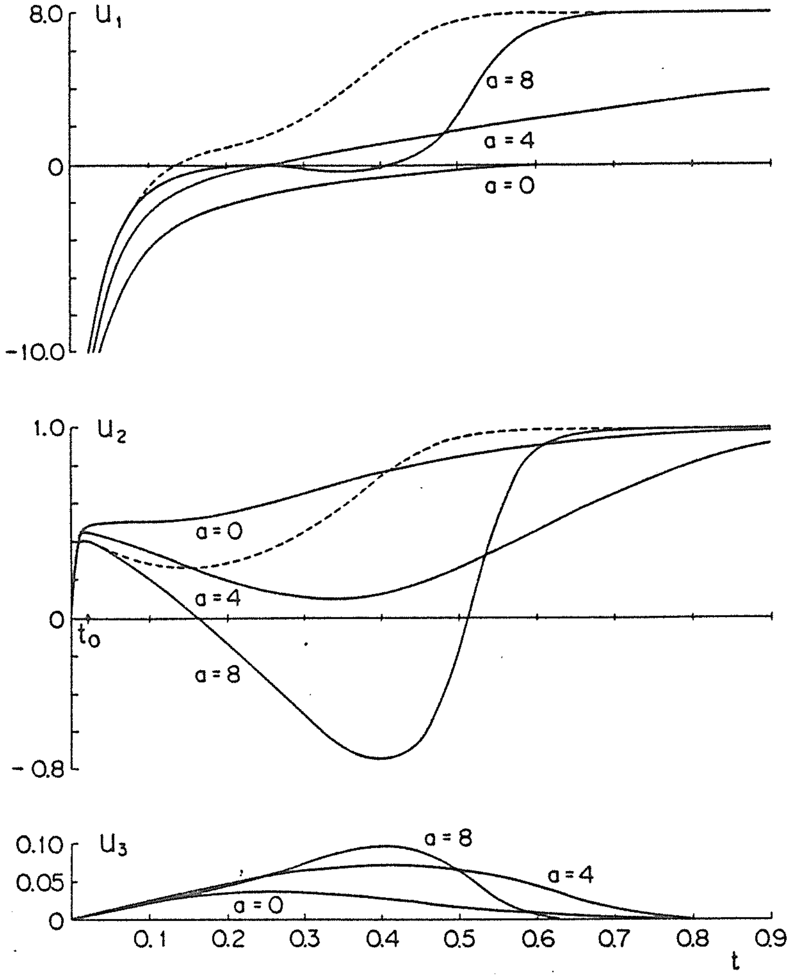

Fig. 1. The integrated three coefficients u_1, u_2 and u_3 in the exponent of the time-dependent laser distribution function for three values of the pump parameter a . The unit of abscissa is the scaled time in accordance with Risken's presentation.[7] For a comparison, the results for the truncation up to n=2($\dot{u}_3=u_3=0$ in Eq.(17)), a=8, are also shown (dotted lines).

expansion method,[9] as follows:

$$\frac{\partial \psi}{\partial t} = I_1 \, R\left(\frac{\partial}{\partial z}(1 + \varepsilon - z^2)\psi + \frac{\varepsilon}{2}\frac{\partial}{\partial z}(1-z^2)\frac{\partial \psi}{\partial z}\right) \tag{20}$$

