

Advances in Hadronic Chemistry and its Applications

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Abstract. In this paper, we outline the foundations of the time invariant, non-unitary covering of quantum chemistry known as hadronic chemistry, we illustrate its validity by reviewing the exact representations of the binding energies of the Hydrogen and water molecules, and present new advances.

1 Introduction

Following decades of research, the Italian-American scientist *Ruggero Maria Santilli* has achieved a new mathematics (hereon referred to as *Santilli's isomathematics* (see the Appendix and Ref. [1] for the original formulation) that has allowed the formulation of the time invariant, non-unitary covering of quantum mechanics and, therefore., of quantum chemistry for broader physical and chemical conditions, respectively.

No doubt quantum mechanics and chemistry have made very fundamental contributions in understanding atomic and chemical aspects thanks to their “majestic axiomatic structure” (in Santilli's words). However, with the advancement of experimental and technological knowledge the increasing limitations of quantum mechanics and chemistry surfaced out. This is the case particularly because the Schrödinger equation does not admit the exact solutions needed for the representation of a complex system, thus forcing the use of either the perturbation or the variational methods [2, 3].

For instance, a good number of 20th century important scientists have characterized quantum mechanics, e.g., as in the following statements:

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<http://www.santilli-foundation.org/docs/Talk-Schedule.docx>

1) Limitations voiced by Bohr in his philosophical writings:

Anyone who is not shocked by quantum mechanics has not understood it [4].

2) Limitations voiced by Einstein in his letter to Max Born, December 12, 1926:

Quantum mechanics is certainly imposing. But an inner voice tells me that it is not yet the real thing. Quantum theory says a lot, but does not really bring us any closer to the secret of the Old One. I, at any rate, am convinced that He (GOD) does not throw dice [5].

He has commented on the “lack of completion” of the theory and referred to it as “a real black magic calculus”.

3) The doubts expressed by Fermi:

Whether quantum mechanics holds in the interior of mesons [6]

4) Limitation voiced by Heisenberg:

From the linear character of the theory as compared to the nonlinearity of real physical world [6]

5) Limitation voiced by Einstein, Podolsky and Rosen:

Quantum mechanics is an incomplete theory.

and so on....

From the above statements by renowned 20th century scientists, it is clear that we need to generalize quantum mechanics and, therefore, quantum chemistry into broader covering theories for a more accurate description of complex physical systems.

On these lines, right from the stage of his graduate studies (1960s) at the University of Torino, Italy, Santilli too had fundamental doubts on the final character of quantum mechanics and chemistry and, therefore, became motivated to construct the covering theories. Although quantum mechanics provided a representation of the structure of *one* Hydrogen atom with incredible accuracy, however when studying *two* Hydrogen atoms bonded into the Hydrogen molecule, clear limitations emerge, such as the inability to achieve an exact representation of binding energies from unadulterated first principles, as well as the limitations get increasingly compounded for more complex molecular structures.

Recall that -

1. Quantum mechanics and chemistry cannot characterize an attractive force among neutral atoms of a Hydrogen molecule.
2. Quantum mechanics and chemistry cannot explain why the Hydrogen and water molecules admit only two H-atoms and not three or more.
3. Characteristics like binding energy, electric and magnetic dipole and multi-pole moments (and sometimes even their signs) of Hydrogen and other molecules have not been represented accurately.
4. So called more accurate representations of binding energies are achieved by the “screening of the Coulomb potential” via the use of an arbitrary multiplicative function of completely unknown physical or chemical origin,

$$V(r) = \frac{e^2}{r} \rightarrow V'(r) = f(r) \frac{e^2}{r} = UV(r)U^\dagger,$$

$$UU^\dagger = f(r) \neq I.$$

However, such a screening occurs with the evident loss of quantized orbits (since the latter are solely admitted by the Coulomb potential), the evident loss of the fundamental Galilean symmetry (and consequential inapplicability of the imprimitivity theorem for a consistent quantization), and other basic insufficiencies.

5. The basic axioms of quantum mechanics and chemistry are known to be reversible over time, while most chemical reactions are known to be irreversible, thus creating the problem of constructing covering theories based on irreversible axioms.

and so on.

More so, quantum mechanics and chemistry are structurally linear theories, thus necessitating the representation of complex multi-body systems via the factorization of the total wave function into its individual components, such as:

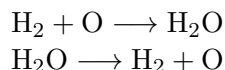
$$\psi_{total} = \psi_1 \times \psi_2 \times \dots \times \psi_n \quad (1.1)$$

This requires the adoption of superposition principle as a prerequisite for consistency in the representation of composite systems. However, composite systems like the water molecule are nonlinear, thus implying the inapplicability of the superposition principle, with consequential inappropriateness of formulating a consistent factorization of the type:

$$H(r, p, \psi, \dots)\psi_{total} \neq H(r, p, \psi, \dots)\psi_1 \times \psi_2 \times \dots \times \psi_n \quad (1.2)$$

thus confirming the inability of quantum mechanics and chemistry as the final theories to represent complex structures.

Additionally, the synthesis of the water molecule from its constituents is a structurally irreversible process, while quantum mechanics and chemistry are reversible theories, thus admitting the possibility of spontaneous decay of water molecule into its atomic constituents, namely (from the time independence of the amplitude and other quantities):



which turns out as a serious drawback of said theories.

Besides all these limitations, quantum mechanics and chemistry admit an additional and rather crucial, inherent limitation, that of divergent or of poorly convergent perturbation series. In fact, the representation of the main features of the water molecule and other complex structures require Gaussian and other methods, all based on expansions whose calculations require the assistance of computers due to their complexities. The insufficiency here referred to is given by the fact that the physical and chemical values of final results under divergent or poorly convergent perturbation series is clearly questionable. Additionally, the time required for basic calculations using big computers is generally excessive, thus implying clear axiomatic limitations from the divergent or poorly convergent character of the series.

For these and other reasons, Santilli never accepted the quantum chemical notion of valence bond. For Santilli, the valence was a merely “nomenclature” without quantitative scientific content because, to achieve the latter, a valence bond must rationally verify the following *requirements*, namely:

1. Represent the force between a pair of valence electrons and its physical or chemical origin.
2. Prove that said force is attractive.

3. The attractive force should provide a quantitative representation of molecular binding energies and other molecular data.

It is well known that quantum mechanics and chemistry could never verify the above basic requirements. On the contrary, according to quantum mechanics and chemistry, identical electrons repel, and certainly do not attract each other even at very short mutual distances.

Therefore, all these limitations motivated Santilli [7] to construct, first, the covering of quantum mechanics known as *hadronic mechanics*, and, subsequently, the corresponding covering of quantum chemistry known as *hadronic chemistry* [1] and these names are nowadays internationally known.

Finally, we should indicate that Santilli conceived hadronic chemistry as a non-unitary covering of quantum chemistry because the map from the Coulomb to the screened Coulomb potential is in fact non-unitary, as recalled earlier. Therefore, by conception and construction, hadronic chemistry admits all infinitely possible screening of the Coulomb law, although formulated within mathematically, physically and chemically consistent covering axioms.

2 Hadronic Chemistry

2.1 Conceptual Foundations

Santilli notes that the main difference between the structure of the Hydrogen atom and of the Hydrogen molecule is the appearance in the latter structure of a deep mutual penetration of the wavepackets of the two valence electrons in singlet couplings. Therefore, Santilli constructs hadronic mechanics and chemistry via the completeness of quantum mechanics and chemistry characterized by the addition of the following effects solely valid at distances of the order of 1 fm (only) [1, 8] (see also review [9])

- *Nonlinearity* - dependence of operators on powers of the wave functions greater than one.
- *Nonlocality* - dependence on integrals over the volume of wave-overlapping that, as such, cannot be reduced to a finite set of isolated points.
- *Nonpotentiality* - consisting of contact interactions caused by the actual physical contact of wavepackets at 1 fm mutual distance with consequential zero range, for which the notion of potential energy has no mathematical or physical meaning.
- *Non-Hamiltonian structure* - lack of complete representability of systems via a Hamiltonian, thus requiring additional terms and, consequently,
- *Non-Unitarity* - the time evolution violating the unitary condition $U \times U^\dagger = U^\dagger \times U = I$.

Notice that the condition of non-unitarity is necessary, otherwise one would fall back fully within the class of unitary equivalence of basic axioms of quantum chemistry.

Santilli applied the mathematical structure of hadronic mechanics to chemical systems thereby achieving results amenable to exact representation of molecular data, precise experimental verifications and novel industrial applications.

In fact, in their important papers of 1999[10] and 2000 [11], Santilli and Shillady have achieved new models for the structure of Hydrogen and water molecules which, apparently for the first time,

1. exhibited a basically new, strongly attractive, non-Coulomb force among pairs of valence electrons in singlet coupling

2. explained, why these molecules have only two Hydrogen atoms,
3. achieved an exact representation of binding energy from unadulterated first axiomatic principle,
4. achieved a representation of the electric and magnetic dipoles of the water molecule which is accurate both in numerical values as well as in the sign, and
5. proved the reduction of computer time by at least a factor of 1000 folds.

