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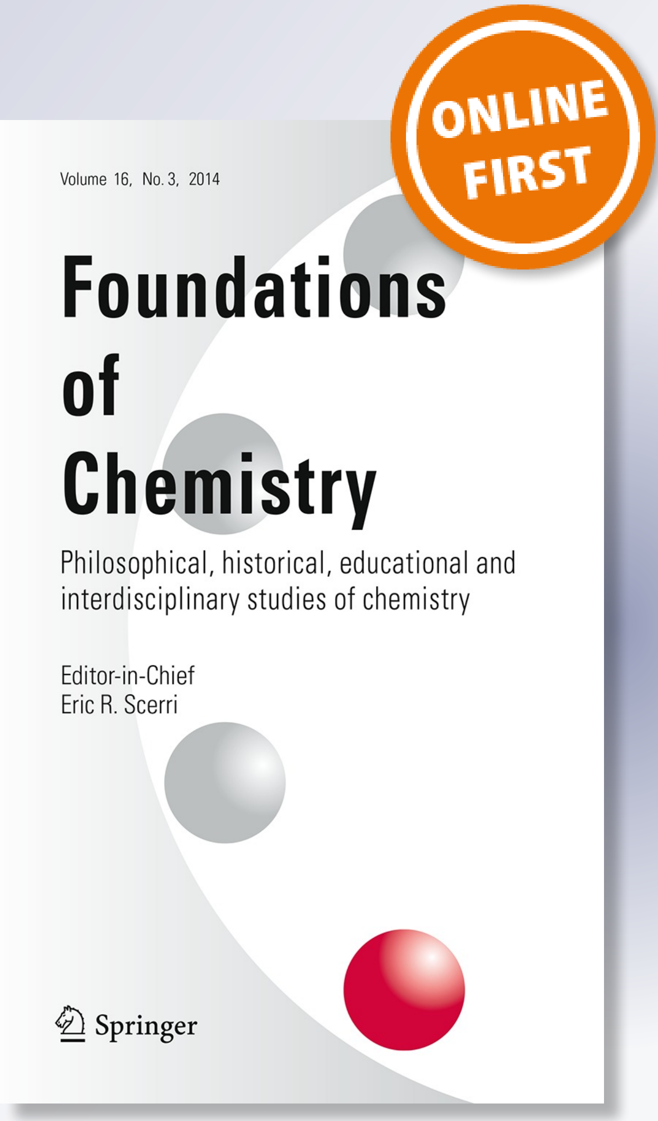

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Advances in hadronic chemistry and its applications

Vijay M. Tangde[1]

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.

Keywords Hadronic chemistry · Quantum chemistry · Isomathematics

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 Animalu 1994 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 when 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 (Kauzmann 1957; Eyring et al. 1961).

For instance, a good number of twentieth century scientists of repute have commented on quantum mechanics, for example recall the following statements:

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(1) Limitations voiced by Bohr in his philosophical writings:

Anyone who is not shocked by quantum mechanics has not understood it (Heisenberg 1971).

(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 (Ankerberg et al. 1996). *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 (Gandzha et al. 2011).

(4) Limitation voiced by Heisenberg:

From the linear character of the theory as compared to the nonlinearity of real physical world (Gandzha et al. 2011).

(5) Limitation voiced by Einstein, Podolsky and Rosen:

Quantum mechanics is an incomplete theory.

and so on...

From the above statements by renowned twentieth 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 in the 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, 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 increasing limitations for more complex molecular structures.

Let us recall a few of the limitations of quantum mechanics:

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. 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,

$$\begin{aligned} &V(r) = \frac{e^2}{r} \rightarrow V'(r) = f(r)\frac{e^2}{r} = UV(r)U^{\dagger}, \\ &UU^{\dagger} = f(r) \neq I. \end{aligned}$$

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.
6. 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:

$$\psi_{total} = \psi_1 \times \psi_2 \times \cdots \times \psi_n \tag{1}$$

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:

$$H(r, p, \psi, \cdots)\psi_{total} \neq H(r, p, \psi, \cdots)\psi_1 \times \psi_2 \times \cdots \psi_n \tag{2}$$

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

7. 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):

$$H_2 + O \longrightarrow H_2O$$
$$H_2O \longrightarrow H_2 + O$$

which turns out as a serious drawback of said theories.

