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A new iso-chemical model of the hydrogen molecule

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Abstract

Despite outstanding advances throughout this century, we still lack final knowledge on the structure of the hydrogen molecule because of a number of insufficiencies in available models identified in the text. In this paper we use the recently achieved covering of quantum chemistry called hadronic chemistry in its iso-chemical branch, and introduce a new model of the hydrogen molecule characterized by a bond at short distances of the two valence electrons into a singlet quasi-particle state called iso-electronium. We study the iso-chemical model of the hydrogen molecule with a stable iso-electronium describing an oo-shaped orbit around the respective two nuclei, and another model with a weaker realization of the iso-electronium as a partially stable state. We show that the new model provides, apparently for the first time, an exact representation of the binding energy and other characteristics of the hydrogen molecules from axiomatic principles, without ad hoc modifications of theory. In subsequent papers we shall show that the new model permits apparently novel advances in the energy, liquefaction and other technological applications of the hydrogen.

1. Limitations of quantum chemistry

Unquestionably, quantum chemistry [1–4] constitutes one of the most important scientific achievements of this century whose multiple and diversified applications have produced clear benefits to all of mankind.

Nevertheless, science will never admit 'final theories', and structural generalizations of pre-existing doctrines are only a matter of time.

Doubts on the final character of quantum mechanics, and, therefore, of quantum chemistry, can be traced back to Einstein, Podolsky and Rosen (E–P–R) [5], who introduced their celebrated argument of 'lack of completion' of the theory.

With the advancement of experimental and technological knowledge, more and more limitations of quantum chemistry have been identified, such as

(1) Quantum chemistry does not characterize an attractive force among the neutral atoms of the H- (and other) molecule(s) sufficient to explain their bond. In fact, the total Coulomb bonding force between atoms is identically null at the semi-classical level. For this reason, the bond is assumed to be due to exchange, van der Waals and other forces originating in nuclear physics whose strength is known to be weak. To state it differently, quantum chemistry still lacks in a molecular bond the equivalent of the strong force in nuclear physics.
(2) Current models of molecular bonds do not explain why the hydrogen (and water) molecules admit only two H-atoms, and not three or more. In fact, the exchange, van der Waals and other forces were constructed for the specific purpose of admitting an arbitrary number of constituents as necessary to represent nuclei. This main characteristic evidently carries over at the level of molecular bonds, thus preventing a scientific explanation why nature has preferred two hydrogen atoms in the hydrogen and water molecule.
(3) A number of main characteristics of H- (and other) molecules have not been represented accurately so far by quantum chemistry. This is the case for the binding energy, electric and magnetic dipole and multi-pole moments, liquid state and other aspects which still miss a few percentages in their representation.

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(4) Quantum chemistry does not allow meaningful thermodynamical calculations. As an example, the 2% currently missing in the representation of molecular binding energies corresponds to about 959 kcal/mole, which is too large an uncertainty for chemical thermodynamics where reaction energies are typically of the order of 20 kcal/mole.
(5) More accurate numerical representations of molecular data can be achieved via the so-called 'screening of the Coulomb potential' which however constitute a structural departure of the theory from the basic axioms of quantum mechanics and chemistry. As an example, Gaussian screening of the Coulomb law generally requires non-unitary transforms of the original Coulomb settings, thus implying the exiting from the class of equivalence of quantum mechanics and chemistry.
(6) Current models of molecular bonds imply a behavior of H- (and other) molecules under external electric and magnetic fields contrary to experimental evidence. As an illustration, the atoms of a molecular bond preserve their individuality according to quantum chemistry. One of the best established disciplines of this century, quantum electrodynamics, then implies that the valence electrons of all atoms of a molecule must assume the same polarization under an external magnetic field. In turn, this implies the capability by water to acquire a paramagnetic character which is contrary to evidence.
(7) Despite the availability of more powerful computers, accurate configuration interactions converge slowly, thus requiring excessive amounts of computer time for calculations. Such amounts of time increase with accuracy, reaching prohibitive amounts in attempting exact representations.
(8) The still unexplained 'correlation energy' is at times advocated to treat the missing percentages; orbital theories work well at qualitative and semi-empirical levels, but they remain afflicted by yet unresolved problems, such as the correlation among many electrons as compared to the evidence that the correlation occurs mainly for electron pairs.
(9) When models achieve 100% representation of the experimental data, this occurs via the introduction of a number of empirical parameters which generally lack physical meaning and motivation; and other problems.

All the above limitations refer to molecular structures which are closed–isolated and reversible (i.e., they verify usual total conservation laws and their time reversal image is causal).

The limitations of quantum chemistry are multiplied when considering irreversible structures, such as chemical reactions involving hydrogen. In fact, we have in this case a structural incompatibility between the basic axioms of quantum chemistry, and the reality represented because said axioms are structurally reversible (as a necessary condition to represent molecules), without any known possibility to modify them in such a way as to reach a credible representation of the irreversibility in chemical reactions from first axiomatic principles.

When passing to more complex biological structures, any claim of final character of quantum mechanics and chemistry implies the exiting of the boundaries of science. In fact, quantum mechanics and chemistry can only represent systems that are closed and isolated from the rest of the universe (conservative), reversible and rigid, as well known. On the contrary, biological systems require the representation of the time rate of variation of characteristics (e.g., their increase at birth, and their decrease at a later age), they are irreversible and flexible. To put it bluntly, under the conditions of the exact validity of quantum mechanics and chemistry everywhere for the microcosm, our body should be perfectly isolated from the rest of the universe, perfectly eternal and perfectly rigid (for studies of these biological aspects one may consult Ref. [15]).

Moreover, biological systems are generally multivalued, in the sense of requiring a structurally novel mathematics expectedly of the so-called hyper-structural type. In any case, the belief of understanding the extremely complex code of a DNA via the single-valued mathematics underlying quantum chemistry is beyond scientific credibility.

In view of these and other occurrences, in this paper we introduce a covering of quantum chemistry which admits the latter as a particular case, yet includes new properties capable of resolving at least some of the above insufficiencies.

We shall then introduce a new model for the structure of the hydrogen molecule which, apparently for the first time, can: explain why the molecule has only two atoms; achieve an exact representation of the binding energy and other characteristics; permit a dramatic reduction of computer time; and reach other advances.

In subsequent papers we plan to indicate that, even though admittedly small, the percentages currently missing in the exact representation of the characteristics of the hydrogen molecule imply rather important technological advances, including possible new structures of the gas itself, new enhancement of the energy content, new means for liquefaction and other applications.

2. Rudiments of hadronic mechanics

In this paper we follow the historical E–P–R teaching on the 'lack of completion' of quantum mechanics and, therefore, of quantum chemistry [5–9].

Among a variety of possible 'completions', we study the addition of effects resulting from the deep overlapping of the wavepackets of valence electrons in chemical bonds.

As it is well known, all massive particles (beginning with the valence electrons) have a wavepacket of the order of 1 fm (10^{-13} cm). We therefore assume quantum chemistry as being exactly valid at distances bigger than 1 fm, while we seek possible, generally small corrections at mutual distances of 1 fm or less due to the deep overlappings of valence electrons.

Deep mutual penetrations of the wavepackets of particles are known to be: non-linear (i.e., dependent on powers of the wavefunctions greater than one), non-local-integral (i.e., dependent on integrals over the volume of overlapping which, as such, cannot be reduced to a finite set of isolated points), and non-potential (i.e., consisting of 'contact' interactions with consequential 'zero range' for which the notion of action-at-a-distance, potential energy has no mathematical or physical sense).

The latter features evidently imply a non-Hamiltonian theory (i.e., a theory which cannot be solely characterized by the Hamiltonian thus requiring additional terms). It then follows that the emerging theory is non-unitary (i.e., its time evolution violates the unitarity conditions $UU^\dagger = U^\dagger U = I$ when formulated on conventional Hilbert spaces over conventional fields).