2.2 Classification of Hadronic Chemistry

Hadronic chemistry is nowadays a diversified discipline with the following main branches:

- **QUANTUM CHEMISTRY:** assumed to be exactly valid for all mutual distances of particles larger than $1 \text{ fm} = 10^{-13} \text{ cm}$;
- **ISOCHEMISTRY:** characterized by a Lie-isotopic, time invariant, axiom-preserving, non-unitary covering of quantum chemistry formulated over Hilbert-Santilli isospaces over Santilli isofields for the representation of *isolated and reversible chemical structures and processes*;
- **GENOCHEMISTRY:** characterized by a Lie-admissible, time irreversible covering of isochemistry formulated on Hilbert-Santilli genospaces over Santilli genofields for the representation of *irreversible chemical structures and processes*;
- **HYPERCHEMISTRY:** characterized by a multi-valued covering of genochemistry for the representation of *multi-valued organic structures and processes*;
- **ISODUALS of ISO-, GENO-, and HYPER-CHEMISTRY:** characterized by the isodual (anti-Hermitean) map of iso-, geno-, and hyper-chemistry for the description of the *antimatter chemical structures and processes*.

For detailed historical and technical descriptions on hadronic chemistry, the reader is advised to study the monograph [1] and original papers quoted therein. In the following, let us first look at the conceptual foundation of isochemical model of molecular bond for the simplest possible case of the H_2 molecule. Since the Hydrogen molecule is stable, thus reversible, we need to use isochemistry.

2.3 Santilli's Isochemistry

While quantum chemistry is based on the conventional mathematics of quantum mechanics (such as Hilbert spaces over conventional numerical fields), hereon referred to as a mathematics based on the conventional left and right unit $\hbar = 1$, *isochemistry* is based on *Santilli's isomathematics* outlined in Appendix A, and hereon referred to as a mathematics admitting a positive-definite, but otherwise arbitrary, quantity \hat{I} as the left and right unit at all levels. Conventional action-at-a-distance interactions are represented with the conventional Hamiltonian $H = H(r, p)$, while contact non-linear, non-local and non-potential interactions are represented with the new (multiplicative) unit $\hat{I} = \hat{I}(r, p, \psi, \dots) > 0$.

By recalling that, besides the Hamiltonian, the unit is a basis invariant for any theory, Santilli selected the unit for the representation of non-linear, non-local and non-potential interactions as a necessary and sufficient condition to achieve "invariance over time," that is, the prediction of the same numerical values under the same conditions at subsequent times. Other representations of non-linear, non-local and non-potential interactions are possible, but they violate the said invariance over time, thus having no known physical or chemical value.

The additional importance of isomathematics is that of permitting a representation of non-linear, non-local and non-potential interactions in such a way that the resulting isochemistry coincides with conventional quantum chemistry at the abstract, realization-free level, thus illustrating the prefix “iso” used by Santilli in the Greek meaning of being “axiom-preserving.”

By assuming a minimal knowledge of isomathematics as reviewed in Appendix A, let us begin with the conventional non-relativistic quantum mechanical equation in relative coordinates and reduced mass for two ordinary electrons in singlet coupling (the conventional Schrödinger’s equation)

$$H \times \psi(r) = \left(\frac{p \times p}{m} + \frac{e^2}{r} \right) \psi(r) = E \times \psi(r), \quad (2.1)$$

where m is the electron mass and \times is the conventional (associative) product. The above equation shows the *repulsive* Coulomb force between the *point-like* charges of the valence electron pair.

But the electrons have *extended wavepackets* of the order of 1 *fm* whose mutual penetration, as necessary for the valence bond, causes *non-linear, non-local* and *non-potential interactions* (see Figure 1). Therefore, a term correspondingly needs to be added to the Hamiltonian to represent these additional interactions at a short distances. These novel interactions characterize the foundations of Santilli’s hadronic mechanics and chemistry [6].

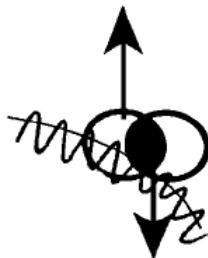


Fig. 1 A schematic view of the the deep overlapping of the wavepackets of valence electrons in singlet coupling resulting in conditions which are known to be *non-linear, non-local*, and *non-potential* (due to the zero-range, contact character of the interactions), thus not being representable via a Hamiltonian (*non-Hamiltonian structure*). As a result, the ultimate nature of valence bonds is outside any representational capability of quantum chemistry. Santilli has build hadronic chemistry for the specific scope of representing the conditions herein considered of the bonding of valence electrons (see the monograph *Hadronic Mathematics, Mechanics and Chemistry* Volume V [8]).

As indicated earlier, the only possibility for a time invariant representation of the bonding of the H-atoms via valence electron couplings is to exit from the class of unitary equivalence of quantum chemistry.

Recall that the axioms of quantum chemistry are invariant under a unitary transformation $U \times U^\dagger = U^\dagger \times U = I$ whose value represented by I is the left and right multiplicative unit of the theory. Therefore, Santilli constructs isochemistry by subjecting all quantities and equations of quantum chemistry to a non-unitary transformation [1],

$$U \times U^\dagger \neq I, \quad U \times U^\dagger = \hat{I} = 1/\hat{T} > 0, \quad (2.2)$$

whose value \hat{I} is then assumed as the basic unit of the new theory. For \hat{I} to be the correct left and right multiplicative unit, Santilli introduces the new multiplication $A \hat{\times} B = A \times \hat{T} \times B$ between arbitrary quantities A, B (such as numbers, matrices, operators, etc.) under which \hat{I} verifies the fundamental axiom of a unit, $\hat{I} \hat{\times} A = A \hat{\times} \hat{I} \equiv A$ for all elements of the set considered.

Santilli's isochemistry then get constructed via the simple application of non-unitary transformation (2.2) to the totality of the quantities and their operators and operation of quantum chemistry. In fact, the new unit is a non-unitary image of the conventional unit, i.e. $\hat{I} = U \times I \times U^\dagger$, the new product is in fact the non-unitary image of the conventional product,

$$U \times (A \times B) \times U^\dagger = \hat{A} \hat{\times} \hat{B} = \hat{A} \times \hat{T} \times \hat{B}, \quad \hat{\psi} = U \times \psi \times U^\dagger, \quad (2.3)$$

and so on. Nowadays, $\hat{I} = 1/\hat{T} > 0$ is called Santilli's isounit, its inverse $\hat{T} = (U \times U^\dagger)^{-1}$ is called the isotopic element and the multiplication between any two generic quantities is called Santilli's isoproduct. This construction then yields the fundamental equation of isochemistry, the *Schrödinger-Santilli isoequation and related isoeigenvalues*,

$$\begin{aligned} U \times (H \times \psi) \times U^\dagger &= (U \times H \times U^\dagger) \times (U \times U^\dagger)^{-1} \times (U \times \psi \times U^\dagger) \\ &= \hat{H} \hat{\times} \hat{\psi} = \hat{H}(\hat{r}, \hat{p}) \times \hat{T}(\hat{r}, \hat{p}, \hat{\psi}, \dots) \times \hat{\psi} \\ &= U \times (E \times \psi) \times U^\dagger \\ &= (U \times E \times U^\dagger) \times (U \times U^\dagger)^{-1} \times (U \times \psi \times U^\dagger) \\ &= \hat{E} \hat{\times} \hat{\psi} = E \times \hat{\psi}. \end{aligned} \quad (2.4)$$

Note that the mathematically correct predictions of isochemistry are the isoeigenvalues \hat{E} . But, in view of their structure $\hat{E} = E \times \hat{I}$, the isounit cancels out with the isotopic element, $\hat{E} = E \times \hat{I} \times \hat{T} \times \hat{\psi} = E \times \hat{\psi}$ and, consequently, the numerical predictions of isochemistry are given by ordinary numbers E .

Following the construction of isochemistry, Santilli proved its crucial invariance over time as follows [1]. All non-unitary transforms (2.2) can be identically rewritten in the form $U = \hat{U} \times \hat{T}^{1/2}$ which turns non-unitary transforms on a Hilbert space over the field of complex numbers into *isounitary transforms* $\hat{U} \hat{\times} \hat{U}^\dagger = \hat{U}^\dagger \hat{\times} \hat{U} = \hat{I}$ thus reconstructing unitarity on the *Hilbert-Santilli isospace* over the field of isocomplex numbers.

It is easy to verify that *the isounit is invariant under isounitary transforms*, $\hat{I} \rightarrow \hat{I}' = \hat{U} \hat{\times} \hat{I} \hat{\times} \hat{U}^\dagger \equiv \hat{I}$, which means that the non-linear, non-local and non-potential interactions in deep wave overlapping of valence electron pairs (that are characterized by \hat{I}) are represented in isochemistry in a way invariant over time. The time invariance of isochemistry is completed by the invariance of the isoproduct under isounitary transforms, as one can verify [1].