8. Beside 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 attractive.

3. The attractive force provides 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 (1978) to construct, first, the covering of quantum mechanics known as *hadronic mechanics,* and, subsequently, the corresponding covering of quantum chemistry known as *hadronic chemistry* (Santilli 2001) 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.

Hadronic chemistry

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) (Santilli 2001, 2008) (see also review Trell 2003)

- *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 path breaking papers, Santilli and Shillady (1999, 2000) 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.

For detailed historical and technical descriptions on hadronic chemistry, the reader is advised to study monograph (Santilli 2001) 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.

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* (see for example, Santilli HMMC-III (2007) and for very elementary account Ref. Bhalekar (2013)), and hereon referred to as a mathematics admitting a positive-definite, but otherwise arbitrary, quantity $\hat{I}$ as the left and right multiplication 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 $\hat{I} = \hat{I}(r, p, \psi, \ldots) > 0$.

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, 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)

$$H \times \psi(r) = \left(\frac{p \times p}{m} + \frac{e^2}{r}\right)\psi(r) = E \times \psi(r), \tag{3}$$

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 Fig. 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 (Gandzha et al. 2011) (Figs. 2, 3).

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 I is the left and right unit of the theory. Therefore, Santilli (2001) constructs isochemistry by subjecting all quantities and equations of quantum chemistry to a non-unitary transformation,

$$U \times U^{\dagger} \neq I, \quad U \times U^{\dagger} = \hat{I} = 1/\widehat{T} > 0, \tag{4}$$

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 unit, Santilli introduces the new multiplication $A \hat{\times} B = A \times \widehat{T} \times B$ 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 can then be constructed via the simple application of non-unitary transformation (4) to the totality of the quantities and their operation of quantum chemistry. In fact, the new unit is a non-unitary image of the conventional unit, $\hat{I} = U \times I \times U^{\dagger}$, the new product is in fact the non-unitary image of the conventional product,

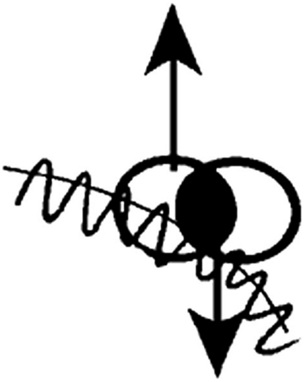

Fig. 1 A schematic view of the the deep overlapping of the wavepackets of valence electrons in singlet coupling resulting in conditions which are known to be *non-linear, non-local,* and *non-potential* (due to the zero-range, contact character of the interactions), thus not being representable via a 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 (Santilli 2008)]

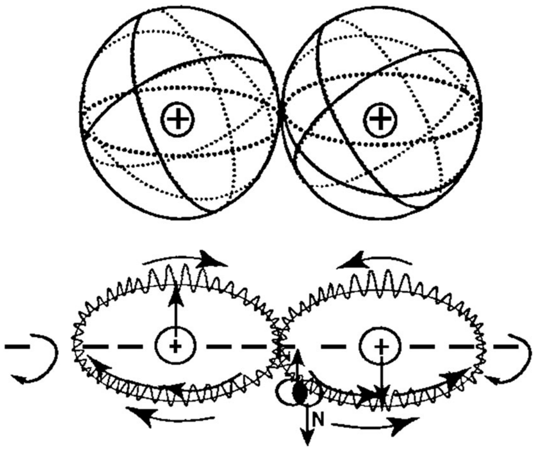

Fig. 2 A view of isochemical model of the Hydrogen molecule at absolute 0° temperature without any rotational degrees of freedom, with the Santilli–Shillady strong valence bond between the valence electrons pair into *isoelectronium* quasi-particle. Note the *oo-shape* orbital of the isoelectronium, 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 (Gandzha et al. 2011)

$$U \times (A \times B) \times U^{\dagger} = \hat{A} \hat{\times} \hat{B} = \hat{A} \times \widehat{T} \times \hat{B}, \quad \hat{\psi} = U \times \psi \times U^{\dagger}, \tag{5}$$

