Chapter 9

EXPERIMENTAL VERIFICATIONS AND APPLICATIONS IN CHEMISTRY

9.1 ISOCHEMICAL MODEL OF THE HYDROGEN MOLECULE

9.1.1 Introduction

Chemistry provides some of the most important experimental verifications and applications of hadronic mechanics in its version known as *hadronic chemistry* essentially consisting of the isotopic methods of Chapter 3 for chemical processes that are invariant under time reversal (*isochemistry*), the genotopic methods of Chapter 4 for irreversible processes (*genochemistry*), the multi-valued methods of Chapter 5 for biological structures (*hyperchemistry*), and their isoduals for the first known formulation of antimatter chemistry (*isodual iso-, geno- and hyper-chemistry*). A comprehensive study of these formulations is presented in monograph [67]. This chapter is essentially dedicated to a review of the experimental verifications and scientific applications of isochemistry. Industrial applications of hadronic chemistry are presented in Chapters 11 and 12.

As an indication, in Sections 1.2 and 1.3 we showed that, following one century of failed attempts, quantum chemistry was unable to represent from unadulterated basic axioms a residual amount of 2% of molecular binding energies with electric and magnetic moments being wrong even in their signs, while the improvement of the representation via the so-called "screenings of the Coulomb law" causes the loss of the quantum of energy as well as other inconsistencies.

By comparison, in this chapter we show that *hadronic chemistry has permitted the first exact and invariant representation from first principles of molecular binding energies and other molecular data without adulteration of the*

basic axioms, while admitting as particular cases conventional screenings of the Coulomb law.

The studies presented in this chapter are devoted to the representation of molecular structures assumed as isolated from the rest of the universe, thus being invariant under time reversal. Consequently, unless otherwise stated, all studies of this chapter are based on *isochemistry.* various experimental verifications and applications of the broader *genochemistry* and *hyperchemistry* and their isoduals are under way by various scholars and they will be reported in their works.

As it is well known, the primary structural characteristics of *quantum chemistry* (see, e.g., Refs. [1]) are those of being:

1) *linear*, in the sense that eigenvalue equations depend on wavefunctions only to the first power;

2) *local-differential*, in the sense of acting among a finite number of isolated points; and

3) *potential*, in the sense that all acting forces are derivable from a potential energy.

Therefore, quantum chemistry is a *Hamiltonian theory*, i.e., models are completely characterized by the *sole* knowledge of the Hamiltonian operator, with a *unitary structure*, i.e., the time evolution verifies the unitarity conditions

$$U = e^{iH \times t}, \quad U \times U^\dagger = U^\dagger \times U = I, \quad H = H^\dagger, \tag{9.1.1}$$

when formulated on conventional Hilbert spaces over the conventional fields of complex numbers.

Despite outstanding achievements throughout the 20-th century, quantum chemistry cannot be considered as "final" because of numerous insufficiencies identified in Chapter 1.

A most important insufficiency is *the inability to represent deep mutual penetrations of the wavepackets of valence electrons in molecular bonds.* The latter interactions are known to be:

$\hat{1}$) *nonlinear*, i.e., dependent on powers of the wavefunctions greater than one;

$\hat{2}$) *nonlocal-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

$\hat{3}$) *nonpotential*, i.e., consisting of "contact" interactions with consequential "zero range," for which the notion of potential energy has no mathematical or physical sense.

A representation of the latter features evidently requires a *nonhamiltonian theory*, i.e., a theory which cannot be solely characterized by the Hamiltonian, and requires additional terms. It then follows that the emerging theory is

nonunitary i.e., its time evolution verifies the law,

$$U \times U^\dagger = U^\dagger \times U \neq I, \tag{9.1.2}$$

when formulated on conventional Hilbert spaces over conventional fields.

It is evident that the above features are beyond any hope of scientific-quantitative treatment via quantum mechanics and chemistry.