In short, we study a 'completion' of quantum mechanics and chemistry via the addition of effects at distances of the order of 1 fm (only) which are assumed to be non-linear, non-local, non-potential, and non-unitary, here generically referred to as 'non-Hamiltonian effects'. Note that the condition of non-unitarity is necessary to exit the class of equivalence of quantum chemistry.

As it is well known by experts in the field, the main technical difficulty of the above completion is that, when treated via the conventional formalism of quantum chemistry, said short range non-Hamiltonian effects have physical inconsistencies so serious to prevent any consistent application to the real world [11, 16].

To give an idea, we indicate that: non-linear theories violate the superposition principle, thus having no meaningful application to composite systems such as molecules; non-local theories violate causality; non-potential theories violate probability laws; non-Hamiltonian theories do not admit invariant basic units of time, length, energy, etc., thus having no meaningful applications to real measurements; non-unitary theories do not preserve the original hermiticity of operators, thus having no physically acceptable observables; and other inconsistencies (see Refs [11, 16] for details).

Quantitative studies on a non-Hamiltonian completion of quantum mechanics, capable of resolving the above problematic aspects, have been recently permitted by hadronic mechanics [10–21], which is an image of quantum mechanics characterized by the novel iso-, geno- and hyper-mathematics [10] for the representation of reversible, irreversible and multi-valued systems, respectively, with Hamiltonian as well as non-Hamiltonian effects. It then follows that hadronic mechanics has three corresponding branches called iso-mechanics, geno-mechanics and hyper-mechanics, respectively.

The latter new mathematics are essentially characterized by the lifting of the conventional unit $I = +1$ of quantum mechanics into invertible generalized units characterized by an $n \times n$ matrix (or operator) $\hat I$ with an arbitrary functional dependence, $I = +1 \to \hat I = \hat I(t, r, \dot r, \psi, \partial\psi, \ldots) = 1/\hat T$, which are Hermitean, $\hat I = \hat I^\dagger$, non-Hermitean, $\hat I \neq \hat I^\dagger$, and multi-valued-non-Hermitean, $\hat I = (\hat I_1, \hat I_2, \ldots) \neq \hat I^\dagger$, respectively.

The new mathematics then emerge via the reconstruction of all conventional algorithms with respect to said generalized units $\hat I$, thus including corresponding lifting of numbers and fields, metric and Hilbert spaces, algebras and geometries, etc. For instance, all conventional (associative) products $A \times B$ of quantum mechanics have to be lifted into the generalized products $A \hat\times B = A \times \hat T \times B$ under which $\hat I = I/\hat T$ is indeed the correct left and right new unit, $\hat I \hat\times A = A \hat\times \hat I \equiv A$, called iso-, geno- and hyper-units. Similar generalizations hold for all other operations, including differentials and derivatives, conventional and special transforms, etc. [15].

The main physical reason for the lifting of the trivial unit $I = +1$ into an operator $\hat I$ is that it provides the only known invariant representation of non-Hamiltonian effects in the pairing of valence electrons [16].

To state it differently, in order to prevent possible misrepresentations of reality, contact–non-potential effects should be represented with anything except a (Hermitean) Hamiltonian. All representations of such effects other than that via Hamiltonians have been proved to be non-variant, thus unsuitable for applications. The representation of contact–non-potential effects via generalized units has been selected because it is the sole known approach yielding an invariant theory which, as such, admits predictions suitable for experimental verifications.

As a simple example, the representation of the novel interactions caused by deep wave-overlappings of the valence electrons as in Fig. 1 can be only done in quantum mechanics and chemistry via the addition of potentials in the Hamiltonian. However, this implies granting potential energy to contact effects which have none (it would be like representing the drag force experienced by the space-shuttle during re-entry with a Hamiltonian), thus implying the description of a system that has no connection with physical reality.

A consistent representation of the same non-Hamiltonian interaction of Fig. 1 can be easily achieved by hadronic mechanics via the generalized unit called isounit

$$\hat I = \exp[C \int d^3 r\, \psi_\uparrow^\dagger(r) \psi_\downarrow(r)], \tag{2.1}$$

where C is a constant (at short range) and $\psi_\uparrow$, $\psi_\downarrow$ are the

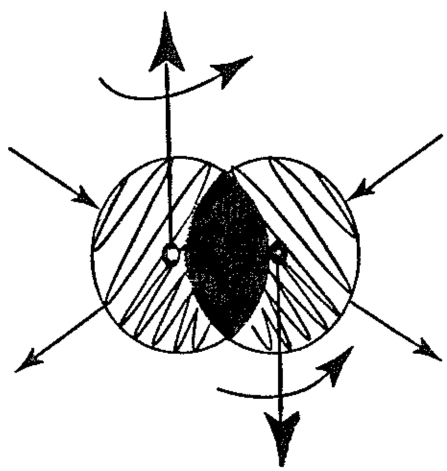

Fig. 1. A schematic view of the fundamental conditions studied in this paper, the deep overlapping of the wavepackets of valence electrons in singlet coupling, as required by Pauli's principle, whose non-linear, non-local and non-potential structure is beyond the capabilities of quantitative treatment via quantum mechanics and chemistry, thus requesting a covering theory.

wavefunctions of the two valence electrons evidently in singlet couplings (from Pauli's principle). Achievement of invariance then requires the step-by-step reconstruction of the entire formalism of quantum mechanics with respect to the new unit (2.1).

Hadronic representation (2.1) of the new interactions of Fig. 1 has a number of advantages over the quantum form, such as: the treatment of non-potential effects without a potential; the achievement of an invariant formulation; the preservation of hermiticity–observability under non-Hamiltonian effects; and others [14, 15].

Whenever the wave-overlapping is no longer appreciable, the exponent of generalized unit (2.1) is null. Then $\hat{I} \equiv +1$, and hadronic mechanics recovers quantum mechanics identically at all levels. This illustrates the covering nature of hadronic over quantum mechanics.

A similar situation occurs for other characteristics which are conceptually, mathematically and physically beyond the representation capabilities of a Hamiltonian, but which admit instead a simple and effective representation via generalized units.

An illustration is given by the representation of actual, extended, non-spherical and deformable shapes of bodies which is impossible for quantum mechanics because it would violate one of its pillars (the rotational symmetry), but which can be readily represented by hadronic mechanics. As an example, a deformable spheroidal ellipsoid can be represented via the iso-unit $\hat{I} = \text{Diag.}(n_1^2, n_2^2, n_3^2)$, where the n's are the variable semi-axes, and the reconstruction of the rotational symmetry with respect to that generalized unit (see Refs [9, 15] for details).

Similarly, Bose–Einstein correlations and condensations are known to be beyond the exact character of quantum mechanics because intrinsically extended in space, thus requiring a suitable non-local topology. Hadronic mechanics can readily represent these effects from first axiomatic principles via an $n \times n$ generalized unit incorporating off-diagonal elements of type (2.1).

We refer the interested reader to Ref. [11] for an outline of numerous applications and experimental verifications of hadronic mechanics in particle physics, nuclear physics, superconductivity, astrophysics and other fields.

A mathematical motivation for the generalization of the unit is that it permits the reconstruction of the linear, local and potential characters on certain generalized spaces (called iso-, geno- and hyper-spaces) over generalized fields (called iso-, geno- and hyper-fields).

The latter features assure the resolution of the problematic aspects indicated earlier for the conventional treatment of non-Hamiltonian effects. The same features also imply that hadronic mechanics coincides with quantum mechanics at the abstract, realization-free level in all its iso-, geno- and hyper-branches, and merely provides broader realizations of conventional quantum axioms.