and so on. Nowadays, $\hat{I} = 1/\widehat{T} > 0$ is called Santilli's isounit, its inverse $\widehat{T} = (U \times U^{\dagger})^{-1}$ 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*,

$$\begin{aligned} & U \times (H \times \psi) \times U^{\dagger} \\ & \quad = (U \times H \times U^{\dagger}) \times (U \times U^{\dagger})^{-1} \times (U \times \psi \times U^{\dagger}) \\ & \quad = \hat{H} \hat{\times} \hat{\psi} = \hat{H}(\hat{r}, \hat{p}) \times \hat{T}(\hat{r}, \hat{p}, \hat{\psi}, \ldots) \times \hat{\psi} \\ & \quad = U \times (E \times \psi) \times U^{\dagger} \\ & \quad = (E \times U \times U^{\dagger}) \times (U \times U^{\dagger})^{-1} \times (U \times \psi \times U^{\dagger}) \\ & \quad = \hat{E} \hat{\times} \hat{\psi} = E \times \hat{\psi}. \end{aligned} \tag{6}$$

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, $\hat{E} = E \times \hat{I} \times \widehat{T} \times \hat{\psi} = E \times \hat{\psi}$ and, consequently, the numerical predictions of isochemistry are given by ordinary numbers E.

Following the construction of isochemistry, Santilli (2001) proved its crucial invariance over time as follows. All non-unitary transforms (4) can be identically rewritten in the form $U = \hat{U} \times \widehat{T}^{1/2}$ 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.

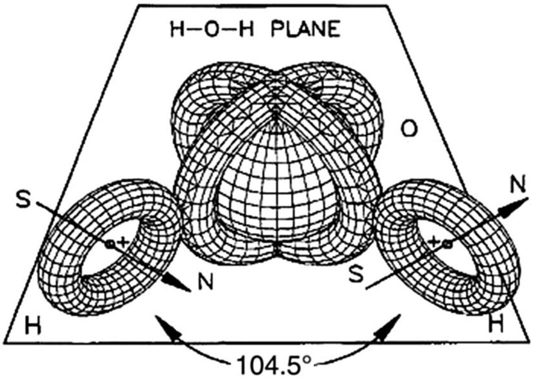

Fig. 3 A view of a water molecule H_2O at absolute 0° of temperature without any rotational degrees of freedom, showing the H–O–H plane, the angle 104.5° between the H–O and O–H dimers and, above all, the natural occurrence according to which the orbital of the H atoms are not spherical, but of toroidal character for their coupling with Oxygen, thus providing direct verification of the isochemical model of the Hydrogen molecule of Fig. 2. *Source*: New Science for a New Era Gandzha et al. (2011)

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 (Santilli 2001).

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* as shown in Fig. 2 which describes an oo-shaped orbit around the respective two nuclei. The oo-orbital 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) molecule admits only two Hydrogen atoms.

Santilli–Shillady strong valence bond (1999)

The fundamental three *requirements* mentioned in the introduction were fulfilled by R. M. Santilli and the American chemist D. D. Shillady in their historical paper (Santilli and Shillady 1999).

The limit case of stable isoelectronium

By using the laws of isochemistry, Santilli and Shillady consider the non-unitary transform of Eq. (3), that reads as,

$$\left(\frac{1}{m}\hat{p}\times\widehat{T}\times\hat{p}\times\widehat{T}+\frac{e^2}{r}\times\widehat{T}-\frac{z\times e^2}{r}\right)\times\hat{\psi}(r)=E_0\times\hat{\psi}(r), \qquad (7)$$

where, $\hat{\psi}(r) = U \times \psi \times U^{\dagger}$ is the isowavefunction and the factor $\widehat{T} = (U \times U^{\dagger})^{-1}$ in the first coulomb term originates from the nonunitary transform of Eq. (3), while the same factor is absent in the second coulomb term because the latter describes the long range Coulomb interaction, hence is conventional. Note that eigenvalue E_0 is different from E of Eq. (3) 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* (Santilli 2001), for the radial component r in the fashion,

$$\begin{aligned} U \times U^{\dagger} = \hat{I} = 1/\widehat{T} &= exp\left(\left[\psi/\hat{\psi}\right] \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r\right) \\ &= 1 + \left[\psi/\hat{\psi}\right] \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r + \cdots, \end{aligned} \tag{8}$$

