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Santilli's Lie-Admissible Mechanics. The Only Option Commensurate with Irreversibility and Nonequilibrium Thermodynamics¹

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Abstract. Our analysis of time reversal symmetry of various dynamical equations of fluid dynamics including Boltzmann integro-differential equation reveals that in a good number of cases there are no unique methods to relegate them to the so-called irreversible category unambiguously though they neither can be grouped into the reversible category. This substantiates Professor Santilli's No Reduction Theorem [1–3] that formed a base to develop genomathematics [4]. Hence, we once again substantiate the assertion of Professor Santilli that the only option commensurate with irreversibility and nonequilibrium thermodynamics is Santilli's Lie-Admissible Mechanics.

Keywords: Time reversal symmetry, Genomathematics, Lie Admissibility, Thermodynamics, Irreversible Thermodynamics, Irreversibility, Kinetic Theory.

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INTRODUCTION

Traditionally there are two different ways one establishes irreversibility of a motion. The dynamical irreversibility is determined and understood using a yard stick of time reversal symmetry. The second yard stick of irreversibility originates from the second law of thermodynamics (see for example [5]) and also via Boltzmann integro-differential equation [6]. Indeed, the dynamical reversibility and irreversibility can be worked out in principle both at microscopic and macroscopic levels of considerations. Whereas the thermodynamic reversibility and irreversibility are determined at the macroscopic level only. It is believed that these reversibility and irreversibility aspects are well understood and their mathematical descriptions are seemingly sound. However, still there exist certain ambiguities that would be presented in this paper. For example, one striking example is that of the following unresolved paradox, the Loschmidt paradox (J. Loschmidt, *Sitzungsber. Kais. Akad. Wiss. Wien, Math. Naturwiss. Classe* 73, 128 -142 (1876)). Consider the case of a non-uniform dilute monatomic gas. Its molecules follow the reversible dynamics, that is these molecules follow the invariant to time reversal Newtonian equations. But when the time variation of Boltzmann- H function is computed, which involves the kinetic theory based averaging for all molecules over all velocities, the result is a negative definite time rate. This is the well known Boltzmann H -theorem. That is the bi-directional dynamics produces uni-directional evolution. This computed behaviour with time of H -function is then juxtaposed with the law of monotonic increase of entropy of thermodynamics and then it is proposed that the Boltzmann constant times the negative of this H -function is equal to Clausius' entropy. Notice that this approach only side tracks the above paradox but not at all is its solution.

The purpose of this presentation is to elaborate the ambiguities that result on applying the time reversal symmetry

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test to a good number of well known dynamical equations from fluid dynamics, discuss thermodynamic and dynamical reversibilities and then conclude that all the existing shortcomings get resolved if one adopts the gemomathematics based dynamics [7].

THERMODYNAMIC REVERSIBILITY

The *thermodynamic reversibility* gets mathematically described as follows,

$$\begin{aligned} dS &= \frac{dQ}{T} \implies (-dS) = \frac{(-dQ)}{T} \implies dS = \frac{dQ}{T} \\ dU &= dQ - p dV \implies (-dU) = (-dQ) - p(-dV) \implies dU = dQ - p dV \\ dU &= T dS - p dV \implies (-dU) = T(-dS) - p(-dV) \implies dU = T dS - p dV \end{aligned} \quad (1)$$

Notice that dQ is the differential amount of heat exchanged by the system in the forward direction and $(-dQ)$ is that in the reverse direction, but dQ is not the state function. Thus an equilibrium state of a closed system gets described by any two state functions out of the five offered by $dU = T dS - p dV$, namely U, S, V, T, p but in this list obviously dQ doesn't appear. This is an amazing outcome and demonstrates the tight hold of thermodynamics on the state of a system in equilibrium [5]. This result is well tested in laboratory.

Thus a *thermodynamic reversible path* is the one on which a system can be equally carried along forward and reverse directions that guarantees the system to assume the identically same equilibrium states but in reverse order on reversing the transition. Notice that this simple and convincing description of reversibility results because no time parameter is involved in the description.