In the preceding Chapter 3 we have submitted the foundations of a generalization covering of quantum chemistry under the name of *hadronic chemistry*, first submitted by Santilli and Shillady in Ref. [2], which is capable of providing an invariant representation of the above-mentioned nonlinear, nonlocal, non-potential, nonhamiltonian, and nonunitary interactions in deep correlations of valence electrons.

In Chapter 3, we have also shown that the conventional "screenings" of the Coulomb potential (which are necessary for a better representation of experimental data) are outside the axiomatic structure of "quantum" chemistry because such screenings can only be reached via nonunitary maps of the Coulomb law, thus resulting in being particular cases of the broader hadronic chemistry.

The main purpose of this chapter is the application of hadronic chemistry to the construction of a new model of molecular bonds and its verification in the representation of experimental data of the hydrogen molecule.

Since molecular structures are considered as isolated, thus being closed, conservative, and reversible, the applicable branch of hadronic chemistry is *isochemistry*, which is characterized by the identification of the nonunitary time evolution with the *generalized unit* of the theory, called *isounit*,

$$U \times U^\dagger = \hat{I}(r, p, \psi, \partial\psi, ...) \neq I, \tag{9.1.3}$$

assumed hereon not to depend explicitly on time, and the reconstruction of the *totality* of the formalism of quantum chemistry into a new form admitting of $\hat{I}$, rather than I, as the correct right and left new unit.

The capability by the isounit to represent nonlinear, nonlocal, and non-hamiltonian interactions is evident. Its selection over other possible choices is mandated by the condition of *invariance*, that is, the prediction of the same numerical values for the same quantities under the same conditions, but at different times. In fact, whether generalized or not, the unit of any theory is the basic invariant.

A central assumption of this chapter is that *quantum mechanics and chemistry are exactly valid at all distances of the order of the Bohr radius ($\simeq 10^{-8}$ cm), and the covering hadronic chemistry only holds at distance of the order of the size of the wavepackets of valence electrons* (1 fm = 10^{-13} cm).

This condition is evidently necessary, on one side, to admit the conventional quantum structure of the hydrogen atom, and, on the other side, to admit
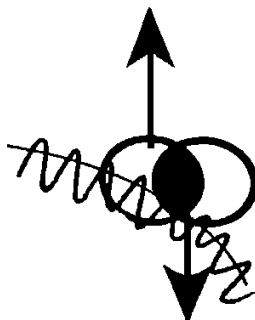
Figure 9.1. A schematic view of the central conditions studied in this chapter, the deep overlapping of the wavepackets of valence electrons in singlet coupling (to verify Pauli's exclusion principle). These conditions are known to be nonlinear, nonlocal, and nonpotential (due to the zero-range, contact character of the interactions), thus not being representable via a Hamiltonian, and, consequently, not being unitary. As a result, the ultimate nature of valence bonds is outside any credible representation via quantum chemistry. Hadronic chemistry (Chapter 3) has been built for the specific scope of representing the conditions herein considered of the bonding of valence electrons.

quantitative studies of the nonhamiltonian interactions of short range valence bonds.

The above condition is readily achieved by imposing that all isounits used in this chapter recover the conventional unit at distances greater than 1 fm,

$$\lim_{r \gg 1\,\text{fm}} \hat{I}(r, p, \psi, \partial\psi, \dots) = I, \qquad (9.1.4a)$$

$$|\hat{I}| \ll 1, \quad |\hat{T}| \gg 1. \qquad (9.1.4b)$$

In fact, under the above condition, hadronic chemistry recovers quantum chemistry everywhere identically. The reader should keep in mind the crucial implications of conditions (9.1.4b) which, as shown in Sect. 3.4, permit a dramatic increase of the convergence of chemical series, with corresponding decrease of computer time, as verified in the models of this chapter and of the following ones.

The reader should also note that, quite remarkably, rather than being imposed, both conditions (9.4a) and (9.4b) are naturally verified by actual chemical models.