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

$$\widehat{T} \approx 1 - \left[\psi/\hat{\psi}\right] \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3r, \tag{9}$$

$$|\, \hat{I} \,| \gg 1, \quad |\, \widehat{T} \,| \ll 1, \tag{10}$$

$$\lim_{r \gg 1fm} \hat{I} = 1 = \widehat{T} \tag{11}$$

that is, for all mutual distances between the valence electrons greater than 1 fm, the volume integral of Eq. (8) is null thereby the hadronic chemistry recovers the quantum chemistry. Additionally, one should note here that the condition of Eq. (10) is automatically verified by expressions (8) and (9) wherein, the explicit form of the isotopic element $\widehat{T}$, emerges in a rather natural way as being smaller than one in absolute value, Eq. (9). This property alone is sufficient to guarantee that all slow convergent series of quantum chemistry converges faster in isochemistry[1] (see sect. 3.4 of reference Santilli HMMC-III 2007).

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

$$\psi \approx N \times exp(-b \times r), \tag{12}$$

---

[1] For example let us consider a divergent canonical series,

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

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

$$\begin{aligned} &\hat{A}(k) = \hat{A}(0) + k \times [A \hat{,} H]/1! + k^2 \times [[A \hat{,} H] \hat{,} H]/2! + \cdots \leq |N| < \infty, \\ &[A \hat{,} H] = A \times \widehat{T} \times H - H \times \widehat{T} \times A, \end{aligned}$$

which holds e.g. for the case $\widehat{T} = \epsilon \times k^{-1}$ where ϵ is sufficiently small positive definite constant. This shows that the original divergent coefficient 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.

where,

$$N = \int \hat{\psi}_{1\downarrow}(r) \times \hat{\psi}_{2\uparrow}(r) d^3 r \tag{13}$$

is approximately a small constant at distances near the hadronic horizon of radius

$$r_c = \frac{1}{b}, \tag{14}$$

while $\hat{\psi}$ behaves like (Santilli and Shillady 1999),

$$\hat{\psi} \approx M \times \left(\frac{1 - exp(-b \times r)}{r} \right), \tag{15}$$

with M being also approximately constant under the same range (Animalu 1994).

We then have

$$\widehat{T} \approx 1 - \frac{V_{Hulthén}}{r} = 1 - V_0 \frac{e^{-b \times r}}{(1 - e^{-b \times r})}, \quad V_0 = \left(\frac{N^2}{M} r \right) \tag{16}$$

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

$$V_{Hulthén} = V_0 \frac{e^{-b \times r}}{1 - e^{-b \times r}} r. \tag{17}$$

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

$$\frac{V_{Hulthén}}{r} \approx \frac{V_0}{b} \times \frac{1}{r} = \frac{N}{b} = \frac{1}{b} \qquad \text{because } N \to 1. \tag{18}$$

Therefore, inside the hadronic horizon we can ignore the repulsive (or attractive) Coulomb forces altogether, and write the columbic terms of Eq. (7) as,

$$+ \frac{e^2}{r} \times \widehat{T} - \frac{z \times e^2}{r} \approx + \frac{e^2}{r} \times \left(1 - \frac{V_{Hulthén}}{r} \right) - \frac{z \times e^2}{r} = -V' \times \frac{e^{-b \times r}}{1 - e^{-b \times r}}, \tag{19}$$

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 (1999, 2000).

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*.

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 (Eyring et al. 1961; Kauzmann 1957),

$$\left(\frac{1}{2\mu_1}p_1 \times p_1 + \frac{1}{2\mu_2}p_2 \times p_2 + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times \mid \psi\rangle = E \times \mid \psi\rangle \tag{20}$$

where $1, 2$ represents the two electrons; a, b represents the two protons; and R is the distance between the protons. 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* (Santilli and Shillady 1999).