The assumption is that pairs of valence electrons from two different atoms bound themselves at short distances into a singlet (mostly, but not totally stable) quasi-particle state called an *isoelectronium* which describes an oo-shaped orbit around the respective two nuclei. The oo-orbit is suggested to represent the diamagnetic character of the H-H molecule, thus being in agreement with experimental verifications.

Note that, once two valence electrons are bonded into the isoelectronium, there is no possibility for bonding additional valence electrons, that explains why Hydrogen- (or water) molecules admit only two Hydrogen atoms.

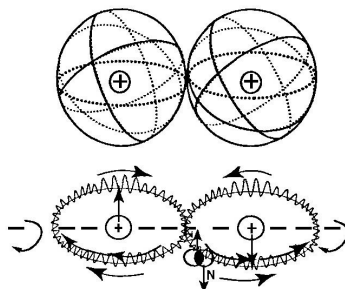


Fig. 2 A view of isochemical model of the Hydrogen molecule at absolute zero degrees temperature without any rotational degree of freedom, with the Santilli-Shillady strong valence bond between the valence electrons pair into *isoelectronium* quasi-particle. Note the oo-shaped orbit of the isoelectronium, thus allowing a representation of the diamagnetic character of the H-molecule since, under an external strong magnetic field, the two H atoms acquire parallel but opposite magnetic polarities with null value of the total magnetic field at sufficient distances.

source: New Science for a New Era [6]

2.4 Santilli-Shillady Strong Valence Bond (1999)

The fundamental three *requirements* mentioned in the introduction were achieved by R. M. Santilli and the American chemist D. D. Shillady in their historical paper [10].

The Limit Case of Stable Isoelectronium

By using the laws of isochemistry, Santilli and Shillady consider the non-unitary transform of equation (2.1), that reads as,

$$\left(\frac{1}{m} \hat{p} \times \hat{T} \times \hat{p} \times \hat{T} + \frac{e^2}{r} \times \hat{T} - \frac{z \times e^2}{r} \right) \times \hat{\psi}(r) = E_0 \times \hat{\psi}(r), \quad (2.5)$$

where, $\hat{\psi}(r) = U \times \psi \times U^\dagger$ is the isowavefunction and the factor $\hat{T} = (U \times U^\dagger)^{-1}$ in the first coulomb term originates from the nonunitary transform of equation (2.1), while the same factor is absent in the second coulomb term because the latter describes the Coulomb interaction at long distance between proton and electron, hence is conventional. Note that eigenvalue E_0 is different from E of equation (2.1) due to the general noncommutativity of the Hamiltonian and the isounit.

At this point, Santilli and Shillady introduced the following realization of the *fundamental isounit of hadronic chemistry* [1], for the radial component r in the fashion,

$$U \times U^\dagger = \hat{I} = 1/\hat{T} = \exp \left(\left[\psi/\hat{\psi} \right] \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r \right) = 1 + \left[\psi/\hat{\psi} \right] \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r + \dots, \quad (2.6)$$

where ψ and $\hat{\psi}$ are the solutions of the unitary and nonunitary Schrödinger wave equations, and ψ_k , $k = 1, 2$, are the conventional quantum mechanical wavefunctions of the two electrons. Correspondingly,

$$\hat{T} \approx 1 - [\psi/\hat{\psi}] \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r, \quad (2.7)$$

$$|\hat{I}| \gg 1, \quad |\hat{T}| \ll 1, \quad (2.8)$$

$$\lim_{r \gg 1 \text{ fm}} \hat{I} = 1 = \hat{T} \quad (2.9)$$

that is, for all mutual distances between the valence electrons greater than 1 fm, the volume integral of equation (2.6) is null wherein the hadronic chemistry recovers the quantum chemistry. Additionally, one should note here that the condition of equation (2.8) gets automatically verified by expressions (2.6) and (2.7) wherein, the explicit form of the isotopic element \hat{T} , emerges in a rather natural way as being smaller than one in absolute value, equation (2.7). This property alone is sufficient to guarantee that all slow convergent series of quantum chemistry converges faster for isochemistry¹ (see sect. 3.4 of reference [12]).

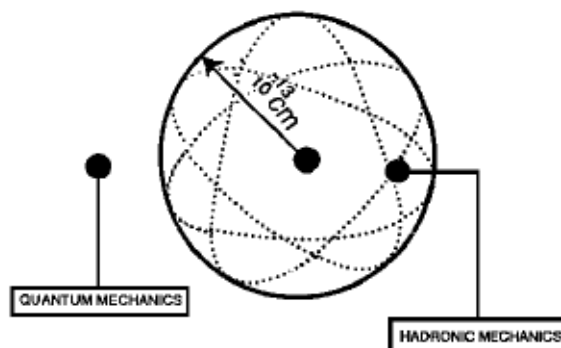


Fig. 3 A schematic unit of the hadronic horizon, namely, of the sphere of radius 1 fm ($= 10^{-13}$ cm) outside which quantum chemistry is assumed to be exactly valid, and inside which nonlinear, nonlocal, and nonpotential effects are no longer negligible, thus requesting the use of hadronic chemistry for their numerical and invariant treatment.

source: Hadronic Mathematics, Mechanics and Chemistry Volume V [8]

Note also that the explicit form of ψ is of a Coulomb type, thus behaving like

¹ For example let us consider a divergent canonical series,

$$A(k) = A(0) + k \times [A, H]/1! + k^2 \times [[A, H], H]/2! + \dots \rightarrow \infty, k > 1,$$

where $[A, H] = A \times H - H \times A$ is the familiar Lie product, and the operators A and H are Hermitian and sufficiently bounded. Then under the isotopic lifting the preceding series becomes

$$\hat{A}(k) = \hat{A}(0) + k \times [A; H]/1! + k^2 \times [[A; H]; H]/2! + \dots \leq |N| < \infty,$$

$$[A; H] = A \times \hat{T} \times H - H \times \hat{T} \times A,$$

which holds e.g. for the case $\hat{T} = \epsilon \times k^{-1}$ where ϵ is sufficiently small positive definite constant. This shows that the original divergent coefficients are now turned into the convergent coefficients. Therefore, by permitting fast convergence of perturbative series, all known applications of hadronic mechanics allows much faster computations. For example, when computer uses iteration method of computation obviously due to the fast convergence of the series having isotopic element as variable it would take drastically less steps of iterations.

$$\psi \approx N \times \exp(-b \times r), \quad (2.10)$$

where,

$$N = \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r \quad (2.11)$$

is approximately a small constant at distances near the hadronic horizon (see Figure 3) of radius

$$r_c = \frac{1}{b}, \quad (2.12)$$

while $\hat{\psi}$ behaves like [10],

$$\hat{\psi} \approx M \times \left(\frac{1 - \exp(-b \times r)}{r} \right), \quad (2.13)$$

with M being also approximately constant within the same range [13].

We then have

$$\hat{T} \approx 1 - \frac{V_{Hulthén}}{r} = 1 - V_0 \frac{e^{-b \times r}}{(1 - e^{-b \times r})}, \quad V_0 = \left(\frac{N^2}{M} r \right) \quad (2.14)$$

Here one recognizes the emergence of the *attractive Hulthén potential*

$$V_{Hulthén} = V_0 \frac{e^{-b \times r}}{1 - e^{-b \times r}}. \quad (2.15)$$

But the Hulthén potential is known to behave like the Coulomb potential at short distances and is much stronger than the latter, that is

$$\frac{V_{Hulthén}}{r} \approx \frac{V_0}{b} \times \frac{1}{r} = \frac{N}{b} = \frac{1}{b} \quad \text{because } N \rightarrow 1. \quad (2.16)$$

Therefore, inside the hadronic horizon we can ignore the repulsive (or attractive) Coulomb forces altogether, and write the columbic terms of equation (2.5) as,

$$\begin{aligned} +\frac{e^2}{r} \times \hat{T} - \frac{z \times e^2}{r} &\approx +\frac{e^2}{r} \times \left(1 - \frac{V_{Hulthén}}{r} \right) - \frac{z \times e^2}{r} \\ &= -V' \times \frac{e^{-b \times r}}{1 - e^{-b \times r}}, \end{aligned} \quad (2.17)$$

where the new constant V' reflects the “absorption” of the repulsive Coulomb potential by the much stronger attractive Hulthén potential.

In this way, *Santilli and Shillady have achieved the strong valence bond for the first time in the history of chemistry namely a valence coupling between two identical electrons in singlet coupling with a strongly attractive force.*

With the above fundamental development we now proceed, in the following subsections, to consider and describe the bonding in Hydrogen and water molecules developed by Santilli and Shillady [10, 11].