It should be recalled that, under the assumption of representing closed-isolated systems, *isochemistry verifies all conventional laws and principles of quantum mechanics* (Chapter 3). Therefore, there is no *a priori* mean for rejecting the validity of hadronic chemistry within the small region of space of valence bonds.

It then follows that the selection of which theory is valid is referred to the capability to represent experimental data. Quantum mechanics has been capable of achieving an exact representation of all experimental data for the structure of *one individual* hydrogen atom. Therefore, quantum mechanics is here assumed as being exactly valid within such a well defined physical system, any possible improvement being redundant at best.

By comparison, quantum mechanics and chemistry have not been able to achieve an exact representation of the experimental data of the *different* conditions of molecular structures, as discussed in detail in Chapter 1. As a result, these theories are *not* considered as being exactly valid for the different conditions of molecular bonds (see Fig. 1.7).

As we shall see in this chapter, hadronic chemistry can indeed provide an exact representation of molecular characteristics, and, therefore, it is consider as being exactly valid for the indicated conditions of applicability.

A knowledge of *isomathematics* of Chapter 3 is essential for a technical understanding of the content of this chapter. A comprehemnsive presentation is available in monograph [67]

(see also representative papers [3, 4]).

For mathematically less inclined readers, we recall from Sect. 3.3.6 that specific applications of isochemistry can be constructed in their entirety via a simple nonunitary transform of conventional quantum chemical models. In fact such a transform adds precisely the desired short range, nonlinear, nonlocal, and nonhamiltonian effects.
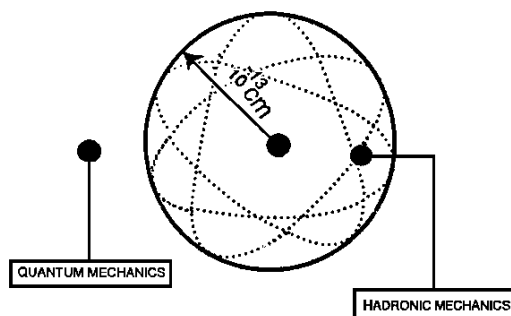

Figure 9.2. A schematic unit of the *hadronic horizon*, namely, of the sphere of radius 1 fm $(= 10^{-13}$ cm) outside which quantum chemistry is assumed to be exactly valid, and inside which nonlinear, nonlocal, and nonpotential effects are no longer negligible, thus requesting the use of hadronic chemistry for their numerical and invariant treatment.

9.1.2   Isochemical Model of Molecular Bonds

We now present the conceptual foundations of our *isochemical model of molecular bonds* for the simplest possible case of the H_2 molecule, which was first submitted by Santilli and Shillady in Ref. [5]. We shall then extend the model to the water and to other molecules in the subsequent chapter.

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 bond of the peripheral valence electrons, as generally acknowledged [1].

Our main assumption [5] is that *pairs of valence electrons from two different atoms can bond themselves at short distances into a singlet quasi-particle state called "isoelectronium," which describes an oo-shaped orbit around the two nuclei similar to that of planets in binary star systems (Fig. 9.3).*

It is important to note that recent studies in pure mathematics [39] have established that the *oo*-shaped orbit, called the *figure eight* solution, is one of the most stable solutions of the N-body problem.

The primary binding force of the isoelectronium is assumed to be of nonlinear, nonlocal, and nonpotential type due to contact effects in deep overlappings of the wavepackets of the valence electrons, as studied in Sect. 9.3.

However, the reader should be aware that the isoelectronium is expected to have a component of the binding force of purely potential type because, when the electrons are in singlet coupling, the magnetostatic *attraction* may be conceivably bigger than the electrostatic *repulsion* at distances of the order of one fermi or less (see Fig. 9.4 for details).

It should be stressed, however, that a purely potential origin of the isoelectronium is not expected to be exactly valid for various reasons, the most visible one being the fact that, at the very small mutual distances here considered, magnetostatic and electrostatic laws diverge, thus prohibiting reliable quantitative studies.