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

$$U \times U^{\dagger} \mid_{r \approx r_c} = \hat{I} = 1/\widehat{T} \neq I, \tag{21}$$

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

$$r_c = b^{-1} = r_{12} \approx 6.8 \times 10^{-11} \text{ cm}, \tag{22}$$

and becomes unitary at relatively large distances

$$U \times U^{\dagger} \mid_{r \leq 10^{-10}\,\text{cm}} \neq I, \quad \hat{I}_{r \gg 10^{-10}\,\text{cm}} = I. \tag{23}$$

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 Eq. (20) can be factorized in the familiar form in which each term is duly symmetrized or antisymmetrized, as

$$\mid \psi\rangle = \mid \psi_{12}\rangle \times \mid \psi_{1a}\rangle \times \mid \psi_{1b}\rangle \times \mid \psi_{2a}\rangle \times \mid \psi_{2b}\rangle \times \mid \psi_R\rangle, \tag{24}$$

$$\mathcal{H}_{Tot} = \mathcal{H}_{12} \times \mathcal{H}_{1a} \times \mathcal{H}_{1b} \times \mathcal{H}_{2a} \times \mathcal{H}_{2b} \times \mathcal{H}_R. \tag{25}$$

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

$$U(r_{12}) \times U^{\dagger}(r_{12}) = \hat{I} = exp\left[\frac{\psi(r_{12})}{\hat{\psi}(r_{12})} \int d^3 r_{12} \hat{\psi^{\dagger}}_{1\downarrow}(r_{12}) \times \hat{\psi}(r_{12})\right], \tag{26}$$

where ψ's represent conventional wavefunctions and $\hat{\psi}$'s represent isowavefunctions. The isounitary transform of Eq. (20) showing the short range terms (isochemistry) and simple addition of long range terms (quantum chemistry) yields the radial equation and again recall here that the Hulthén potential behaves, at small distances, like the Coulomb one, the isounitary transform of Eq. (20) produces the isochemical model of the Hydrogen molecule as a four-body system:

$$\begin{gathered}\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2\right. \\ \left.-V \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times \mid \hat{\psi}\rangle = E \times \mid \hat{\psi}\rangle\end{gathered} \tag{27}$$

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 H_2 molecule admits only two H-atoms and provides the exact representation of the binding energy and other molecular characteristics.

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 values, [2]

$$r_{12} \leq r_{1a} \text{ and } r_{1b}, \quad r_{12} \approx 0, \tag{28}$$

$$r_{1a} \approx r_{2a} = r_a, \quad r_{1b} \approx r_{2b} = r_b. \tag{29}$$

Moreover, the H-nuclei are about 2,000 times heavier than the isoelectronium. Therefore, the model of Eq. (27) 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

$$\left(-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_2^2 - V \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R}\right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \tag{30}$$

where the system does admit an analytic solution in its restricted form under the assumption that the *isoelectronium* is stable. Note also that Eq. (30) is purely quantum chemical because all distances between the constituents are much bigger than 1 fm.

Now in next section we describe the isochemical model of water molecule as above described model is conveniently applicable to it (Santilli and Shillady 2000).

The water molecule (2000)

Subsequent to the successful study of the isochemical molecular model of *isoelectronium* for Hydrogen molecules in the historical paper of, Santilli and Shillady (1999) proposed their second historical study (Santilli and Shillady 2000) 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 bond as shown in Fig. 3. The bonding force between the two H- and one 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 bonded atoms as being restricted to a three body system (two protons of Hydrogen

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[2] In usual quantum chemistry the allowed approximations 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 Eqs. (28) and (29) are in order.

and Oxygen atoms respectively and an *isoelectronium* of H–O bonded atoms)[3] with an exact solution. The addition of another Hydrogen to H–O has been proposed as a perturbation via other means.