2.5 The Isochemical Model of the Hydrogen Molecule with Stable Isoelectronium (1999)

The model of *isoelectronium* therefore gave the clear understanding of the fact that *the Hydrogen molecule admits only two H-atoms and not three or more* and the model also gave the satisfactory reason for the *force of attraction between two valence electrons in singlet coupling*. Now herein, we shall see, how this has been successfully utilized to identify the equation for the structure of the Hydrogen molecule.

According to quantum chemistry, the Hydrogen molecule is a four body system comprising two protons and two electrons with conventional equation for the molecule at rest, that is, the two protons are considered at rest as conventionally done [3, 2],

$$\left(\frac{1}{2\mu_1} p_1 \times p_1 + \frac{1}{2\mu_2} p_2 \times p_2 + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\psi\rangle = E \times |\psi\rangle \quad (2.18)$$

where 1, 2 represents the two electrons; a, b represents the two protons; and R is the distance between the protons as shown in Figure 4. Due to its four body character, the above equation, *does not admit any analytic solution; misses at least 2% of the binding energy; and predicts that the Hydrogen molecule is paramagnetic due to the evident independence of the electrons* [10].

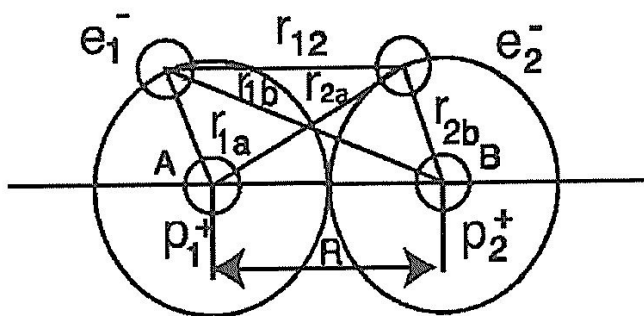


Fig. 4 A schematic view of the representation of distances between two H-protons, respective electrons and distance between protons and electrons.

Therefore, again the task is of subjecting the above model to a nonunitary transform, using,

$$U \times U^\dagger |_{r \approx r_c} = \hat{I} = 1/\hat{T} \neq I, \quad (2.19)$$

in which the nonunitary behavior is only at short mutual distances, namely:

$$r_c = b^{-1} = r_{12} \approx 6.8 \times 10^{-11} \text{cm}, \quad (2.20)$$

and becomes unitary at bigger distances

$$U \times U^\dagger |_{r \leq 10^{-10} \text{cm}} \neq I, \quad \hat{I}_{r \gg 10^{-10} \text{cm}} = I. \quad (2.21)$$

Therefore, the isochemical model coincides with the conventional model everywhere except for small contributions at small distances.

The Hilbert space of systems described by the wave function in equation (2.18) can be factorized in the familiar form in which each term is duly symmetrized or antisymmetrized, as

$$|\psi\rangle = |\psi_{12}\rangle \times |\psi_{1a}\rangle \times |\psi_{1b}\rangle \times |\psi_{2a}\rangle \times |\psi_{2b}\rangle \times |\psi_R\rangle, \quad (2.22)$$

$$\mathcal{H}_{Tot} = \mathcal{H}_{12} \times \mathcal{H}_{1a} \times \mathcal{H}_{1b} \times \mathcal{H}_{2a} \times \mathcal{H}_{2b} \times \mathcal{H}_R. \quad (2.23)$$

The nonunitary transform under consideration would act only on the r_{12} variable while leaving all other terms unchanged. The simplest possible solution is given by

$$U(r_{12}) \times U^\dagger(r_{12}) = \hat{I} = \exp \left[\frac{\psi(r_{12})}{\hat{\psi}(r_{12})} \int d^3r_{12} \hat{\psi}_{1\downarrow}^\dagger(r_{12}) \times \hat{\psi}(r_{12}) \right], \quad (2.24)$$

where ψ 's represent conventional wavefunctions and $\hat{\psi}$'s represent isowavefunctions. The isounitary transform of equation (2.18) showing the short range terms (isochemistry) and simple addition of long range terms (quantum chemistry) yields the radial equation as,

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \hat{T} \times \nabla_1 \times \hat{T} \times \nabla_1 - \frac{\hbar^2}{2 \times \mu_2} \hat{T} \times \nabla_2 \times \hat{T} \times \nabla_2 + \frac{e^2}{r_{12}} \times \hat{T} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle \quad (2.25)$$

Again recall here that the Hulthén potential behaves, at small distances, like the Coulomb one, the isounitary transform of equation (2.18) produces the isochemical model of the Hydrogen molecule as a four-body system:

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2 - V' \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (2.26)$$

showing the effect of the Santilli-Shillady strong valence bond of Hulthén type that absorbs all Coulomb potentials. The equation also explains the reason why the H₂ molecule admits only two H-atoms and provides the exact representation of the binding energy and other molecular characteristics.

2.6 Exactly Solvable Three-Body Isochemical Model of the Hydrogen Molecule

A fundamental implication of hadronic chemistry is that of restricting the above four-body model to a three-body structure evidently composed of the two protons at mutual distance R and the two valence electrons strongly bonded into the isoelectronium quasiparticle. In particular, the charge radius of the isoelectronium is sufficiently small to permit the values²,

² In usual quantum chemistry the allowed approximations from Figure 4 are $r_{1a} \approx r_{2b}$ and $r_{2a} \approx r_{1b}$ but since we are dealing at much shorter distances, viz. r_{12} the approximations of equations (2.27) and (2.28) are in order.

$$r_{12} \leq r_{1a} \text{ and } r_{1b}, \quad r_{12} \approx 0, \quad (2.27)$$

$$r_{1a} \approx r_{2a} = r_a, \quad r_{1b} \approx r_{2b} = r_b. \quad (2.28)$$

Moreover, the H-nuclei are about 2,000 times heavier than the isoelectronium. Therefore, the model of equation (2.26) can be reduced to a restricted three body problem similar to that possible for the conventional H_2^+ ion, but not for the conventional H_2 molecule. By recalling that Hulthén potential behaves at small distances like the Coulomb one and therefore, the isochemical model of Hydrogen molecule as a three-body system can be written as

$$\left(-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_2^2 - V' \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (2.29)$$

where the system does admit an analytic solution in its restricted form under the assumption that the *isoelectronium* is stable. Note also that equation (2.29) is purely quantum chemical because all distances between the constituents are much bigger than 1 fm.

2.7 Isochemical Model of the Hydrogen Molecule with Unstable Isoelectronium

The stable character of the isoelectronium is crucially dependent on the use of the attractive Hulthén potential, which absorbs repulsive Coulomb forces at short distances resulting in attraction. Therefore, the weakening of the Hulthén potential into the Gaussian form of the type

$$\frac{e^{-rb}}{1 - e^{-rb}} \approx \frac{1 - Ae^{-br}}{r}, \quad (2.30)$$

has the direct consequence of turning the isoelectronium into an unstable state. Where, the use of above Gaussian form implies the technical difficulty in using the Hulthén potential $e^{-rb}/(1 - e^{-rb})$. Therefore, an isochemical model of the Hydrogen molecule which is somewhat intermediary between the conventional chemical bond and the isochemical model with a fully stable isoelectronium has been studied (For details ref. [8]).

Unstable isoelectronium refers to the period of time in which the two valence electrons remain within the hadronic horizon of 6.8×10^{-11} cm. The main achievement of this study is the exact representation of molecular characteristics even for the case of one Gaussian approximation of equation (2.30). The question whether the isoelectronium is stable or unstable evidently depends on the amount of instability and its confrontation with experimental data, e.g. magnetic susceptibility, etc.

Under the above assumption, the model of equation (2.29) has been studied using the standard method of variational calculations by setting up the matrix algebra form in a nonorthogonal basis which has been normalized to one. On carrying out the detailed calculations for the Gaussian orbital it was evident that the bond length of the three body model is much shorter than the usual value of 1.4011 Bohr (= 0.74143 Å). Readers may obtain the details from the references [8, 10]. Thereby the bond length was re-optimized after optimization of the scaling for each principal shell. The scaling constants and the orbital contractions are of the order of Angströms at an energy of -7.61509174 Hartrees (= -207.2051232 eV) where the achievement of an exact representation of the binding energy is studied in detail. While it is

expected that a collapsed isoelectronium pair would be even more unstable than a collapsed positronium quasi particle due to the repulsive interaction of the electrons, this three body model of Hydrogen predicts over 6 Hartrees of added molecular stability and a substantial decrease in bond length.

Moreover, as indicated earlier, it is possible that the valence electrons bound themselves into the isoelectronium not in a permanent fashion, but rather in a statistical fashion with only a percentage of their time in a bonded state, wherein the three-body model is evidently insufficient. Therefore, a full four-body isochemical model has been reviewed separately in ref. [8], which also permits the achievement of an exact representation of the binding energy from the first principles without ad hoc adulteration, known as *the Gaussian approximation of the isochemical model of the Hydrogen molecule as a four body system*.