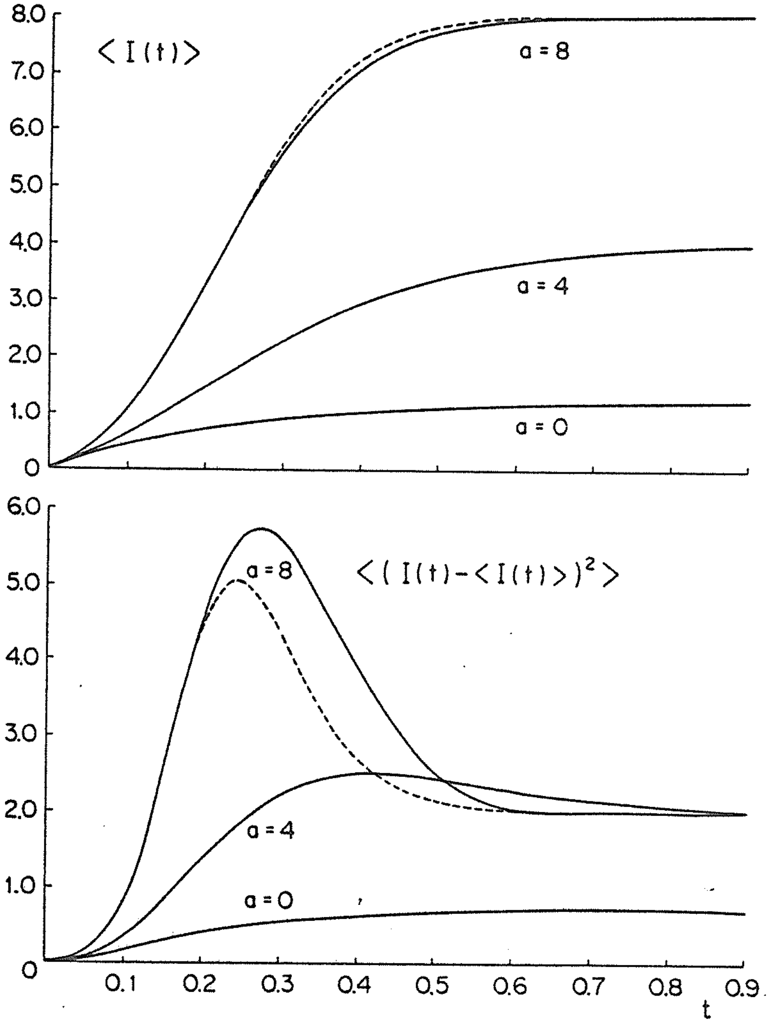

Fig. 2 The mean and the variance of the calculated intensity (in the same unit as Risken's) of the radiation for the laser. The n=2 truncation (dotted lines for a=8) disagrees with the corresponding curves due to Risken[7] (especially for the intensity variance between t=0.2 and 0.5). This is improved by taking into account the I^3-term (i.e., the n=3 truncation).

where $R=\varepsilon^{-1}$, the magnitude of the "spin", represents the system size (one-half of the number of active two-level atoms), and the variable z represents the cosine of the Bloch angle (measured from the north pole) so that

$$-1 \leq z \leq 1 \ . \tag{20a}$$

Here, the Prigogine's variational principle (4)-(4a,b) (the "local potential") is used to determine the approximate solution of Eq. (20) by taking a trial distribution function as

$$\psi(z) = \text{const.}\ \exp[-\frac{R}{2\sigma}(z-m)^2] \quad , \tag{21}$$

which also conforms to the spirit of the system-size expansion. By considering the mean m and the variance σ of z as two variation parameters, we have derived a set of differential equations for them as follows:

$$\frac{dm}{d\tau} = m^2 - 1 - \varepsilon(m+1-\sigma) \tag{22a}$$

$$\frac{d\sigma}{d\tau} = 1 - m^2 + 4m\sigma - 3\varepsilon\sigma \quad . \tag{22b}$$

Here we have scaled time t such that $\tau = I_1Rt$, as usual.

The stationary points of Eqs.(22a,b) i.e., the zeroes of the r.h.s., can be easily located. In the physical region of the m-σ plane, $-1 \leq m \leq 1$, $0 \leq \sigma$, they are:

(i) $m = -1$, $\sigma = 0$ (stable equilibrium point)

(ii) $m = \frac{\varepsilon}{2}$, $\sigma = \frac{1}{\varepsilon} \gg 1$ (unstable "saddle point").

Thus, it is naturally expected that the system starting at any point inside the above physical region will tend to the stable equilibrium (i), as $\tau \rightarrow \infty$, i.e., to the "south pole" of the dipole pendulum around which the system becomes sharply distributed.

The nonlinear differential equations (22a,b) are easier to handle than Eq.(17) for the laser, some typical solutions of which are presented in Fig. 3. A significant point of discussion from the present result must be that our method yields the evolution equations for the mean and variance in order of the smallness parameter $\varepsilon(=1/R)$, one higher than that which has been formulated.[9] Thus, the familiar superradiance equation of the hyperbolic tangent type for the atomic inversion m is modified by the additional term which arises from the diffusion part of Eq.(20). Consequently, the present result yields a finite period in order of O(log R) to attain the maximum intensity of the emitted radiation, starting from the complete inversion with a small, or even vanishing, dipole-fluctuation. Since the diffusion part of Eq.(20) is purely quantum in origin (as can be realized by checking its derivation and its existence in the case of vanishing thermal photons), we can say