Hadronic chemistry has been built to resolve all divergences in the study of the isoelectronium thanks to the isomathematics with product $A \hat{\times} B = A \times \hat{T} \times B$, and the isotopic element $\hat{T}$ restricted to have absolute values much smaller than 1. In this way, the hadronic component of the isoelectronium binding force will "absorb" all divergent or otherwise repulsive effects, resulting in convergent numerical values.

The reader is also discouraged to reduce the isoelectronium to a purely quantum structure because, in this way, the theory would preserve all the insufficiencies of chemistry studied in Chapter 1, most importantly, the inability to reach an exact representation of molecular characteristics from the strict application of first quantum principles without *ad hoc* adulterations. In fact, as now well established, such an exact representation requires screenings of the Coulomb law, which can only be obtained via nonunitary transforms. The
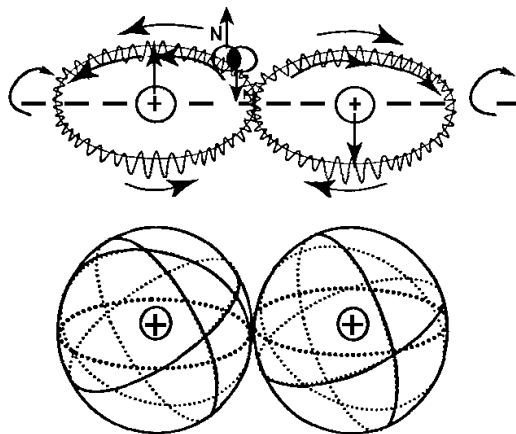
Figure 9.3. A schematic view of the proposed *isochemical model of the hydrogen molecule with fully stable isoelectronium*, where the top view refers to absolute zero degree temperature and in the absence of any motions, while the lower view includes rotations, thus recovering the conventional spherical distribution. The view is complementary to that of Fig. 9.7 for the unstable isoelectronium. The model is here depicted in terms of *orbits of the valence electrons*, rather than in terms of *orbitals, or density distributions*. The fundamental assumption is that the two valence electrons, one per each atom, correlate themselves into a bonded singlet state at short distance we have called *isoelectronium*, which is assumed in this figure to be stable. In this case the only orbit yielding a stable H-molecule is that in which the isoelectronium describes a *oo*-shaped orbit around the respective two nuclei, as it occurs for planets in certain systems of binary stars. The isoelectronium is then responsible for the *attractive force* between the two atoms. The *binding energy* is instead characterized by the *oo*-shaped orbit of the isoelectronium around the two nuclei, conceptually represented in this figure via a standing wave for a particle of spin 0, charge $-2e$, and null magnetic moment. As we shall see in this chapter, 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; the resolution of some of the inconsistencies of the conventional model; and other advances. Note finally that the model is easily extendable to dimers such as HO, HC, *etc.*, as studied in Chapter 3. The novelty in predictive character of the model can be seen from these preliminary lines. For instance, the model depicted in this figure predicts that *the hydrogen molecule becomes asymmetric, thus acquiring an infrared signature, under sufficient magnetic polarization, which removes its rotational motions*.

same nonunitary broadening of quantum chemistry is requested on numerous other counts independent from the isoelectronium.