The approximation that the H–O–H molecule as being composed of two intersecting identical H–O with evidently only one O-atom requires a first correction due to the lack of independence of said bonded state. Moreover, in each H–O 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 bond can be represented via a nonunitary image of the Coulomb law resulting in screening of Gaussian type

$$2e^2/r \longrightarrow 2e^2(1 \pm e^{-\alpha r})/r, \tag{31}$$

where, the double value 2e 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 bonded state with the Oxygen assumed to have only one elementary charge $+e$ in the nucleus is given by,

$$\left(\frac{1}{2\mu_1}p_1 \times p_1 + \frac{1}{2\mu_2}p_2 \times p_2 + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\,\psi\rangle = E \times |\,\psi\rangle \tag{32}$$

where R denotes the internuclear distance between H and O atoms. Again, on following what has been described above in the case of the H_2 molecule, the transformation of short-range terms (isochemistry) of the isochemical model and adding un-transformed long range ones (chemistry), we are led to the following radial equation,

$$\begin{aligned}&\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2\right.\\ &\left.-V \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\,\hat{\psi}\rangle = E \times |\,\hat{\psi}\rangle\end{aligned} \tag{33}$$

This model has been further simplified as in the case of Hydrogen molecule to a *restricted three body problem* and further Santilli and Shillady (2000) produced the following *isochemical model of the water molecule*,

$$\begin{aligned}&\left[-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_2^2\right.\\ &\left.-V \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \frac{2e^2}{r_{2a}} - \frac{2e^2(1 - e^{-\alpha r_{1b}})}{r_{1b}} + \frac{e^2(1 + e^{-\alpha R})}{R}\right]\hat{\psi}(r) = E'\hat{\psi}(r),\end{aligned} \tag{34}$$

where E' is half of the binding energy of the water molecule, and α is a positive parameter needs to be evaluated experimentally. Under the above approximation, plus the assumption that the isoelectronium is stable, model (34) constitutes the first model of the water

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[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.

molecule admitting the exact analytic solution from first principle in scientific history. Being exactly solvable Eq. (34) 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.

Variational calculations of isochemical models

As reviewed in the references (Santilli and Shillady 1999, 2000) the variational methods 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 considerably detailed and independent studies on the models of Santilli and Shillady (1999, 2000) was conducted by Aringazin et al. (2000) via exact solution, Aringazin (2000) using Ritz variational method, and by Pérez-Enríquez et al. (2007). All of them confirm all numerical results of Santilli and Shillady (1999, 2000).

The Aringazin–Kucherenko study (Aringazin–Kucherenko 2000) *of the restricted, three body isochemical model of the Hydrogen molecule* confirms that the isochemical model of Eq. (30) is indeed valid, but only in first approximation, in accordance with the intent of the original proposal Santilli and Shillady (1999). Using the Born–Oppenheimer approximation, i.e. at fixed nuclei, Aringazin and Kucherenko (2000) 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 which finally recover the values obtained in Ref. Santilli and Shillady (1999)

$$E_{min} = -7.61509174 a.u., \quad R_{opt} = 0.2592 a.u., \tag{35}$$

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 in first approximation and therefore, that *the two valence electrons of the Hydrogen molecule cannot be permanently bound inside the hadronic horizon with a radius of one Fermi*.

Whereas, *Aringazin's variational study* (Aringazin 2000) *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 Eq. (27) 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 Eq. (27). 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 and Shillady (1999) via SASLOBE variational approach to Gaussian model.

An interesting result of the Ritz variational approach to the Hulthén potential studied by Aringazin (2000) 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 (Pérez-Enríquez et al. 2007), 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 Scrödinger 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*.

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 Santilli 2001; Santilli and Shillady 1999, 2000 and the recent monographs (Gandzha et al. 2011; Santilli 2008)]. 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 twentieth 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,

$$H(r,p,\psi,\cdots) = H_0(r,p)T(\psi,\cdots), \tag{36}$$

   thus restoring the superposition principles with exact factorization,

$$H_0(r,p)T(\psi,\cdots)\psi_{total} = H_0T(r,p,\psi,\cdots)\psi_1 \times \psi_2 \times \cdots \psi_n, \tag{37}$$

   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 Eq. (8) is much bigger than one and, consequently, the isotopic element is much smaller than one, by therefore turning 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 OH bonds.

Moreover, hadronic chemistry admits the broader genochemical and hyperchemical models (not reviewed in this paper for brevity, see Gandzha et al. 2011; Santilli 2008) 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 1961):

$$X + X + M \longrightarrow X_2 + M,$$

   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.

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