It is also interesting to note that the above model can be used for the study of the bonding of an H-atom to another generic atom, such as HO, thus permitting, again for the first time, novel exact calculations on the water as HOH, namely, as two intersecting isotopic bonds HO and OH, each admitting an exact solution, with possible extension to molecular chains, and extensions to other molecules.

2.8 The Water Molecule (2000)

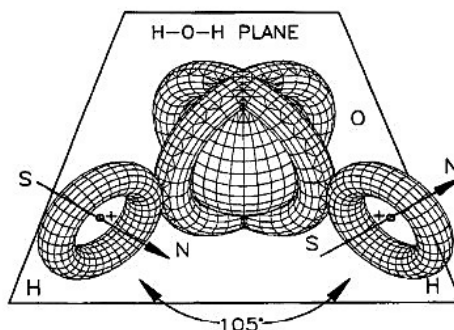


Fig. 5 A view of a water molecule H₂O at absolute zero degrees of temperature without any rotational degrees of freedom, showing the H-O-H plane, the angle 105⁰ between the H-O and O-H dimers and, above all, the natural occurrence according to which the orbital of the H atoms are not spherical, but of toroidal character for their coupling with Oxygen, thus providing direct verification of the isochemical model of the Hydrogen molecule of Figure 2

source: New Science for a New Era [6]

Subsequent to the successful study of the isochemical molecular model of *isoelectronium* for Hydrogen molecules in the historical paper of (1999) [10], Santilli and Shillady proposed their second historical study [11] of hadronic chemistry for the water molecule resulting from the first axiomatic unadulterated principles of binding energy, sign and values of electric and magnetic moments and other data.

The hypothesis is that the two valence electrons, one per each pair of Hydrogen and Oxygen atoms, correlate themselves into a bonded singlet state at a short distance resulting

in two *isoelectronia*, one per each H-O dimer. The bonding force between the two H- and O-atoms was justified by Hulthén force between the two valence electrons in the *isoelectronia*. Therefore, the binding energy is characterized by two oo-shaped orbits of *isoelectronia* around the H-O-H nuclei; and molecule itself is characterized by two *isoelectronia*, one per each H-O dimer. This then renders the system of H-O dimer as being restricted to a three body system (two protons of Hydrogen and Oxygen atoms respectively and an *isoelectronium* H-O dimer³) with an exact solution. The addition of another Hydrogen to the dimer has been proposed as a perturbation via other means.

The approximation that the H-O-H molecule as being composed of two intersecting identical dimers H-O with evidently only one O-atom requires a first correction due to the lack of independence of said dimer. Moreover, in each H-O dimer we shall assume that the Oxygen appears to the *isoelectronium* as having only net positive charge +e located in the nucleus. This evidently requires a second correction which essentially represents the screening of the other 7 electrons of the Oxygen. That is, the additional H-atom bonded with the first H-O dimer can be represented via a nonunitary image of the Coulomb law resulting in screening of Gaussian type

$$2e^2/r \longrightarrow 2e^2(1 \pm e^{-\alpha r})/r, \quad (2.31)$$

where, the double value $2e^2$ originates from the duality of the bonds in H-O-H; α is positive parameter to be determined from the data; the sign “-” applies for screened O-nucleus as seen from an H-electron (because of the repulsion caused by the electron clouds of the Oxygen); and the sign “+” applies for the screened O-nucleus as seen from the H-nucleus (due to the attraction caused by said electron cloud). By denoting with the sub-indices 1 and a to Hydrogen; 2 and b , to Oxygen, and assuming the absence of all hadronic effects, the conventional quantum chemical representation for above H-O dimer with the Oxygen assumed to have only one elementary charge +e in the nucleus is given by,

$$\left(\frac{1}{2\mu_1} p_1 \times p_1 + \frac{1}{2\mu_2} p_2 \times p_2 + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\psi\rangle = E_0 \times |\psi\rangle \quad (2.32)$$

where R denotes the internuclear distance between H and O atoms. Again, as we have seen in the case of the H_2 molecule, here the task is to transform the above model to the nonunitary settings but only at short mutual distances $r_c = b^{-1} = r_{12}$ of the two valence electrons (hadronic horizon), and that should become unitary at relatively larger distances $\hat{I}_{r \leq 10^{-10} \text{cm}} \neq I, I_{r \gg 10^{-10} \text{cm}} = I$.

Moreover, the assumption that the state and related Hilbert space of systems described by the wave function in equation (2.32) can be factorized in the familiar form where each term is duly symmetrized or antisymmetrized,

$$|\psi\rangle = |\psi_{12}\rangle \times |\psi_{1a}\rangle \times |\psi_{1b}\rangle \times |\psi_{2a}\rangle \times |\psi_{2b}\rangle \times |\psi_R\rangle, \quad (2.33)$$

$$\mathcal{H}_{Tot} = \mathcal{H}_{12} \times \mathcal{H}_{1a} \times \mathcal{H}_{1b} \times \mathcal{H}_{2a} \times \mathcal{H}_{2b} \times \mathcal{H}_R. \quad (2.34)$$

³ As described in the following paragraph it is assumed that each *isoelectronium* sees only one positive charge located at the nucleus of Oxygen atom.

The nonunitary transform now shall act only on the r_{12} variable characterizing the isoelectronium while leaving all other variables unchanged. The simplest possible solution for this is to propose the isounit of the form,

$$U(r_{12}) \times U^\dagger(r_{12}) = \hat{I} = \exp \left[\frac{\psi(r_{12})}{\hat{\psi}(r_{12})} \int d^3 r_{12} \hat{\psi}_{1\downarrow}^\dagger(r_{12}) \times \hat{\psi}_{2\uparrow}(r_{12}) \right], \quad (2.35)$$

where ψ 's represents conventional wavefunctions and $\hat{\psi}$'s represents isowavefunctions for which, again the fundamental condition of fast convergence exists as,

$$|\hat{T}| = |(U \times U^\dagger)^{-1}| \ll 1. \quad (2.36)$$

Therefore, by transforming short-range terms (isochemistry) of the isochemical model and adding un-transformed long range ones (chemistry), we are provided the following radial equation,

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \hat{T} \times \nabla_1 \times \hat{T} \times \nabla_1 - \frac{\hbar^2}{2 \times \mu_2} \hat{T} \times \nabla_2 \times \hat{T} \times \nabla_2 + \frac{e^2}{r_{12}} \times \hat{T} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle \quad (2.37)$$

By recalling that the Hulthén potential behaves at small distances like Coulomb one, equation (2.37) becomes,

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2 - V' \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (2.38)$$

This model can be subjected to an important simplification. Now, under the assumption considered herein, the H-O dimer in equation (2.38) can be reduced to a *restricted three body problem* similar to that is possible for H_2^+ molecule, but not for H_2 molecule, accordingly we have the following equation,

$$\left(-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_2^2 - V' \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (2.39)$$

The above indicated corrections/lifting are due to the screening of the other 7 electrons of the Oxygen atom and other corrections needed in the “sensing” of the O-nucleus by the isoelectronium as well as by the H-nucleus, which then yields the *isochemical model of the water molecule* in its projection in the conventional Hilbert space over conventional fields,

$$\left[-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_2^2 - V \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \frac{2e^2}{r_{2a}} - \frac{2e^2(1 - e^{-\alpha r_{1b}})}{r_{1b}} + \frac{e^2(1 + e^{-\alpha R})}{R} \right] \hat{\psi}(r) = E' \hat{\psi}(r), \quad (2.40)$$

where E' is half of the binding energy of the water molecule, and α is a positive parameter that needs to be evaluated experimentally. Under the above approximation, plus the assumption that the isoelectronium is stable, the model (2.40) constitutes the first model of the water molecule admitting the exact analytic solution from first principle in scientific history. Being exactly solvable equation (2.40) exhibits a new explicitly attractive “strong” force among neutral atoms of the H-O dimer, which is absent in conventional quantum chemistry. The equation also explains the reason why the water molecule admits only two H-atoms. The model yields much faster convergence of series with much reduced computer times and resolves many other insufficiencies of quantum theory. Finally, the model is evidently extendable with simple adjustments to an exact solution of other dimers involving the Hydrogen, such as H-C.

3 Variational Calculations of Isochemical Models

As reviewed in the references [10, 11] the variational methods of hadronic chemistry showed the capability of the isochemical models to reach an essentially exact representation of experimental data on the Hydrogen and water molecules, as well as resolving the other issues of inconsistencies of conventional quantum chemistry.

More so, a greatly detailed, independent studies on the models described in [10, 11] was conducted by Aringazin et al [14] via exact solution, Aringazin [15] using Ritz variational method, and by R. Pérez-Enríquez, J. L. Marín and R. Riera [16]. All of them confirm all numerical results of Santilli and Shillady [10, 11].