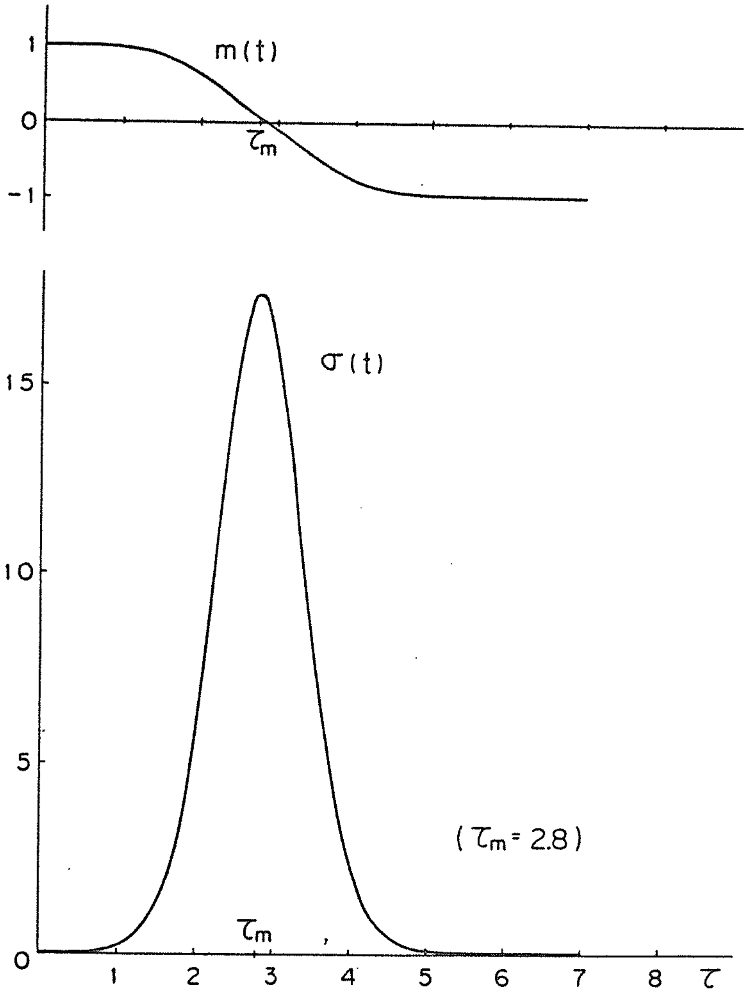

Fig. 3 The integrated mean m and variance σ of the normalized atomic inversion, $z=R_z/R$, for the superradiance with initial values: $m=\sigma=0$, at $\tau=0$ $(R=100)$, where $\tau=RI_1t$.

that the quantum fluctuation assures us of this result.

4. A TEST OF THE GLANSDORFF-PRIGOGINE INEQUALITY AND OTHER REMARKS

We had conjectured that the evolution criterion (6) might be true in a much wider circumstance than restricted to near the steady state: in view of the idealized characteristic of entropy,[10] it might be true for any solution of the Fokker-Planck equation, so far as it exists. The present computer results for the laser have provided evidence that this is not the case, as shown in Fig. 4. Thus, the Glansdorff-Prigogine inequality can be violated for stochastic systems with instability such as the laser.[11]

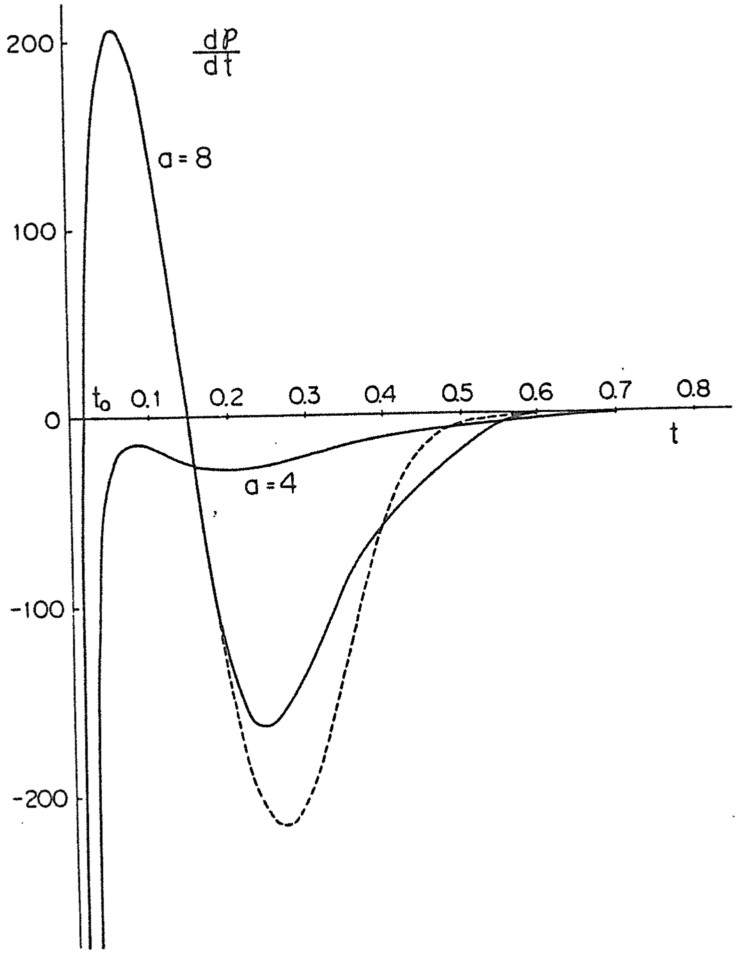

Fig. 4 The derivative in time of the calculated dissipation function (i.e., the entropy production rate) for the laser instability. For a=4, the Glansdorff-Prigogine inequality is fulfilled all the time, while for a=8 the curve crosses abscissa (which is unaltered by going from the n=2 (dotted lines) to n=3 truncations), showing that the instability action violates the said inequality.