In particular, hadronic mechanics preserve all conventional laws and principles of quantum mechanics, such as Pauli's exclusion principle, Heisenberg's uncertainties, causality and probability laws, etc.

The understanding of this note requires a knowledge of hadronic mechanics and its underlying new mathematics that we cannot possibly outline here. Readers are therefore referred to Ref. [10] on the new mathematics, Ref. [11] on the latest formulation of hadronic mechanics, and Ref. [16] on the inconsistencies of conventional formulations of non-Hamiltonian effects.

3. Rudiments of hadronic chemistry

In this paper we use the covering of quantum chemistry characterized by hadronic mechanics, here called hadronic chemistry. As such, the new discipline too has three main branches called iso-, geno- and hyper-chemistry for the representation of reversible, irreversible and multi-valued chemical structures, respectively, with Hamiltonian (long range) and non-Hamiltonian (short range) effects.

Since the hydrogen molecule is stable and reversible, in this paper we shall focus solely on iso-chemistry.

However, the reader should be aware that, as it occurred for conventional chemistry, iso-chemistry too is insufficient to represent chemical reactions, or, more generally, irreversible complex biological structures. When studying these cases in future papers the use of the broader geno-chemistry and hyper-chemistry, respectively, will be necessary for consistency.

Again, by conception and construction, hadronic and quantum chemistry coincide everywhere, except at distances of 1 fm or less in which the former admits novel contributions over the latter under the exact validity of all conventional quantum laws. As we shall see, the novel short range contributions are generally small, yet they permit the apparent resolution of at least some of the insufficiencies outlined in Section 1.

The completion of quantum into hadronic mechanics along the historical E–P–R teaching is studied in detail in Ref. [9]. The same results hold for the completion of quantum into hadronic chemistry. For this reason, the topic is ignored hereon for brevity.

Quantum mechanics and chemistry have only one formulation, the conventional one [1–4]. On the contrary, hadronic theories have two different formulations [10–21], that on generalized spaces over generalized fields and its projection on conventional spaces over conventional fields [10–16]. The reader should be aware that, to avoid excessive complexities for non-initiated readers, in this paper we shall solely consider the projection of hadronic theories on conventional spaces over conventional fields, and leave the mathematically correct formulation to mathematical studies.

Moreover, systems are characterized by quantum mechanics and chemistry via the sole assignment of the Hamiltonian and the tacit assumption of the simplest possible unit $I = +1$. By comparison, systems are characterized by hadronic mechanics and chemistry via the assignment of two quantities, the Hamiltonian for the representation of all conventional interactions, plus the generalized unit for the representation of the short range non-Hamiltonian effects.

Despite apparent mathematical complexities, iso-chemistry can be uniquely and unambiguously constructed in its entirety via a non-unitary transform characterizing precisely the iso-unit

$$U \times U^{\dagger} = \hat{I} \neq I, \tag{3.1}$$

which must be applied to the totality of the conventional formalism as a necessary condition to achieve invariance [16].

This procedure yields the iso-unit itself, the iso-numbers, the iso-Hilbert space, etc.

$$I \rightarrow U \times I \times U^{\dagger} = \hat{I} = 1/\hat{T}, \quad \hat{T} = (U \times U^{\dagger})^{-1},$$

$$c \rightarrow U \times c \times U^{\dagger} = c \times (U \times U^{\dagger}) = c \times \hat{I} = \hat{c},$$

$$A \times B \rightarrow U \times (A \times B) \times U^{\dagger}$$

$$= (U \times A \times U^{\dagger}) \times (U \times U^{\dagger})^{-1} \times (U \times B \times U^{\dagger}) = \hat{A} \hat{\times} \hat{B},$$

$$H \times |\psi\rangle \rightarrow U \times (H \times |\psi\rangle)$$

$$= (U \times H \times U^{\dagger}) \times (U \times U^{\dagger})^{-1} \times (U \times |\psi\rangle) = \hat{H} \hat{\times} |\hat{\psi}\rangle,$$

$$\langle\phi| \times |\psi\rangle \rightarrow U \times (\langle\phi| \times |\psi\rangle) \times U^{\dagger}$$

$$= (\langle\phi| \times U^{\dagger}) \times (U \times U^{\dagger})^{-1} \times (U \times |\psi\rangle) \times (U \times U^{\dagger})$$

$$= \langle\hat{\phi}| \hat{\times} |\hat{\psi}\rangle \times \hat{I}, \text{etc.} \tag{3.2}$$

Once achieved via the above simple map, iso-chemistry remains invariant under any other possible non-unitary transform, provided that it is evidently expressed in the iso-unitary form on the iso-Hilbert space over iso-fields, under which we have the invariance of the numerical value of the iso-unit, the invariance of the iso-product (where the numerical value of $\hat{T}$ is not changed), etc.

$$W \times W^{\dagger} = \hat{I} \neq I, \quad W = \hat{W} \times \hat{T}^{1/2},$$

$$W \times W^{\dagger} \equiv \hat{W} \hat{\times} \hat{W}^{\dagger} = \hat{W}^{\dagger} \hat{\times} \hat{W} = \hat{I},$$

$$\hat{I} \rightarrow \hat{I}' = \hat{W} \hat{\times} \hat{I} \hat{\times} \hat{W}^{\dagger} = \hat{I},$$

$$\hat{A} \hat{\times} \hat{B} \rightarrow \hat{W} \hat{\times} (\hat{A} \hat{\times} \hat{B}) \hat{\times} \hat{W}^{\dagger} = \hat{A}' \times \hat{T} \times \hat{B}' = \hat{A}' \hat{\times} \hat{B}', \text{etc.} \tag{3.3}$$

The main problem of completing chemistry into iso-chemistry is, therefore, the identification of a transform which is:

(1) non-unitary for $r < 1$ fm, $U \times U^{\dagger} r \approx 1$ fm $= \hat{I} \neq I$;
(2) unitary for $r > 1$ fm. $U \times U^{\dagger} r > 1$ fm $= I$; and
(3) capable of representing the desired short-range, non-linear, non-local and non-potential effects due to the overlapping of the wavepackets of the valence electrons, e.g., as in iso-unit (2.1).

All original axiomatic properties of quantum chemistry are preserved everywhere (including at short distances) and only realized in a broader way. This implies the preservation of all quantum laws and principles, such as Pauli's exclusion principle, Heisenberg uncertainty principle, causality and probability laws, etc.

Regrettably, to remain within the limitation on length of this journal, we cannot provide additional details. A comprehensive presentation of hadronic chemistry, including its application to hydrogen, is forthcoming in Ref. [22].

We should finally mention that, by its very structure, iso-chemistry assures much faster convergence of power series. This can be illustrated by the fact that, any given divergent quantum series can always be turned into an isotopically convergent form via the selection of isotopic elements $\hat{T}$ sufficiently smaller than one [15], as in the example

$$A(k) = A(0) + k[A, H]/1! + \cdots \rightarrow \infty, \quad k > 1,$$

$$A(k) = A(0) + k[A \hat{,} H]/1! + \cdots = N < \infty, \quad \hat{T} = k^{-n},$$

$$[A, H] = A \times B - B \times A \cdot [A \hat{,} H] = A \hat{\times} H - H \hat{\times} A. \tag{3.4}$$

As we shall see, the above feature permits the reduction of computer time in chemical calculations by a factor of at least 1000, thus rendering feasible calculations that would be otherwise prohibitive.

Needless to say, the studies presented below are deeply linked to numerous preceding studies in quantum chemistry (see, e.g., Refs [23–28]). In fact, we essentially provide a 'completion' of available contributions via novel non-Hamiltonian effects at short distances without exiting from the axiomatic structure of the theory, as inherent in Coulomb screenings and other ad hoc modifications of quantum chemistry. We shall then show the achievement of exact and invariant representations of main data of the hydrogen molecule. Other advances will be presented in future papers.