DYNAMIC REVERSIBILITY

From the above thermodynamic description of reversibility it may look that one cannot have reversibility in dynamical description. However, in practice if one throws a stone vertically straight up it travels through a succession of positions upward and while coming down it follows the same succession of heights and positions but in reverse order. This demonstrates the dynamical reversibility if time factor is ignored. This gets well described by Newtonian equation say, $\mathbf{v} = \mathbf{u} + \mathbf{f}t$, where \mathbf{v} and \mathbf{u} are the velocities, \mathbf{f} is the per unit mass force and t is time. The above so-called dynamic reversibility is usually considered as described well by time reversal symmetry of the preceding equation just by substituting $-t$ for t and its effect is the change of sign of velocities,

$$\mathbf{u} = \frac{d\mathbf{r}}{dt} \xrightarrow{t \rightarrow -t} \frac{d\mathbf{r}}{d(-t)} = -\mathbf{u}. \quad (2)$$

Hence we have,

$$\mathbf{v} = \mathbf{u} + \mathbf{f}t \xrightarrow{T} -\mathbf{v} = -\mathbf{u} + \mathbf{f}(-t) \longrightarrow \mathbf{v} = \mathbf{u} + \mathbf{f}t \quad (3)$$

where we have represented $(\mathbf{r}, \mathbf{u}, t) \rightarrow (\mathbf{r}, -\mathbf{u}, -t)$ as \xrightarrow{T} . That is the same equation describes equally well the forward and backward motions and hence it is termed as a reversible equation. But can we say that the dynamic state of the stone at a chosen height remains identically same for both upward and downward motions. The answer is a straight no. Because the velocity vectors have opposite directions. It simply means that one needs to devise a mathematical language to unambiguously represent this distinction. In fact, this problem gets well attended in Santilli's gemomathematics [4].

DETERMINATION OF TIME REVERSAL SYMMETRY

Let us consider a few examples of fluid dynamical equations [8] both where the time reversal symmetry test produces so-called unambiguous results and those ones where the ambiguity is encountered.

Simple Time Reversal Symmetric Equations

The relation between *convective and local time derivatives* transforms as:

$$\begin{aligned}\frac{d}{dt} &= \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \xrightarrow{T} \frac{d}{d(-t)} = \frac{\partial}{\partial(-t)} + (-\mathbf{u}) \cdot \nabla \\ &\Rightarrow \frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\end{aligned}$$

where \mathbf{u} is the barycentric velocity.

The *Kinetic energy balance equation in Eulerian form* transforms as:

$$\begin{aligned}\frac{\partial \frac{1}{2} \rho \mathbf{u}^2}{\partial t} &= -\nabla \cdot \left(\frac{1}{2} \rho \mathbf{u}^2 \mathbf{u} \right) + \rho \mathbf{F} \cdot \mathbf{u} \\ \xrightarrow{T} \frac{\partial \frac{1}{2} \rho \mathbf{u}^2}{\partial(-t)} &= -\nabla \cdot \left(\frac{1}{2} \rho \mathbf{u}^2 (-\mathbf{u}) \right) + \rho \mathbf{F} \cdot (-\mathbf{u}) \\ \Rightarrow \frac{\partial \frac{1}{2} \rho \mathbf{u}^2}{\partial t} &= -\nabla \cdot \left(\frac{1}{2} \rho \mathbf{u}^2 \mathbf{u} \right) + \rho \mathbf{F} \cdot \mathbf{u}\end{aligned}$$

where \mathbf{F} is the body force per unit mass.

The above equations are no doubt time reversal symmetric in the traditionally understood sense but not in the sense of identical dynamic states as described in section on dynamic reversibility.

Ambiguous to Time Reversal Symmetry Equations

The *Lagrangian form of internal energy balance equation* in the case of a rigid body reads as:

$$\rho \frac{du}{dt} = -\nabla \cdot \mathbf{J}_u = -\nabla \cdot \mathbf{q}$$

Thus \mathbf{J}_u is nothing else but the heat flux density, \mathbf{q} . Now we have the following time reversal transformation,

$$\rho \frac{du}{dt} \xrightarrow{T} \rho \frac{du}{d(-t)} = -\rho \frac{du}{dt}$$

it implies that: $-\nabla \cdot \mathbf{q} \xrightarrow{T} -(-\nabla \cdot \mathbf{q})$ which can happen only when: $\mathbf{q} \xrightarrow{T} -\mathbf{q}$.