We can show by a more analytic means that a similar situation occurs in superradiance when the atomic dipoles are set in initially at the point of full inversion with 0-fluctuations. It can be said that the entropy production decreases rapidly to attain a minimum value which is different from that corresponding to the final equilibrium (or, steady-) state: instead, it increases once and then decreases again, according to the real evolution criterion (see Fig. 5). The "anomalous fluctuation" produced in such instability action could be characterized by this entropy production increase or entropy overproduction. Hence, one might attribute the so-called "dissipative structure" formation to a kind of compensation effect for such an overproduction of fluctuations.

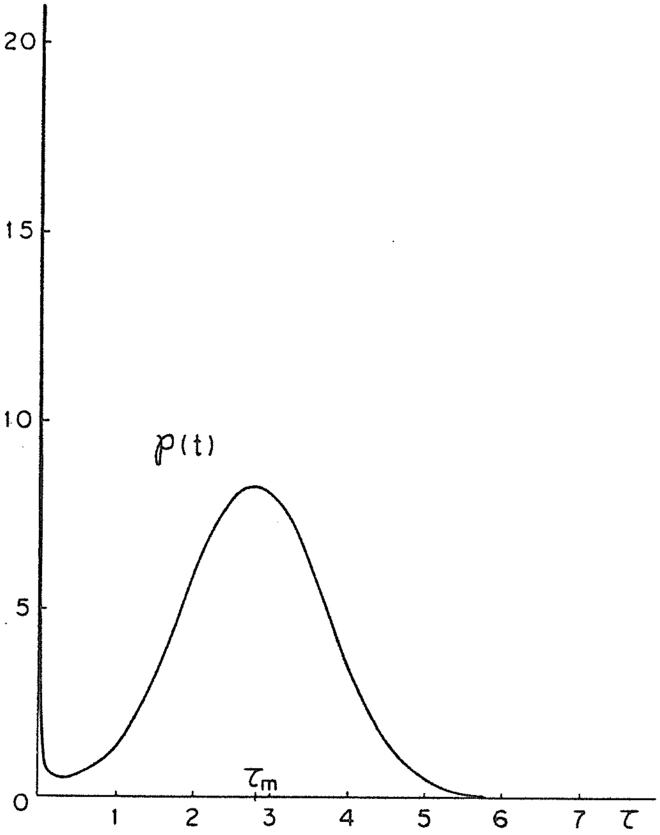

Fig. 5 The time behavior of the calculated dissipation function (i.e., the entropy production) for the superradiance showing a minimum point before τ_m (time of the maximum intensity), another "entropy production minimum".

In conclusion, the typical optical instabilities, the laser and superradiance, can be characterized from a thermodynamic point of view by saying that a unique principle governs the process, that is the least dissipation principle of Onsager.

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11. This statement deserves a careful account of its implication, which we point out here in order to avoid any misleading reference to the Glansdorff-Prigogine original expression,[2]:

$$J_\mu \dot{X}_\mu \le 0 \quad . \qquad \text{(A)}$$

As noted by these authors, the inequality guarantees that $(d/dt)(J_\mu X_\mu) \le 0$ in the near steady-state for which $J_\mu = L_{\mu\nu} X_\nu$ ($L_{\mu\nu} = L_{\nu\mu}$ and constant), but generally the l.h.s. of (A) cannot be identified with the total time-derivative of any scalar function of the potential nature. Therefore, one should look at the quantity $(d/dt)(J_\mu X_\mu)$, if at all concerned with the time behaviour of the "entropy production". (Note that the

laser gives a typical example of the violation of (A) around the unstable point, when Graham's potential lnP is chosen as the entropy.) In the present context, the l.h.s. of (A) may be replaced by the average $\int J_\mu(\partial X_\mu/\partial t)\psi\ dx$, where $J_\mu = (1/2)K_{\mu\lambda}X_\lambda$ and $X_\mu = (\partial/\partial x_\mu)\log(\psi_0/\psi)$, showing that (A) is always valid.[3] However, what we consider here is the total derivative of $\mathcal{P} = \int J_\mu X_\mu \psi\ dx$.

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