4. Iso-chemical molecular bonds

We now present, apparently for the first time, the conceptual foundations of our iso-chemical model of molecular bonds for the simplest possible case of the H_2 molecule. We shall then extend the model to the water and to other molecules in subsequent papers.

Since the nuclei of the two H-atoms remain at large mutual distances, the bond of the H_2 molecule is evidently due to the peripheral electrons, as generally acknowledged [1–4].

Our main assumption is that pairs of valence electrons from two different atoms bond themselves at short distances into a singlet quasi-particle state, here called iso-electronium, which describes an oo-shaped orbit around the respective two nuclei, as it is the case of a planet in certain binary stars.

We should stress that the above hypothesis is strictly prohibited by quantum mechanics and chemistry because of the repulsive Coulomb force which prevents any possible bound state of identical electrons at short distances.

However, as we shall see in the next section, the hypothesis is fully plausible for hadronic mechanics and chemistry because the novel non-Hamiltonian interactions due to deep wave-overlappings become so attractive when in singlet couplings at short distance, to overcome repulsive Coulomb forces.

The above occurrence is important to see that the new model of the hydrogen molecule presented in this paper is strictly impossible for quantum mechanics and chemistry, and requires a covering theory.

Iso-chemistry therefore introduces a new attractive force for the representation of the molecular bond among neutral atoms given by the coupling of valence electrons into singlet states. The binding energy is represented by the orbital motion of the iso-electronium around the respective nuclei.

In this paper we show that the emerging new model of the hydrogen molecule can: provide an exact representation of the binding energy from first axiomatic principles; explain the reason why the hydrogen molecule has only two atoms; achieve a much faster convergence of power series with consequential large reduction in computer times; and permit other advances.

The explanation by iso-chemistry of the reasons why the H- (or water) molecule admit only two hydrogen atoms is inherent in the very notion of iso-electronium. In fact, once two valence electrons are bonded into the iso-electronium, there is no possibility for bonding additional atoms.

The exact representation of the binding energy and other characteristics will be presented in the subsequent sections.

Two notions of hadronic chemistry are important for further advances:

(a) the hadronic horizon, which is the ideal sphere of radius 1 fm outside which quantum chemistry is assumed to be exact and within which hadronic chemistry applies; and
(b) the trigger, which is given by external (conventional) interactions causing identical electrons to move one toward the other and to penetrate the hadronic horizon against their repulsive Coulomb interactions. Once inside said horizon, the attractive hadronic forces overcome the repulsive Coulomb interaction, resulting in a bound state.

The hypothesis of the bonding of electrons at short distances was first introduced by Santilli [29] in 1978 for the structure of the π^0 meson as a hadronic bound state of one electron and one positron. Animalu [30] and Animalu and Santilli [31] extended the model to the Cooper pair in superconductivity as a hadronic bound state of two identical electrons.

In the case of the π^0 model there is no need of a trigger because the constituents have opposite charges, thus naturally attracting each other. On the contrary, the existence of the Cooper pair does indeed require a trigger, which was identified by Animalu [30] and Animalu and Santilli [31] as being constituted by the Cuprate ions. For the case of an isolated hydrogen molecule, we conjecture that the trigger is constituted by the two H-nuclei which do indeed attract the electrons. We essentially argue that the attraction of the electrons by the two nuclei is sufficient to cause the overlapping of the two wavepackets, thus triggering the electrons beyond the hadronic horizon.

We should finally indicate that the hypothesis of the iso-electronium can also be explained via the use of the intrinsic magnetic moments of the electrons which, in singlet couplings, are opposite to each other, thus implying an attraction that can counterbalance the electric repulsion.

However, the approach requires alteration (called mutation) of the electromagnetic fields of the electrons which is directly representable by the Poincaré–Santilli iso-symmetry [12, 13]; namely, an isomorphic reconstruction of the conventional Poincaré symmetry with respect to the iso-unit. This requires, for quantitative treatment, the lifting, this time, of relativistic quantum mechanics into relativistic hadronic mechanics which is here ignored for brevity [15].

The latter occurrence also explains that the term 'iso-electronium' is motivated by the fact that its constituents are not ordinary electrons (i.e., unitary representations of the Poincaré symmetry), but rather electrons in mutated forms called iso-electrons (i.e., iso-unitary iso-representations of the Poincaré–Santilli iso-symmetry).

5. The stable iso-electronium

We begin our quantitative analysis with the non-relativistic quantum mechanical equation of two ordinary electrons in singlet couplings, $e_\downarrow$ and $e_\uparrow$, represented by the wavefunction $\psi_{\uparrow\downarrow}(r) = \psi(r)$ and the conventional Schrödinger's equation

$$H \times \psi(r) = \left(\frac{1}{m} p \times p + \frac{e^2}{r}\right) \times \psi(r) = E \times \psi(r). \quad (5.1)$$

To transform this state into the iso-electronium representing the bonding of one valence electron with a valence electron of another atom of generic charge ze, we need first to submit eqn (5.1) to a non-unitary transform $U \times U^\dagger = \hat{I} \neq I$ characterizing the short range hadronic effects, and then we must add the trigger, namely; the Coulomb attraction by the nuclei.

By recalling rules (3.2), this procedure yields the iso-Schrödinger equation for the iso-electronium (see [22] for details)

$$\begin{aligned} &U \times H \times \psi(\beta r) + \text{trigger} \\ &= U \times H \times U^\dagger \times (U \times U^\dagger)^{-1} \times U \times \psi(r) + \text{trigger} \\ &= H \hat{\times} \hat{\psi}(r) + \text{trigger} \\ &= \left(\frac{1}{m} \hat{p} \times \hat{T} \hat{p} \times \hat{T} + \frac{e^2}{r} \times \hat{T} - \frac{2e^2}{r}\right) \times \hat{\psi}(r) = E_0 \times \hat{\psi}(r), \\ &\hat{p} \hat{\times} \hat{\psi}(r) = -i \times \hat{T} \times \nabla \hat{\psi}(r), \end{aligned} \quad (5.2)$$

where $\hat{\psi} = U \times \psi$, $\hat{H} = U \times H \times U^\dagger$, $\hat{p} = U \times p \times U^\dagger$, the factor $\hat{T} = (U \times U^\dagger)^{-1}$ in the first Coulomb term originates from the non-unitary transform of model (5.1), while the same factor is absent in the second Coulomb term because the latter is long range, thus being conventional.

The angular component of model (5.2) is conventional [1–4] and it is hereon ignored. For the radial component $r = |r|$ we assume the iso-unit [29–31]

$$\begin{aligned} &\hat{I} = e^{N \times \psi/\hat{\psi}} \approx 1 + N \times \psi/\hat{\psi}, \\ &N = \int dr^3 \hat{\psi}^\dagger(r)_\uparrow \times \hat{\psi}(r)_\downarrow, \\ &\hat{T} \approx 1 - N \times \psi/\hat{\psi}. \end{aligned} \quad (5.3)$$

Note that the explicit form of ψ is of Coulomb type, thus behaving like $C \times \exp(-b \times r)$, with C approximately constant at distances near the hadronic horizon of radius $r_c = 1/b$, while $\hat{\psi}$ behaves like $D \times (1 - \exp(-b \times r))/r$, with D being also approximately constant under the same range [29]. We then have

$$\hat{T} \approx 1 - V^h/r = 1 - V_0 \frac{e^{-b \times r}}{(1 - e^{-b \times r})/r}, \quad (5.4)$$

but the Hulten potential behaves at small distances as the Coulomb one:

$$V^h r \approx 1/b \approx \frac{V_0}{b} \times \frac{1}{r}. \quad (5.5)$$

As a result, inside the hadronic horizon we can ignore the repulsive Coulomb force altogether and write

$$+\frac{e^2}{r} \times \hat{T} - \frac{z \times e^2}{r} \approx +\frac{e^2}{r} \times (1 - V^h/r) - \frac{z \times e^2}{r}$$

$$= -V \frac{e^{-b \times r}}{1 - e^{-b \times r}}, \quad (5.6)$$

by therefore resulting in the desired overall attractive force among the identical electrons inside the hadronic horizon, as desired.