The Aringazin-Kucherenko study [14] of the restricted, three body isochemical model of the Hydrogen molecule confirms that the isochemical model of equation (2.29) is indeed valid, but only in first approximation, in accordance with the intent of the original proposal [10]. Using the Born-Oppenheimer approximation, i.e. at fixed nuclei, Aringazin and Kucherenko [14] calculated the energy levels via the use of recurrence relations and have computed some 27 tables, each with the identification of the minimum of the total energy, together with the corresponding optimal distances R . Then, they collected all the obtained energy minima and optimal distances in tabular form. With the fourth order interpolation / extrapolation, the graphical representation of the tabular data have shown that minimal total energy behaves as,

$$E_{min}(M) \approx -3.808M$$

and the optimal distance behaves as

$$R_{opt}(M) \approx 0.517/M.$$

At $M = 2m_e$, one has

$$E_{min}(M) = -7.617041 \text{ a.u.}, \quad R_{opt}(M) = 0.258399 \text{ a.u.},$$

which recover the values obtained in Ref. [10]

$$E_{min} = -7.61509174 \text{ a.u.}, \quad R_{opt} = 0.2592 \text{ a.u.}, \quad (3.1)$$

to the remarkable accuracy. The conclusion by Aringazin-Kucherenko was that the Santilli-Shillady restricted three-body model of the Hydrogen molecule is indeed valid as in first approximation.

Whereas, *Aringazin's variational study* [15] of the four-body isochemical model of the Hydrogen molecule uses the application of Ritz variational method to Santilli-Shillady four-body isochemical model of the Hydrogen molecule in equation (2.26) without the restriction that the isoelectronium has the dimension of about one Fermi. In particular the objective was to identify the ground state energy and bond length of the Hydrogen molecule in Born-Oppenheimer approximation, via a Gaussian screening of the Coulomb potential, as well as the original Hulthén potential of equation (2.26). The resulting analysis has proved to be quite sophisticated wherein the Coulomb and exchange integrals were calculated only for Gaussian screening of the Coulomb potential while for the Hulthén potential Aringazin achieved analytical results for the Coulomb integrals. The conclusion of Ritz variational treatment is capable to provide an exact fit of the experimental data of the Hydrogen molecule in confirmation of the results obtained by Santilli-Shillady [10] via SASLOBE variational approach to Gaussian model.

An interesting result of the Ritz variational approach to the Hulthén potential studied by Aringazin [15] is that only some fixed values of the effective radius of the one-level isoelectronium are admitted in the Santilli-Shillady model when treated via the Ritz approach.

Raúl Pérez-Enríquez, José Luis Marín and Raúl Riera in 2007 [16], gave for the first time an exact solution for restricted three-body model of the Hydrogen molecule by following the Ley-Koo solution to the Schrödinger equation for a confined Hydrogen molecular ion, H_2^+ . They obtained for the restricted three-body Santilli-Shillady model *the value of the minimum energy of the ground state of the Hydrogen molecule* and have shown that the confined model to 3-body molecule reproduce the ground state curve as calculated by Kolos, Szalewics and Monkhorst with a precision up to the 4-th digit and a precision in the representation of the binding energy up to the 5-th digit.

4 Conclusions

In the preceding sections, we have reviewed Santilli's covering of quantum chemistry known as hadronic chemistry with particular reference to its isochemical branch (see [1, 10, 11] and the recent monographs [6, 8]). We have then reviewed molecular structures based on the bonding of a pair of valence electrons from different atoms into a singlet quasi-particle state called *isoelectronium* that provides realistic hopes to overcome the 20th century insufficiencies of quantum chemistry thanks to the following results:

1. Exact representation of molecular binding energies from first axiomatic principles without *ad hoc* adulteration.
2. An explanation why the Hydrogen molecule has only two Hydrogen atoms.
3. Reconstruction of the superposition principle at the isotopic level, thus permitting an axiomatically consistent study of composite systems under non-linear, non-local and non-Hamiltonian interactions. This is achieved by embedding of all non-linear terms in the isotopic element,

$$H(r, p, \psi, \dots) = H_0(r, p)T(\psi, \dots), \quad (4.1)$$

thus restoring the superposition principles with exact factorization,

$$H_0(r, p)T(\psi, \dots)\psi_{total} = H_0T(r, p, \psi, \dots)\psi_1 \times \psi_2 \times \dots \times \psi_n, \quad (4.2)$$

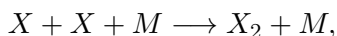
with consequential validity of isochemistry for complex systems.

4. Reduction of computer time by at least 1000-fold. This is permitted by the fact that the absolute value of the isounit as in equation (2.6) is much bigger than one and, consequently, the isotopic element is much smaller than one, that turns all slow convergent series into strong (fast) convergent forms.
5. Admission of a restricted three body structure in the Hydrogen molecule with consequential exact analytic solution that, even though approximate, has nevertheless major implications for deeper studies of molecular structures at large, such as the study of the water molecule at the intersection of two exactly solvable dimers OH.

Moreover, hadronic chemistry admits the broader genochemical and hyperchemical models (not reviewed in this paper for brevity, see [6]) that Santilli respectively developed for the representation of single-valued irreversible processes (such as the water synthesis from Hydrogen and Oxygen), and for multi-valued irreversible biological structures and processes (as expected in biological structures and events).

To conclude, Santilli isochemistry has indeed resolved most, if not all, of the insufficiencies of quantum chemistry for reversible structures and processes by offering an axiomatically consistent framework for further basic advances. Some of the problems needing further investigation are:

1. With the advent of the isoelectronium we need to reinterpret the Morse curve of diatomic molecules.
2. The stability of a diatomic molecule has been interpreted via a three body reaction (see, for example, Frost and Pearson [17]):



thus suggesting its reinterpretation via the isoelectronium.

3. There is the need to develop an isochemical theory of bond angles, molecular geometries, double and triple valence bonds and related fundamental aspects.
4. There is also the need to develop the isochemical theory of valence bonds for excited states as it would be important for a deeper understanding of photochemical and biological photosynthetic processes, as well as several additional open problems in chemistry and biology.
5. Finally, there is the need to develop a comprehensive theory of chemical reactions via the structurally irreversible genomechanics.

5 Appendix

Elements of Santilli Isomathematics.

In an attempt to resolve the scientific insufficiencies of the conventional 20th century theories, when at the Department of Mathematics of Harvard University in the late 1970s, Santilli proposed an axiom-preserving generalization of conventional mathematics, today known as Santilli's "isotopic" mathematics or the isomathematics a [18, 19] (see also the important reviews [20] [21]). It should be recalled that the prefix "iso" in the word "isotopic" is used in the Greek meaning of preserving the original axioms, and the prefix "geno" in the word "genotopic" is used in the sense of including new axioms.

In this appendix, we can only review the most relevant aspects of isomathematics. The reader interested in mathematical details of Santilli's iso- and geno-mathematics should study

the original references [1, 7, 8, 12, 18, 19]. It should be noted that, in this paper, we only use Santilli's isomathematics since we solely consider reversible structures, such as the structure of the Hydrogen and water molecules. By contrast, Santilli's broader genomathematics is necessary for the representation of irreversible processes, such as chemical reactions at large, that are not considered in this paper.

The lifting of the trivial unit $I = +1$ into a generalized unit, \hat{I} , is the first basic step of the isomathematics. Thus the lifting of I to N -dimensional *isounit* is represented as,

$$I = +1 \longrightarrow \hat{I}(t, r, \dot{r}, p, T, \psi, \psi^\dagger, \partial\psi, \partial\psi^\dagger, \dots\dots\dots) \tag{5.1}$$

where t is time, r is the position vector, \dot{r} is the velocity vector, p is the momentum vector, T is the temperature function, ψ is the wave function and ψ^\dagger its transpose, and $\partial\psi$ and $\partial\psi^\dagger$ are the corresponding partial differentials. The positive definiteness of the *isounit*, \hat{I} , is prescribed by,

$$\hat{I}(t, r, \dot{r}, p, T, \psi, \psi^\dagger, \partial\psi, \partial\psi^\dagger, \dots\dots\dots) = \frac{1}{\hat{T}} > 0 \tag{5.2}$$

where \hat{T} is called the *isotopic element* a positive definite quantity.

The *isonumbers*, \hat{n} , are generated as,

$$\hat{n} = n \times \hat{I}, \quad n = 0, 1, 2, 3, \dots\dots\dots \tag{5.3}$$

Thus the *isonumbers* are $\hat{0}, \hat{1}, \hat{2}, \hat{3}, \dots\dots\dots$.

The above realization of *isonumbers* implies,

$$a^{\hat{0}} = \hat{I} = \frac{1}{\hat{T}} > 0 \tag{5.4}$$

Compare this with the traditional algebra where we have $a^0 = 1$.