Despite these limitations, the purely magnetostatic-electrostatic structure of the isoelectronium remains important *in first approximation*, because it recovers in a very simple way the hadronic horizon (Fig. 9.2), as well as the prediction by hadronic mechanics dating back to 1978 that triplet couplings are highly unstable. In fact, in the latter case, both electrostatic and magne-
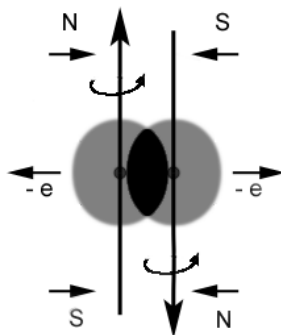
Figure 9.4. A schematic view of the conventional Coulomb forces of electrostatic and magnetostatic type in the structure of the isoelectronium. Since the charges are equal, they cause a *repulsion*. However, since the coupling is in singlet, the magnetic polarities are opposite, thus implying an *attraction*. Elementary calculations show that the magnetostatic attraction equals the electrostatic repulsion at a mutual distance of the order of 1 fm, while it becomes bigger at smaller distances, thus explaining the reason why the hadronic horizon has been set at 10^{-13} cm. This evidence establishes that the bonding force of the isoelectronium can also see its origin on purely Coulomb forces and, more particular, on the dominance of magnetic over electric effects at short distances, which is a rather general occurrence under the proper conditions (see the new chemical special of *magnecules* in Chapter 8). Despite this fully potential attractive total force, it should be stressed that the isoelectronium cannot be treated within a purely quantum mechanics context for various reasons. The first reason is that with the decrease of the distance, both electrostatic and magnetostatic effects diverge, thus preventing any serious scientific study. Hadronic mechanics and chemistry have been built precisely to remove these divergencies via the isotopies of generic products $A \hat{\times} B = A \times \hat{T} \times B$ with $|\hat{T}| \ll 1$ (Chapter 3). Therefore, the hadronic treatment of the isoelectronium permits convergent numerical predictions which would be otherwise impossible for quantum chemistry. Independently from that, the nonunitary lifting of quantum chemistry is mandated by the need to achieve an exact representation of experimental data on molecules which, as now established, requires screenings solely obtainable via nonunitary transforms of the Coulomb potential. Thus, any attempt to preserve old theories as exactly valid is doomed to failures. Despite that, the electrostatic and magnetostatic effects depicted in this figure illustrate that conventional potential effects should also be expected in the structure of the isoelectronium. In other words, rather than assuming either a purely quantum or a purely hadronic setting, we have *in media virtus*, i.e., the most plausible origin of the bonding force of the isoelectronium is that partially of potential and partially of nonpotential type. Still in turn, this implies the possibility of a significant (negative) binding energy for the isoelectronium, which is evidently that characterized by the potential component (Sect. 9.3).

tostatic forces would be *repulsive*, thus prohibiting any possible bound state, in beautiful agreement with Pauli's exclusion principle.

It is easy to predict that *the isoelectronium cannot be permanently stable when interpreted as a quasi-particle of about 1 fm charge diameter.* In fact, the

mere presence of exchange forces, which remain fully admitted by isochemistry, prevents the achievement of a complete stability under the indicated small mutual distances of the electrons. As we shall see in more details in Chapter 6, there are additional technical reasons which prevent the complete stability at short distances, and actually render the isoelectronium a short lived quasi-particles when the valence electrons are assumed at mutual distances of 1 fm.

However, it is easy to see that *the isoelectronium must be fully stable when the mutual distance of the two valence electrons is permitted to be of the order of molecular size. In fact, any instability under the latter long range conditions would imply a necessary violation of the fundamental Pauli's exclusion principle.*

In different words, *the isoelectronium is one of the first known quantitative representations of Pauli's principle*, in the sense that:

1) When assumed to be of potential type, the interaction responsible for Pauli's principle implies catastrophic inconsistencies, such as shifts of experimentally established energy levels, deviations from all spectroscopic lines, etc. As a result, a quantitative representation of Pauli's principle is *impossible* for quantum mechanics, evidently due to its strictly potential character. For this reason, Pauli's principle is merely imposed in quantum mechanics without any explanations, as well known. By comparison, a quantitative representation is possible for hadronic mechanics precisely because of its admission of *nonpotential* interactions, that is, interactions which have no bearing on energy levels and spectroscopic lines.