However, one may have another argument, viz. *the empirical Fourier law*, $\mathbf{q} = -\lambda \nabla T$, would allow the change of the sign of \mathbf{q} only if ∇T changes sign. But the time reversal operation leaves the sign of ∇T unchanged, therefore, \mathbf{q} will remain invariant on time reversal.

Moreover, in kinetic theory [6, 9, 10] the expression of heat flux is $\mathbf{q} = \overline{\rho \frac{1}{2} \mathbf{C}^2 \mathbf{C}}$ for a non-uniform monatomic gas, where $\mathbf{C} (= \mathbf{c} - \mathbf{u})$ is the chaotic velocity of a molecule and \mathbf{c} is the molecular velocity. In view of this definition \mathbf{C} would change its sign on time reversal as the sign of both \mathbf{c} and \mathbf{u} changes on time reversal. Therefore, $\mathbf{q} = \overline{\rho \frac{1}{2} \mathbf{C}^2 \mathbf{C}}$ would change its sign on time reversal.

Furthermore, in classical irreversible thermodynamics (CIT) [11] the entropy source strength, σ_s , due to heat transfer is quantified as $\sigma_s = \mathbf{q} \cdot \nabla T^{-1} > 0$. Thus if on time reversal \mathbf{q} changes its sign then the second law of thermodynamics appears to stand violated on the time reversed path. Whereas, in extended irreversible thermodynamics (EIT) [12] we have $\sigma_s = \beta \mathbf{q} \mathbf{q}^2 > 0$ hence even if \mathbf{q} changes sign on time reversed path the second law is not violated. From the above elaboration *one may perhaps assume that, in general \mathbf{q} is not time reversal symmetric* but it is not an unambiguous conclusion.

Time reversal symmetry of Boltzmann integro-differential equation

The Boltzmann integro-differential equation for monatomic gas on neglecting body forces reads as [13],

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} = J(f|f)$$

where f is the distribution function corresponding to the molecular velocity \mathbf{c} , \mathbf{r} is the position vector and $J(f|f)$ is the Boltzmann collisional integral given by:

$$J(f|f) = \int \int (f'_1 f' - f_1 f) g \sigma(g, \Omega) d\Omega d\mathbf{c}_1$$

where $\sigma(g, \Omega)$ is the collision cross section that depends on the relative velocity $g = |\mathbf{c}_1 - \mathbf{c}|$ and the scattering solid angle Ω . The primes and indices in the distribution function have the usual meaning, namely, $f'_1 = f(\mathbf{c}'_1, \mathbf{r}, t)$ is the distribution function of particle 1 after collision, etc.

The left hand side of the Boltzmann equation changes sign on time reversal operation, namely:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} \xrightarrow{T} \frac{\partial f}{\partial(-t)} + (-\mathbf{c}) \cdot \frac{\partial f}{\partial \mathbf{r}} \Rightarrow - \left(\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} \right)$$

but the right hand side of Boltzmann equation is obtained as time reversal invariant, namely:

$$J(f|f) = \int \int (f'_1 f' - f_1 f) g \sigma(g, \Omega) d\Omega d\mathbf{c}_1 \xrightarrow{T} J(f|f) = \int \int (f'_1 f' - f_1 f) g \sigma(g, \Omega) d\Omega d\mathbf{c}_1$$

because it does not contain t explicitly.

So far so good but let us analyze it further. On instantaneous time reversal all molecules would reverse their motion then the distribution functions before collision should become those of after collision and vice versa. However, the effecting of this time reversal operation does imply $f(\mathbf{c}, \mathbf{r}, t) = f(-\mathbf{c}, \mathbf{r}, -t)$. Hence, we would have $(f'_1 f' - f_1 f) \xrightarrow{T} (f_1 f - f'_1 f') \Rightarrow -(f'_1 f' - f_1 f)$. With this insight the Boltzmann equation is obtained as time reversal invariant.