By assuming in the first approximation $|\hat{T}| = \rho \approx 1$, the radial equation of model (5.2) reduces to the model of π meson or of the Cooper pair, although with different values of V and b, which has been studied in great detail in Refs [29–31], including all necessary boundary conditions. The solution is the typical one of the Hulten well:

$$|E_0| = \frac{\rho^2 \times \hbar^2 \times b^2}{4 \times m} \left(\frac{m \times V}{\rho^2 \times \hbar^2 \times b^2} \times \frac{1}{n} - n\right)^2. \quad (5.7)$$

To reach a numerical solution, we introduce the parametrization as in Ref. [29], $k_1 = 1/\lambda \times b$, $k_2 = m \times V/\rho^2 \times \hbar^2 \times b^2$. We note again that, from the boundary conditions, k_2 must be bigger than but close to 1 [29–31]. We therefore assume in first non-relativistic approximation that $k_2 = m \times V/\rho^2 \times \hbar^2 \times b^2 = 1$. By assuming that V is of the order of magnitude of the total energy of the iso-electrons at rest as in the preceding models [29–31], we reach the numerical value of the depth of the hadronic well (Hulten potential):

$$V \approx 2 \times \hbar \times \omega \approx 2 \times 0.5\,\text{MeV} = 1\,\text{MeV}. \quad (5.8)$$

By recalling that $\rho \approx 1$, we reach the following numerical value of the radius of the hadronic horizon (radius of the iso-electronium):

$$r_c = b^{-1} \approx (\hbar^2/m \times V)^{1/2} = (\hbar/m \times \omega_0)^{1/2}$$

$$= (1.054 \times 10^{-27}\,\text{erg sec}$$

$$1.82\times 10^{-27}\,\mathrm{gr}\times 1.236\times 10^{20}\,\mathrm{Hz})^{1/2}$$
$$= 6.8432329\times 10^{-11}\,\mathrm{cm} = 0.015424288\,\mathrm{bohrs}$$
$$= 0.006843\,\text{Å}. \tag{5.9}$$

It should be noted that: (1) the above value is only an upper boundary in the center-of-mass frame of the iso-electronium, i.e., it is the largest possible value under the assumptions of this section; (2) the value has been computed under the approximation of identically null relative kinetic energy of the iso-electrons with individual total energy equal to their rest energy; and (3) the value evidently decreases with the addition of the relative kinetic energy of the iso-electrons (because this implies the increase of m in the denominator).

The actual radius of the iso-electronium is also expected to vary with the trigger, that is, with the nuclear charges, as supported by the calculations presented in the next sections. This illustrates again the upper boundary character of value (5.9).

The value k_1 is then given by $k_1 = V/2\times k_2\times b\times c_0 = 0.19$. Intriguingly, the combined two values $k_1 = 0.19$ and $k_2 = 1$ for the iso-electronium are quite close to the corresponding values of the π° [29] and of the Cooper pair [30, 31].

It is important to see that, at this non-relativistic approximation, the binding energy of the iso-electronium is not only unique, but also identically null.

The notion of a bound state with only one allowed energy level (called 'hadronic suppression of the atomic spectrum') is foreign to conventional quantum mechanics and chemistry, although it is of great importance for hadronic mechanics and chemistry. In fact, any excitation of the constituents, whether the π°, the Cooper pair or the iso-electronium, causes their exiting the hadronic horizon, by, therefore re-acquiring the typical atomic spectrum. Each of the considered three hadronic states has, therefore, only one possible energy level.

In fact, it is easy to see that the generally finite Hulten spectrum reduces to only one energy value according to

$$|E_0| = \frac{\rho^2\times\hbar^2\times b^2}{4\times m}\left(\frac{m\times V}{\rho^2\times\hbar^2\times b^2}-1\right)^2$$
$$= \frac{V}{4\times k_2}\times(k_2-1)^2 = 0. \tag{5.10}$$

The additional notion of a bound state with null binding energy is also foreign to quantum mechanics and chemistry, although it is another fundamental characteristic of hadronic mechanics and chemistry. In fact, the hadronic interactions admit no potential energy and, as such, they cannot admit any appreciable binding energy, as typical for ordinary contact zero-range forces of our macroscopic Newtonian reality.

The null value of the binding energy can be confirmed from the expression of the meanlife of the iso-electronium which can be written [29]

$$\tau = \hbar/4\times\pi\times\lambda^2|\hat\psi(0)|\times\alpha\times E_{\mathrm{e}}^{\mathrm{Kin}}$$
$$= 7.16\times 10^4\times\frac{k_1}{(k_2-1)^3\times b\times c_0} = \infty. \tag{5.11}$$

The full stability of the iso-electronium, $\tau = \infty$, therefore, requires the exact value $k_2 \equiv 1$ which, in turn, implies $E_0 \equiv 0$.

According to the above non-relativistic model, the iso-electronium is a stable bound state (at ordinary conditions). This property is at the foundation of our representation of the stability of the H_2 and other molecules. We should, however, indicate that, under a relativistic treatment [11], the iso-electronium admits a small instability due to the exchange, van der Waals and other forces.

By comparison, the Cooper pair is not permanently stable already at the non-relativistic level because its binding energy is very small, yet finite [30], thus implying a large yet finite meanlife. Also by comparison, the π° cannot be stable, and actually has a very small meanlife, evidently because the constituents are a particle–antiparticle pair and, as such, they annihilate each other when bound at short distances. By comparison, no such annihilation may occur in the iso-electronium.

Another important result of this section is that the iso-electronium is sufficiently small in size, as per value (5.9), to be treated as a single quasi-particle. This property will permit rather important simplifications in the iso-chemical structure of molecules studied in the following sections.

By comparison, the Cooper pair has a size much bigger than that of the iso-electronium. This property is fundamental in preventing the Cooper pair taking the role of the iso-electronium in molecular bonds, i.e., even though possessing the same constituents and similar physical origins, the iso-electronium and the Cooper pair are different, non-interchangeable, hadronic bound states because they originate from different triggers and conditions.

The lack of binding energy of the iso-electronium is perhaps the most important information of this section. In fact, it transfers the representation of the binding energy of molecular bonds to the motion of the iso-electronium in a molecular structure, as studied in the following sections.

A novelty of iso-chemistry over quantum chemistry is that the mutual distance (charge diameter) between the two iso-electrons in the iso-electronium could, as a limit case, also be identically null, that is, the two iso-electrons are superimposed in a singlet state. Rather than being far fetched, this limit case is intriguing because it yields the value $-2e$ for the charge of the iso-electronium, the null value of the relative kinetic energy, and an identically null magnetic field. This is a perfectly diamagnetic state which evidently allows a better stability of the iso-chemical bond as compared to a quasi-particle with non-null magnetic moment.

Note that, if conventionally treated (i.e., represented on conventional spaces over conventional fields), the non-unitary image of model (5.1) would yield non-invariant numerical results which, as such, are unacceptable (Section 2 and Ref. [16]). This occurrence mandates the use of the covering iso-chemistry and related iso-mathematics which assures the achievement of invariant results.

Note also that the main physical idea of iso-unit (5.3) is the representation of the overlapping of the wavepackets of the two electrons under the condition of recovering conventional quantum chemistry identically, whenever such overlapping is no longer appreciable. In fact, for sufficiently large relative distances, the volume integral of iso-unit (5.3) is null, the exponential reduces to I, the non-unitary transform becomes conventionally unitary, and quantum chemistry is recovered identically.