Notice that the use of *isounit* \hat{I} constitutes the *nonunitary transform*. A simple way to preserve the said nonunitary transform is to express \hat{I} as,

$$\begin{aligned} U \times U^\dagger &\neq I \\ \hat{I} &= U \times U^\dagger = \frac{1}{\hat{T}} > 0 \end{aligned} \tag{5.5}$$

and the Hermiticity of \hat{I} is guaranteed by the prescription,

$$U \times U^\dagger = (U \times U^\dagger)^\dagger \tag{5.6}$$

where the superscript (\dagger) denotes the transpose. Thus it implies that $U \times U^\dagger$ must be a positive definite N -dimensional matrix other than the conventional unit matrix and hence it is no where singular because we then have,

$$0 < \text{Det} (U \times U^\dagger) \neq I \tag{5.7}$$

Thus the lifting to isounit gets represented as,

$$I = +1 \longrightarrow U \times I \times U^\dagger = \hat{I} \quad (5.8)$$

which is the noncanonical-nonunitary transform of the conventional unit.

On the same lines the *isoproduct* is also a noncanonical-nonunitary transform of the conventional product, that gets illustrated as,

$$\begin{aligned} A \times B &\longrightarrow U \times (A \times B) \times U^\dagger \\ &= (U \times A \times U^\dagger) \times (U \times U^\dagger)^{-1} \times (U \times B \times U^\dagger) \\ &= \hat{A} \times \hat{T} \times \hat{B} = \hat{A} \hat{\times} \hat{B} \end{aligned} \quad (5.9)$$

Thus we have obtained the following *isotopicliftings*, namely:

$$\times \longrightarrow \hat{\times} = \times (U \times U^\dagger)^{-1} \times = \times \hat{T} \times \quad (5.10)$$

$$A \longrightarrow U \times A \times U^\dagger = \hat{A} \quad (5.11)$$

The *isoproducts* of iso- and conventional quantities get expressed as,

$$\hat{A} \hat{\times} \hat{B} = \hat{C} = A \times \hat{I} \times \hat{T} \times B \times \hat{I} = (A \times B) \times \hat{I} = C \times \hat{I} = \widehat{AB} \quad (5.12)$$

$$A \hat{\times} B = A \times \hat{T} \times B \quad (5.13)$$

Thus \hat{I} being a *multiplicative isounit* we identically have,

$$\hat{I} \hat{\times} \hat{A} = \hat{A} \hat{\times} \hat{I} = \hat{A} \quad (5.14)$$

$$\hat{I} \hat{\times} A = A \hat{\times} \hat{I} = A \quad (5.15)$$

Hence, in general we have,

$$\hat{n} \hat{\times} A = n \times \hat{I} \times \hat{T} \times A = nA$$

The *isoproducts* are not necessarily *isocommutative*

$$\hat{A} \hat{\times} \hat{B} \neq \hat{B} \hat{\times} \hat{A}$$

but are *isoassociative*, namely:

$$\hat{A} \hat{\times} (\hat{B} \hat{\times} \hat{C}) = (\hat{A} \hat{\times} \hat{B}) \hat{\times} \hat{C} \quad (5.16)$$

The *isosums* are given as,

$$A \hat{+} B = A + B, \quad \hat{A} \hat{+} \hat{B} = \hat{A} + \hat{B} \quad \text{implying} \quad + = \hat{+} \quad (5.17)$$

The *isosums* are commutative and associative

$$\hat{A} + \hat{B} = \hat{B} + \hat{A} \quad (5.18)$$

$$(\hat{A} + \hat{B}) + \hat{C} = \hat{A} + (\hat{B} + \hat{C}) \quad (5.19)$$

There exists an *additive isounit*, $\hat{0}$, such that,

$$\hat{A} + \hat{0} = \hat{0} + \hat{A} = \hat{A} \quad (5.20)$$

where the lifting to *isozero*, $\hat{0}$, is expressed as $0 \rightarrow U \times 0 \times U^\dagger \equiv \hat{0}$, and the negative isonumber, $-\hat{A}$ follows the following relationship with its positive counterpart, namely:

$$\hat{A} + (-\hat{A}) = \hat{0} \tag{5.21}$$

The isoproducts and isosums follow the right and left *isodistributive law*, namely:

$$\hat{A} \hat{\times} (\hat{B} + \hat{C}) = \hat{A} \hat{\times} \hat{B} + \hat{A} \hat{\times} \hat{C}, \quad (\hat{A} + \hat{B}) \hat{\times} \hat{C} = \hat{A} \hat{\times} \hat{C} + \hat{B} \hat{\times} \hat{C} \tag{5.22}$$

From the above *liftings* we have,

$$\begin{aligned} \hat{A}^{\hat{n}} &= \hat{A} \hat{\times} \hat{A} \hat{\times} \hat{A} \hat{\times} \hat{\times} \dots \hat{\times} \hat{A} \hat{\times} \hat{A} \\ &= A \times \hat{I} \times \hat{T} \times A \times \hat{I} \times \hat{T} \times A \times \hat{I} \times \hat{T} \times \dots \times \hat{T} \times A \times \hat{I} \\ &= A^n \hat{T}^{n-1} \hat{I}^n = A^n \hat{I} \end{aligned} \tag{5.23}$$

$$\begin{aligned} A^{\hat{n}} &= A \hat{\times} A \hat{\times} A \hat{\times} \dots \hat{\times} A \\ &= A \times \hat{T} \times A \times \hat{T} \times A \times \hat{T} \times \dots \times \hat{T} \times A \\ &= A^n (\hat{T})^{n-1} = A^n \hat{T} \end{aligned} \tag{5.24}$$

Notice the difference between the result of multiplication to A^n by \hat{I} and \hat{T} . The *isosquareroot* gets depicted as,

$$\hat{A}^{\hat{1}/2} = A^{1/2} \times \hat{I}^{1/2} \tag{5.25}$$

But as \hat{I} is the *isounit* we have,

$$\widehat{\hat{I}^{1/2}} = \hat{I} = \hat{I}^{1/2} \tag{5.26}$$

that gets illustrated as,

$$\widehat{\hat{I}^{1/2}} = (a^{\hat{0}})^{1/2} = a^{1/2 \hat{\times} \hat{0}} = a^{\hat{0}} = \hat{I} \tag{5.27}$$

$$\hat{I}^{1/2} = (a^{\hat{0}})^{1/2} = a^{1/2 \hat{\times} \hat{0}} = a^{\hat{0}} = \hat{I} \tag{5.28}$$

Thus the iso- and conventional products of isounit, \hat{I} gets illustrated in general as,

$$\hat{I}^{\hat{n}} = (a^{\hat{0}})^{\hat{n}} = a^{\hat{n} \hat{\times} \hat{0}} = a^{\hat{0}} = \hat{I} \tag{5.29}$$

$$\hat{I}^n = (a^{\hat{0}})^n = a^{n \hat{\times} \hat{0}} = a^{\hat{0}} = \hat{I} \tag{5.30}$$

where we have used $\hat{0} \hat{\times} \hat{n} = \hat{0} = \hat{0} \hat{\times} n$. Hence we have,

$$(\hat{I})^n = (\hat{I})^{\hat{n}} = \hat{I}, \quad n = 1, 2, 3, \dots \tag{5.31}$$

$$(\widehat{\hat{I}})^n = (\widehat{\hat{I}})^{\hat{n}} = \widehat{\hat{I}}, \quad n = 1, 2, 3, \dots \tag{5.32}$$

but we have,

$$\hat{I}^{\hat{0}} = \hat{I} \quad \text{and} \quad \hat{I}^0 = I = 1, \quad \widehat{\hat{I}}^{\hat{0}} = \widehat{\hat{I}} \quad \text{and} \quad \widehat{\hat{I}}^0 = I = 1 \tag{5.33}$$

Moreover, \hat{I} being an *isounit* there we have,

$$\hat{A}^{\hat{I}} = \hat{A} = A \times \hat{I} \quad (5.34)$$

(Compare: $A^1 = A$ or $A^I = A$ as $I = +1$).

The lifting of the conventional division to the *isodivision* is shown as,

$$\begin{aligned} A \div B &\longrightarrow U \times (A \div B) \times U^\dagger \\ &= U \times \frac{A}{B} \times U^\dagger \\ &= \frac{U \times A \times U^\dagger}{U \times B \times U^\dagger} (U \times U^\dagger) \\ &= \frac{\hat{A}}{\hat{B}} \times \hat{I} = \frac{A}{B} \times \hat{I} \\ &= \hat{A} \hat{\div} \hat{B} = \hat{A} / \hat{B} \end{aligned} \quad (5.35)$$

Thus we have obtained the following nonunitary transform:

$$\div \longrightarrow \hat{\div} = \div \times \hat{I} \quad \text{or} \quad / \longrightarrow \hat{/} = (/) \times \hat{I} \quad (5.36)$$

Now the *isoinverse* is represented as,

$$\hat{A}^{-\hat{I}} = \hat{I} \hat{\div} \hat{A}^{\hat{I}} = \frac{\hat{I}}{\hat{A}^{\hat{I}}} \times \hat{I} = \frac{\hat{I}^2}{A \times \hat{I}} = A^{-1} \times \hat{I} \quad (5.37)$$

Thus we see that \hat{I} being an *isounit* we correctly have $\hat{I} \times \hat{I} = \hat{I}$ and $\hat{I} \div \hat{I} = \hat{I}$.