But in essence the time reversal operation means the substitution of $-t$ for t without any alteration in the equation. Thus we see that both the options of time reversal operation have their shortcomings.

With these two options for time reversal symmetry of Boltzmann integro-differential equation, now let us examine the famous Boltzmann's H -theoem. Boltzmann defined kinetic theory based H function [6, 13] whose negative is the kinetic theory definition of entropy function³. Its expressions are,

$$\rho s = -k_B \int f(\ln f - 1) d\mathbf{c}, \quad \frac{\partial \rho s}{\partial t} = -div(\rho s \mathbf{u} + \mathbf{J}_s) + \sigma_s$$

where k_B is the Boltzmann constant and the entropy flux density, \mathbf{J}_s , and the entropy source strength, σ_s , are given by,

$$\mathbf{J}_s = -k_B \int \mathbf{C} f(\ln f - 1) d\mathbf{c}, \quad \sigma_s = -k_B \int J(f|f) \ln f d\mathbf{c}$$

The entropy source strength, σ_s , is further mathematically manipulated that produces,

$$\sigma_s = \frac{1}{4} k_B \int \int \int \left(\ln \frac{f'_1 f'_1}{f f_1} \right) (f'_1 f' - f_1 f) g^3 \sigma(g, \Omega) d\Omega d\Omega' d\mathbf{g} d\mathbf{c}_{(1)} \geq 0$$

where $\mathbf{c}_{(1)}$ is the center of mass velocity of the colliding molecular pair. The positive definiteness shown in the preceding equation stems from the fact that if $\ln \frac{f'_1 f'_1}{f f_1} > 0$ then we have $(f'_1 f' - f_1 f) > 0$ and if the former is < 0 then the latter is also < 0 the rest of the terms of the integrands are positive numbers by definition. This is the Boltzmann's H -theorem [11]. Now we see that the positive definiteness of the preceding equation is time reversal invariant in both the above stated options of change or no change of the roles of the distribution functions on time reversal operation. This is a paradoxical situation because irrespective of the Boltzmann equation is taken time reversal invariant or variant the H -theorem that results from it is obtained as time reversal invariant.

The purpose of the present adequately detailed description of deriving the time reversal symmetry of dynamic mathematical descriptions was to highlight the ambiguities in which we are driven to. The present discussion clearly elucidates it.

³ Actually the H -function has been defined by Boltzmann as,

$$H = \int f \ln f d\mathbf{c}$$

which was later related to the entropy function as given in the main text above.

CONCLUDING REMARKS

The above described elaborations unambiguously surface out the fact that on applying time reversal symmetry test to various fluid dynamical equations including the Boltzmann integro-differential equation we are led to the ambiguous results. Indeed, there is a distinction between thermodynamic and dynamic reversibility that is in the former case the identically same states are encountered on reversing the direction because the state of the system doesn't depend on the sign of the exchange differentials. Whereas in the latter case the direction of a vector associated with the system determines its dynamic state. In view of this we recall the *no reduction theorem* of Santilli, namely *the reversible molecular dynamics cannot produce macroscopic irreversible description and vice-versa the irreversible macroscopic motion cannot be reduced to reversible molecular motion of its constituents* [1–3]. This then demands a mathematical apparatus inherited with unidirectionality of the description. This demand is met by Santilli's genomathematics and the corresponding mechanics. In Santilli's genomathematics for forward and backward motions one uses different multiplying genounits namely, for forward motion it is $\hat{I}^>$ and for the backward motion it is $\hat{I}^<$ and $\hat{I}^> \neq \hat{I}^<$. It means we have separate mathematical descriptions for forward and backward motions as they in reality are not reverse of each other. That is no time reversal symmetry test is required. Hence, we conclude that the *Santilli Lie-admissible mechanics* [1, 3, 14] turns out as an only option for mathematical description of irreversibility and hence for nonequilibrium thermodynamics too.

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