It is also important to see that, under transform (5.3), model (5.1) is implemented with interactions which are: non-linear, due to the factor $\psi/\hat{\psi}$ in the exponent; non-local, because of the volume integral in (5.3); and non-potential, because it is not represented by a Hamiltonian.

We finally note that the explicit form of the isotopic element $\hat{T}$, eqn (5.3b), emerges in a rather natural (and unique) way as being smaller than one in absolute value, $|\hat{T}| \ll 1$. This property alone is sufficient to guarantee that all slowly convergent series of quantum chemistry converge faster for iso-chemistry.

6. Iso-chemical model of the hydrogen molecule with stable iso-electronium

We are now sufficiently equipped to present, apparently for the first time, the iso-chemical model of the H_2 molecule. The understanding of the reasons why the molecule has only two H-atoms is inherent in the very concept of iso-electronium (Sections 4 and 5). In this section we shall, therefore, identify the equation of structure of the H-molecule. The exact representation of the binding energy and other characteristics is studied in the subsequent sections.

Our foundation is the conventional quantum model of the H_2 molecule [1–4]. The task is that of subjecting such a model to a transform which is non-unitary only at the short mutual distances $r_c = b^{-1} = r_{12}$ of the two valence electrons (here assumed to be inside the hadronic horizon), and becomes unitary at bigger distances $\hat{I}_r \leqq 10^{-11}$ cm $\neq I$, $I_r \gg 10^{-11}$ cm $= I$. This guarantees that our iso-chemical model coincides with the conventional model except for small contributions at $r_c = b^{-1}$.

We assume that the state and related Hilbert space can be factorized in the familiar form (in which each term is duly symmetrized or anti-symmetrized) as in Refs [1–4].

The non-unitary transform we are looking for shall act only on the r_{12} variable, while leaving all others unchanged. The simplest possible solution is given by $U(r_{12}) \times U^{\dagger}(r_{12}) = \hat{I} = \exp([\psi(r_{12})/\hat{\psi}(r_{12})] \int dr_{12} \hat{\psi}^{\dagger}(r_{12})_{\uparrow\downarrow} \times \hat{\psi}(r_{12})_{\downarrow\uparrow})$, where the ψ's represent conventional wavefunction and the $\hat{\psi}$'s represent iso-wavefunctions.

As a variant to the approach of Section 5 yielding the same end results, we construct the model by transforming short-range terms (iso-chemistry) and adding untransformed long-range ones (chemistry), thus resulting in the radial equation

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \hat{T} \times \nabla_1 \times \hat{T} \times \nabla_2 - \frac{\hbar^2}{2 \times \mu_2} \hat{T} \times \nabla_2 \times \hat{T} \times \nabla_2 + \frac{e^2}{r_{12}} \times \hat{T} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (6.1)$$

By recalling that the Hulten potential behaves at small distances like the Coulomb one, eqn (6.1) then becomes

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \nabla_2^2 - V \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (6.2)$$

The above equation does indeed achieve our objectives. In fact, it exhibits a new explicitly attractive force among the neutral atoms of the molecule which is absent in conventional quantum chemistry. The equation also explains the reasons why the H_2 molecule admits only two H-atoms (Section 5). As we shall see in the remaining sections, eqn (6.2) also permits the exact representation of the binding energy, yields much faster convergence of series with much reduced computer times, and resolves other insufficiencies of conventional models.

Our iso-chemical model of the hydrogen molecule, eqns (6.2), can be subjected to an additional simplification which is impossible for quantum chemistry. In our isotopic model the two iso-electrons are bonded together into a single state we have called iso-electronium. In particular, the charge radius of the latter is sufficiently small to permit that in first approximation, for $r_{12} \ll r_{1a}$ and r_{1b}, we have $r_{1a} \approx r_{2a} = r_a$ as well as, separately, $r_{1b} \approx r_{2b} = r_b$. Moreover, the H-nuclei are about 2000 times heavier than the iso-electronium.

Therefore, our isotopic model of the H_2 molecule can be reduced to a restricted three-body problem similar to that possible for the conventional H_2^+ ion [1–4], but not for the conventional H_2 molecule. It consists of two H-protons at rest and the iso-electronium moving around

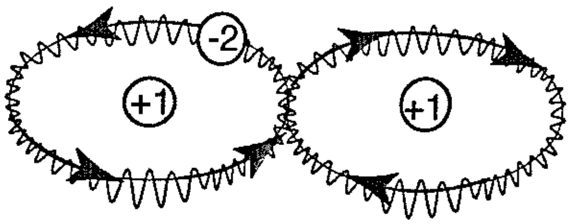

Fig. 2. A schematic view of the proposed iso-chemical model of the hydrogen molecule as well as of other two-body molecules or, more generally, of the bond of one H-atom to a generic other element, e.g., HO, HC, etc., here assumed at absolute K and in the absence of rotations, vibrations, translations and other effects. The fundamental assumption is that the two valence electrons, one per each atom, correlate themselves into a bonded singlet state at a short distance we have called 'iso-electronium', which is assumed in this case to be stable, with infinite lifetime as in eqn (5.9) and describing an oo-shaped orbit around the respective two nuclei. The iso-electronium is then responsible for the attractive force between the two atoms. The binding energy is instead characterized by the oo-shaped orbit of the iso-electronium around the two nuclei, conceptually represented in this figure via a standing wave. The model then permits a representation of the reason why the H_2 and H_2O molecules have only two hydrogen atoms, the exact representation of the binding energy and other advances studied in the text.

them in the oo-shaped orbit of Fig. 2, according to the structural equation

$$\left(-\frac{\hbar^2}{2\mu_1}\nabla_1^2-\frac{\hbar^2}{2\mu_2}\nabla_2^2-V\times\frac{e^{-r_{12}b}}{1-e^{-r_{12}b}}-\frac{2e^2}{r_a}-\frac{2e^2}{r_b}+\frac{e^2}{R}\right)\times|\hat{\psi}\rangle=E\times|\hat{\psi}\rangle. \quad (6.3)$$

Under the latter approximation, the model permits, for the first time, the achievement of an exact solution for the structure of the H-molecule, as it is the case for all restricted three-body problems. This exact solution will be studied elsewhere. In the next sections we shall study the solution of model (6.3) via conventional variational methods.

Note that the above exact solution of the hydrogen molecule is only possible for the case of the fully stable iso-electronium. In fact, for the case of the unstable iso-electronium the model is a full four-body structure which, as such, admits no exact solution.

Note also that model (6.3) is the iso-chemical model of the H_2 molecule inside the hadronic horizon. The matching representation outside the hadronic horizon is presented below. Note also that the above restricted three-body 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, with possible extension to molecular chains and other molecules.

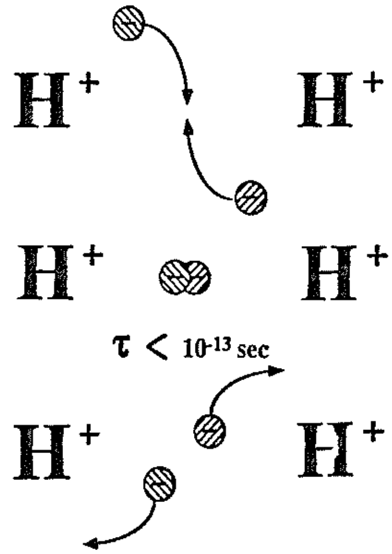

Fig. 3. A schematic view of the iso-chemical model of the hydrogen molecule with unstable iso-electronium due to the weakening of the Hulten potential and consequential relaxation of the infinite lifetime (5.11). In this case the notion of iso-electronium essentially represents a tendency of pairs of valence electrons to correlate in singlet states at short distances. The use of iso-chemistry, rather than conventional chemistry, is necessary because even this weaker form of the iso-electronium, as well as all screenings of the Coulomb potential at large, are non-unitary images of the conventional Coulomb settings as established in Section 5. As such, all these models require a representation on iso-spaces over iso-fields for their invariant formulation. In the text we present the projection of such an invariant formulation on conventional spaces over conventional fields for simplicity.