The isoproduct of an isoquantity with its isoinverse obviously produces isounit, \hat{I} , namely:

$$\hat{A}^{\hat{I}} \hat{\times} \hat{A}^{-\hat{I}} = A \times \hat{I} \times \hat{I} \times A^{-1} \times \hat{I} = 1 \times \hat{I} = \hat{I} = \hat{A}^{\hat{0}} \neq I \quad (5.38)$$

Thus it represents the isorule: anything raised to $\hat{0}$ is equal to \hat{I} . The same remains true for the conventional quantities too, namely:

$$A^{\hat{0}} = \hat{I} = \hat{A}^{\hat{0}} \quad (5.39)$$

Similarly,

$$\hat{a}^0 = (a \times \hat{I})^0 = a^0 \hat{I}^0 = 1 \times 1 = 1 \quad (5.40)$$

which is the mathematical expression of the rule: anything raised to power 0 is equal to 1.

The isolifting of a complex number, say c , is similar to non-complex number,

$$c = (a + i \times b) \longrightarrow \hat{c} = c \times \hat{I} = (a + i \times b) \times \hat{I} = (\hat{a} + i \times \hat{b}) \quad (5.41)$$

where i is the imaginary unit $i = \sqrt{-1}$.

The *isonorm* is represented as,

$$|\hat{A}| = |A| \times \hat{I} \quad (5.42)$$

The *isonorm* of *isoproducts* transform as,

$$|\hat{A} \hat{\times} \hat{B}| = |\hat{A}| \times |\hat{B}|$$

Now if $\hat{I} = i$, then the isonumber say \hat{a} transforms as,

$$\hat{a} = a \times \hat{I} = ai, \quad \hat{T} = \hat{I}^{-1} = \frac{1}{i} = -i \tag{5.43}$$

that transforms the isoproduct of isoquantities as,

$$\hat{a} \hat{\times} \hat{b} = (a \times \hat{I}) \times \hat{T} \times (b \times \hat{I}) = (ai)(-i)(bi) = abi = ab\hat{I} = \hat{a}\hat{b} \tag{5.44}$$

and the isodivision of isoquantities transform as,

$$\hat{a} \hat{\div} \hat{b} = a \times \hat{I} \times (\div) \times \hat{I} \times b \times \hat{I} = a \times i \times (\div) \times i \times b \times i = -\frac{a}{b} \times i \tag{5.45}$$

The *isofunctions* get represented as,

$$\hat{f}(\hat{r}) = f(r \times \hat{I}) \times \hat{I}, \tag{5.46}$$

the *isologarithm* as,

$$\hat{\log}_e a = \hat{I} \times \log_e a, \quad \hat{\log}_e \hat{e} = \hat{I}, \quad \hat{\log}_e \hat{I} = 0 \tag{5.47}$$

Other iso-operations on *isologarithms* are,

$$\begin{aligned} e^{\hat{\log}_e \hat{a}} &= \hat{a} \\ \hat{\log}_e(\hat{a} \hat{\times} \hat{b}) &= \hat{\log}_e \hat{a} + \hat{\log}_e \hat{b} \\ \hat{\log}_e(\hat{a} \hat{\div} \hat{b}) &= \hat{\log}_e \hat{a} - \hat{\log}_e \hat{b} \\ \hat{\log}_e(\hat{a}^{-\hat{I}}) &= -\hat{\log}_e \hat{a} \\ \hat{b} \hat{\times} \hat{\log}_e \hat{a} &= \hat{\log}_e(\hat{a}^{\hat{b}}) \end{aligned}$$

and the *isoeponentiation* as,

$$\begin{aligned} \hat{e}^{\hat{a}} &= \hat{I} \hat{+} \hat{a} / \hat{1}! \hat{+} \hat{a} \hat{\times} \hat{a} / \hat{2}! \hat{+} \dots = e^a \times \hat{I} \\ &= \left[1 + \frac{\hat{a} \times \hat{T}}{1!} + \frac{\hat{a} \times \hat{T} \times \hat{a} \times \hat{T}}{2!} + \dots \right] \times \hat{I} \\ &= (e^{\hat{a} \times \hat{T}}) \times \hat{I} = \hat{I} \times (e^{\hat{a} \times \hat{T}}) \end{aligned} \tag{5.48}$$

The *isodifferentiation* may be arrived at as follows. One of the transformations for an *isodifferential* is,

$$dr = \hat{T} \times dr \times \hat{I} \longrightarrow \hat{T} \times d(r \times \hat{I}) = \hat{d}\hat{r}; \hat{I} = const \tag{5.49}$$

Now assume $\hat{I} \neq constant$ that leads us to,

$$\hat{d}\hat{r} = \hat{T}d\hat{r} = \hat{T}d(r \times \hat{I}) \neq dr \tag{5.50}$$

Similarly, the *isoderivatives* get represented as,

$$\hat{\partial} / \hat{\partial}\hat{r} = \hat{I} \times \partial / \partial r \tag{5.51}$$

The *isointegration* gets obviously represented as,

$$\hat{\int} = \hat{I} \times \int \tag{5.52}$$

and hence we have,

$$\hat{\int} \hat{d}\hat{r} = \hat{I} \times \int \hat{T} \times d(r \times \hat{I}) = \hat{I} \times \int dr \tag{5.53}$$

The isotopiclifting of Schrödinger wave equation may be achieved in two ways:

1. As adopted in the recent monograph entitled “New Sciences for A New Era” the said *isotopic lifting* is described as,

$$\begin{aligned}
 H \times |\psi\rangle &= E^0 |\psi\rangle \rightarrow U \times (H \times |\psi\rangle) \times U^\dagger \\
 &= (U \times H \times U^\dagger) \times (U \times U^\dagger)^{-1} \times (U \times |\psi\rangle \times U^\dagger) \\
 &= \hat{H} \times \hat{T} \times |\hat{\psi}\rangle = \hat{H} \hat{\times} |\hat{\psi}\rangle \\
 &= U \times (E \times |\psi\rangle) \times U^\dagger \\
 &= (U \times E \times U^\dagger) \times (U \times U^\dagger)^{-1} \times (U \times |\psi\rangle \times U^\dagger) \\
 &= \hat{E} \hat{\times} |\hat{\psi}\rangle = E |\hat{\psi}\rangle
 \end{aligned} \tag{5.54}$$

That is we have arrived at the *iso-Schrödinger* equation,

$$\hat{H} \hat{\times} |\hat{\psi}\rangle = E |\hat{\psi}\rangle \tag{5.55}$$

Notice that the involved definition of *isowavefunction* is.

$$|\hat{\psi}\rangle = U \times |\psi\rangle \times U^\dagger \tag{5.56}$$

and we have not lifted E^0 to its iso-counterpart because the new iso-Hamiltonian operator *isoperates* on isowavefunction which is bound to produce a different value of corresponding energy eigenvalue.

2. The second option, that has been extensively used in the Hadronic mechanics literature, is:

$$\begin{aligned}
 H \times |\psi\rangle &= E^0 |\psi\rangle \rightarrow U \times (H \times |\psi\rangle) \\
 &= (U \times H \times U^\dagger) \times (U \times U^\dagger)^{-1} \times (U \times |\psi\rangle) \\
 &= \hat{H} \times \hat{T} \times |\hat{\psi}\rangle = \hat{H} \hat{\times} |\hat{\psi}\rangle \\
 &= U \times (E \times |\psi\rangle) = E \times (U \times |\psi\rangle) \\
 &= E |\hat{\psi}\rangle
 \end{aligned} \tag{5.57}$$

In this choice the *isowavefunction* gets defined as,

$$|\hat{\psi}\rangle = U \times |\psi\rangle \tag{5.58}$$

and the arguments to use E instead of E^0 on isotopiclifting remains the same.

In this paper we have used the first choice.

The *isoinner product* is defined as,

$$\langle \hat{\psi} | \hat{\phi} \rangle = \hat{I} \int d^3r \hat{\psi}^\dagger \hat{T}(r, \dots) \hat{\phi} \tag{5.59}$$

and the *isonormalization* is defined as,

$$\langle \hat{\psi} | \hat{\psi} \rangle = \hat{I} \tag{5.60}$$

The *isouncertainties* are defined in general as,

$$\Delta x \Delta k \geq \frac{1}{2} \langle \hat{I} \rangle, \quad \Delta x \approx a/\hat{T}^{1/2}, \quad \Delta k \approx 1/(a\hat{T}^{1/2}), \quad I = \hbar \tag{5.61}$$

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