7. Iso-chemical model of the hydrogen molecule with unstable iso-electronium

In this section we study the solution of the restricted iso-chemical model of the hydrogen molecule, eqn (6.3), via conventional variational methods [1–4]. For this purpose we note that the solution of the full model with the Hulten potential $\exp(-rb)/[1-\exp(-rb)]$, where $r_c = b^{-1}$ is the horizon, implies rather considerable technical difficulties. Therefore, we shall study model (6.3) under an approximation of the Hulten potential given by one Gaussian of the type $[1-A\exp(-br^2)]/r$ with A a constant identified below.

Recall from Section 5 that the stable character of the iso-electronium, eqn (5.11), is crucially dependent on the use of the attractive Hulten potential which 'absorbs' repulsive Coulomb forces at short distances resulting in a strong attraction. Therefore, the weakening of the Hulten potential into the above Gaussian form has the direct consequence of turning the iso-electronium into an unstable state.

In this and in the following sections, we shall, therefore, study a new iso-chemical model of the hydrogen molecule which is somewhat intermediary between the conventional chemical model and the iso-chemical model with a fully stable iso-electronium.

It should be indicated that the assumption of an unstable iso-electronium implies the capability for more hydrogen atoms to bond to the H-molecules, as well as other features (such as the capability for the hydrogen and water molecules to acquire a paramagnetic character under external magnetic fields) for values depending on the lifetime of the iso-electronium. These features will be studied in detail in subsequent papers.

The main objective of this section is to show the achievement of the exact representation of molecular characteristics even for the case of one Gaussian approximation of the Hulten potential. Since a sufficient number of Gaussians can reproduce any potential, the achievement of the exact representation with one Gaussian assures its preservation for additional Gaussians, thus also for the Hulten potential.

The question whether the iso-electronium is stable or unstable evidently depends on the amount of instability and its confrontation with experimental data, e.g., on magnetic dipole moments. As such, the issue will be addressed theoretically and experimentally in a future paper.

We begin with the approximation of the Hulten potential with the Coulomb one, and then add a Gaussian 'screening'. The reader should be aware that the latter brings us squarely within the applicability of iso-chemistry because the map from the Coulomb potential to Gaussian screened potentials is generally characterized by a non-unitary transform, thus exiting the class of equivalence of quantum mechanics and chemistry. In fact, model (6.3) was constructed precisely via a non-unitary transform of the conventional quantum model.

Under the above assumption, our first step is, therefore, the study of model (6.3) in an exemplified Coulomb form characterized by the following equation, hereon expressed in atomic units (au) (see Ref. [21] for details):

$$H \times \Psi = (-\nabla^2/4 - 2/r_a - 2/r_b + 1/R) \times \Psi, \tag{7.1}$$

where the differences from the corresponding equation for the H_2^+ ion [1–4] are the replacement of the reduced mass ($\mu =$) 2 with 4, and the increase of the electric charge from (e$=$) 1 to 2.

The standard method for solving the above equation is the following [1–4, 32, 33]. The variational calculation is set up in matrix algebra form in a non-orthogonal basis set which has been normalized to 1. The metric of this non-orthogonal system of equations (S) is used to set up the orthogonal eigenvalue problem and the eigenvalues are sorted to find the lowest value. H is a Hermitean (square) matrix as well as C and S; E is a diagonal matrix with the energy eigenvalues

$$HC = ESC; \text{define } C = S^{-1/2}C', HS^{-1/2}C' = ES^{-1/2}C',$$
$$(S^{-1/2}HS^{+1/2}C') = H'C' = E(S^{-1/2}SS^{-1/2})C' = EC', \tag{7.2}$$

where the last equation is obtained by multiplying the first equation from the left by $S^{-1/2}$ and using the unitary property that $S^{-1/2} = S^{+1/2}$ to form an orthogonal eigenvalue problem. Finally we solve C' by diagonalizing H' and obtain $C = S^{-1/2}C'$.

The detailed calculations have been done for both the restricted three-body model of the hydrogen molecule, as well as the full four-body versions. They are rather lengthy and cannot be presented here for brevity. We shall, therefore, only outline the main results below and refer to [22] for a comprehensive presentation, including related references.

8. Summary of results

In order to demonstrate the advantage of the iso-chemical model using a Gaussian-screened-Coulomb attraction between electrons, a standard Boys–Reeves [22] calculation was carried out. This included all single- and double-excitations (CISD) from the ground state Hartree–Fock–Roothaan SCF orbitals for a 99 × 99 'codetor' [23–28] interaction. Only the 1s orbitals were optimized with a scaling of 1.191 for the least-energy 6G–1s orbitals, but the basis also included 1G–2s, 2G–2p, 1G–3s, 1G–3p, 3G–3d, Td1G–4sp (tetrahedral array of four Gaussian spheres), and 4G–4f orbitals scaled to hydrogenic values as previously optimized.

The additional basis functions provide opportunity to excite electrons to higher orbitals as is the standard technique in configuration interaction (contrary to the main hypothesis of this work which is that there is an attractive 'hadronic' force for electrons inside the r_c critical radius). The results of the above calculations are summarized in Table 1 below.

The Boys–Reeves C.I. achieved an energy of −1.14241305 hartrees based on an SCF energy of −1.12822497 hartrees. This was followed by one additional iteration of 'natural orbitals' (CINO) in which the first-order density matrix is diagonalized to improve the electron pairing to first-order [29]. The fact that this procedure lowered the energy only slightly to −1.14241312 hartrees (-7.0×10^{5} hartrees) indicates the 99-configuration representation is close to the lower energy bound using this basis set while the iso-chemistry calculation produced the same exact energy with a comparatively much smaller basis set.

Since the Santilli–Animalu–Shillady LOBE (SASLOBE) has only an n^7 routine for the necessary integral transformation instead of the most efficient n^5 algorithm (n is

Table 1
Summary of results for the hydrogen molecule

Species basis screening	H_2	H_2 [2]	H_2
1s	1.191	6.103	1.191
2s	0.50	24.35	0.50
2p	0.50	24.35	2.36
3s	0.34	16.23	*
3p	0.34	16.23	*
3d	0.34	− 16.2[1]	*
4sp	0.25	12.18	*
4f	0.25	12.18	*
Variational energy (au)	*	− 7.61509174	*
SCF energy (au)	− 1.12822497	*	− 1.13291228
CI energy (au)	− 1.14231305	*	*
CINO energy (au)	− 1.14241312	*	*
SAS energy (au)	*	*	− 1.174444
Exact energy (au) [30]	− 1.174474	*	− 1.174474
Bond length (bohr)	1.4011	0.2592	1.4011
Electronium radius (bohr)	*	*	0.01124995

[1] The negative 3d scaling indicates five equivalent three-sphere scaled to 16.20 rather than 'canonical' 3d shapes.
[2] Three-body Hamiltonian (5.1).

the number of basis functions). the SASLOBE C.I. runs are somewhat slow and required about 20 h on a 300 MFLOPS Silicon Graphics computer.

With more efficient routines this time can be reduced to about three hours. However, the screened-Coulomb attraction method used a smaller basis and achieved lower energies in a few seconds. It is also estimated that careful spacing of fewer quadrature points in the new integral routine can certainly reduce the SASLOBE run times by a factor of 2 at least.

Therefore, it is clear that iso-chemistry calculations are (conservatively) at least 1000 times faster than a C.I. calculation. Another estimate is that since the new integral corrections require a little more time than the usual Coulomb integrals (but do not take any additional storage space), the computer run-times for an iso-chemistry calculation should only be about three times the run-times for the corresponding Hartree–Fock–Roothaan calculation in any given basis set.

The extension of the iso-chemical model of the H_2 molecule to other molecules is conceptually straightforward. In particular, the notion of iso-electronium essentially restricts all possible bonds to the established ones, as it is the case for the water molecule.

In order to generalize the underlying quantitative treatment to molecules containing H-to-F, the pole-spike was re-optimized to obtain 100% of the correlation energy below the SCF energy in the given basis set since the SCF energy here was not quite at the Hartree–Fock limit (see Table 1 for details).

The energy obtained here results from the calibration of the pole-spike to the experimental value of HF and is below the Quantum Monte Carlo energy of Luchow and Anderson [33] which requires hours on a much larger computer, as compared to less than 10 min for this work. In fact, the run times for HF were abut 8 cpu min on a 100 MFLOP Silicon Graphics 'O2' workstation.

The principal value of the pole (9.5 d) was calibrated for 100% energy of HF, H_2O has two tight sigma bonds and two diffuse lone-pairs so a single compromise value is a good test of the method. In HF the F^- is nearly spherical so an average r_c value does a better job of describing the 'correlation hole' of transient iso-electronium.

The computed dipole moments are in excellent agreement with the experimental values. The use of the same pole value for H_2O and HF degrades the H_2 energy slightly. The results of our studies for H-to-F based molecules are summarized in Table 2 below.

A comparison of the above data (particularly those on computer times) with corresponding data obtained via conventional approaches is instructive.

9. Concluding remarks

The fundamental notion of the new model of molecular bonds introduced in this paper is the bonding at short distances of pairs of valence electrons from two different atoms into a singlet quasi-particle state we have called iso-electronium, which travels as an individual particle on an oo-shaped orbit around the two respective nuclei.

Table 2
Iso-electronium results for selected molecules

	H_2	H_2O	HF
SCF-energy (DH)	−1.132800[1]	−76.051524	−100.057186
Hartree–Fock[4]			−100.07185[4]
Iso-energy	−1.174441[3]	−76.398229[3]	−100.459500[3]
Horizon R_c (A)	0.00671	0.00038	0.00030
QMC energy[4,5]	−1.17447	−76.430020[5]	−100.44296[4]
Exact non-rel.	−1.174474[6]		−100.4595[4]
% correlation	99.9[2]	91.6[2]	103.8
SCF-dipole (D)	0.0	1.996828	1.946698
Iso-dipole (D)	0.0	1.847437	1.841378
Exp. dipole	0.0	1.85[7]	1.82[7]
Times (min : s)	0 : 15.49	10 : 08.31	6 : 28.48

(HD^+) Dunning-Huzinaga (10S/6P), [6, 2, 1, 1, 1/4, 1, 1]+H_2P_1+3D1.
[1] LEAO-6G1S+optimized GLO-2S and GLO-2P.
[2] Relative to the basis set used here, not quite HF-limit.
[3] Iso-energy calibrated to give exact energy for HF.
[4] Hartree–Fock and QMC energies from Luchow and Anderson.
[5] QMC energies from Hammond et al. [22].
[6] First 7 sig. fig. from Kolis and Wolniewicz [22].
[7] Data from Chemical Rubber Handbook, 61st ed., p. E60.
Horizon radius in Angstroms.
Run times on an O2 Silicon Graphics workstation (100 MFLOPS max.).

The iso-electronium and related methodology are then assumed to characterize a covering of contemporary chemistry we have called iso-chemistry.

The attractive short-range interactions needed to overcome the repulsive Coulomb force in the iso-electronium structure originate from non-linear, non-local and non-Hamiltonian effects in deep wave-overlappings; they are described by the recently achieved covering of quantum mechanics known as hadronic mechanics [11]; and their invariant formulation is permitted by the recently achieved broadening of conventional mathematics called iso-mathematics [10].

Specific experimental studies are needed to confirm the existence of the iso-electronium, by keeping in mind that the state may not be stable outside a molecule in which the nuclear attraction terms bring the electron density to some critical threshold for binding.

Non-relativistic studies yield a radius of the iso-electronium of 0.69×10^{-10} cm. This 'horizon' is particularly important for iso-chemical applications and developments because outside the horizon the electrons repel one another, while inside the horizon there is a 'hadronic attraction'. The value of the hadronic horizon obtained in this paper for H_2 via a Gaussian-lobe basis set (0.00671 A) confirms the value independently obtained via non-relativistic studies. Nevertheless, the value of the hadronic horizon must also be resolved via experiments. Similar considerations apply also for the depth of the hadronic well of the iso-electronium which has been estimated at about 1 MeV.

The same non-relativistic studies also predict that the iso-electronium is stable within a molecule, although partially stable configurations also yield acceptable results. The question of the stability vs instability of the iso-electronium must, therefore, also be left to experimental resolutions.

The foundations of the iso-electronium can be seen in a paper by Santilli [29] of 1978 on the structure of the π^0-meson which contains the first identification of the attractive character of non-linear, non-local and non-Hamiltonian interactions due to deep wave-overlappings in singlet coupling (and their repulsive character in triplet coupling). The iso-electronium also sees its foundations in subsequent studies by Animalu [30] of 1994 and Animalu and Santilli [31] of 1995 for the Cooper pair in superconductivity, as well as in other examples of electron bondings existing in nature, such as ball lightning.

The iso-electronium also results in having deep connections with a variety of studies in chemistry conducted throughout this century [23–28, 32, 33], and actually provides the physical–chemical foundations with a more adequate mathematical formulation for most of them.

Therefore, the iso-chemical model of molecular bonds results in being consistent with a number of important occurrences in particle physics, superconductivity, chemistry and other fields, such as:

(1) The iso-electronium introduces a new attractive force among the neutral atoms of a molecular structure which is absent in quantum chemistry and certainly improves our understanding of the strength of molecular bonds and its stability.
(2) The iso-electronium permits an immediate interpretation of the reasons why the H_2 and H_2O molecules only admit two H-atoms.
(3) The iso-electronium permits the achievement of a representation of the missing 2% in the binding energy, thus allowing meaningful thermodynamical calculations.
(4) The iso-electronium provides an explanation of the long known, yet little understood Pauli exclusion principle, according to which electrons correlate themselves in singlet when on the same orbit without any exchange of energy, thus via interactions essentially outside the representational capabilities of quantum mechanics and chemistry.
(5) The iso-electronium is consistent with the known existence of superconducting electron-pairs which bond themselves so strongly to tunnel together through a potential barrier.
(6) The iso-electronium provides a quantitative model for the explanation of 'electron correlation'. Instead of a complicated 'dance of electrons' described by positive energy excitations, the iso-chemistry explanation is that electrons are energetically just outside the horizon of a deep attractive potential well due to their wavefunctions overlapping beyond the critical threshold of the hadronic horizon.
(7) The iso-electronium is consistent with the 'Coulomb hole' documented by Boyd and Yee as found from subtracting accurate explicitly-correlated wavefunctions from self-consistent-field wavefunctions. In our studies the 'hole' is re-interpreted as a 'hadronic well'.
(8) The iso-electronium is also in agreement with the 'bi-polaron' calculated for anion vacancies in KCl by Fois, Selloni, Parinello and Car and bi-polaron spectra reported by Xia and Bloomfield.
(9) The iso-electronium permits an increase of the speed in computer calculations at least 1000-fold.

As we hope to illustrate in future works, a promising feature of the proposed iso-chemical model of the hydrogen molecule is not only the capability to permit accurate representations of experimental data in shorter computer times, but also the capability to predict and quantitatively treat new features and reactions.

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