2) Quantum mechanics admits, in general, both singlet and triplet couplings because particles are assumed to be point like as per the very topological structure of the theory. By comparison, hadronic mechanics represents particles as expended at mutual distances smaller than their wavepackets, and solely admits singlet couplings due to highly repulsive-unstable forces predicted for all triplet couplings. The latter repulsive forces originate from the drag experienced by one wavepackets when rotating within and against the rotation of the other wavepacket, as well as by the fact that in triplet couplings both magnetostatic and electrostatic effects are repulsive (Fig. 9.4); and

3) Quantum mechanics cannot provide an exact representation of an *attraction* between *identical* electrons at very short distances, as discussed earlier, in disagreement with the experimental evidence, e.g., that the two electrons of the helium are bonded most of the time, to such an extent that they are emitted in such a bonded form during photodisintegrations, and in other events. By comparison, hadronic mechanics has been built to represent precisely the *bonding* of identical electrons in *singlet* coupling under interactions *not* derivable from a potential.

The assumption of the isoelectronium as being unstable when its valence electrons are at mutual distances of molecular order, implies a violation of Pauli's principle, e.g., because of the automatic admission of triplet couplings for two electrons at the same energy level.

When assumed as being stable in the limit case of a quasi-particle of 1 fm charge radius, *the most stable trajectory of the isoelectronium is of oo-type, each o-branch occurring around each nucleus* (Fig. 9.3). As illustrated in Fig. 9.4 (see also Chapter 8), such a shape automatically prevents the inconsistent prediction of ferromagnetic character of all molecules.

When the correlation-bond is distributed over the entire molecular orbit, *the trajectory of the isoelectronium is also expected to be oo-shaped around the two nuclei with inverted direction of rotation from one o-branch to the other.* This is suggested by a variety of reasons, such as: the need of avoiding the inconsistent prediction of ferromagnetic character, the compatibility with the limit case of a fully stable particle at short distance (which, as we shall see, can describe several *oo*-shaped orbits prior to separation), and others.

It should be indicated that the assumption of a finite lifetime of the isoelectronium irrespective of size implies the possibility of adding several H-atoms to the H_2 molecule for the duration of the unbound valence electrons, as well as other inconsistencies, such as the capability by hydrogen and water to be paramagnetic (Chapter 8).

In this chapter, we apply the above hypothesis to the construction of a new model of the hydrogen molecule and prove its capability to:

1) provide an essentially exact representation of the binding energy and other characteristics of the hydrogen molecules;

2) said representation occurs from first axiomatic principles without exiting from the underlying class of equivalence as occurring for Coulomb screenings;

3) explain for the first time to our knowledge the reason why the hydrogen molecule has only two atoms;

4) introduce an actual "strongly" attractive molecular bond;

5) achieve a much faster convergence of power series with consequential large reduction in computer times;

6) prevent inconsistencies such as the prediction that the hydrogen is ferromagnetic. In fact, whatever magnetic polarity can be acquired by the orbit around one nucleus, the corresponding polarity around the second nucleus will necessarily be opposite, due to the opposite direction of the rotations in the two *o*-branches, thus preventing the acquisition of a net total polarity North-South of the molecule.

By recalling from Chapter 3 that Gaussian screenings of the Coulomb law are a particular case of the general nonunitary structure of hadronic chemistry, one can see from these introductory lines that our first achievement on scientific records of an essentially exact representation of molecular characteristics
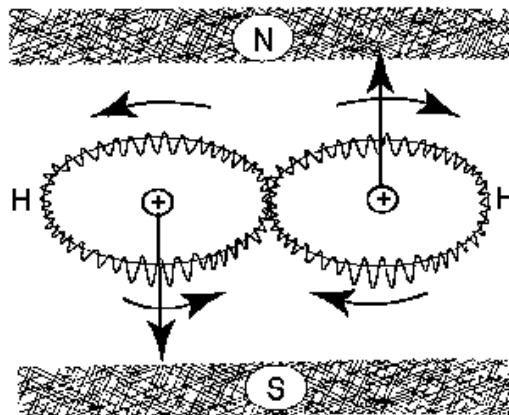
Figure 9.5. A schematic view of the impossibility for the isochemical model of the hydrogen molecule to acquire a net magnetic polarity, thus resolving a serious inconsistency of quantum chemistry. Recall from Chapter 1 that current molecular models are based on exchange, van der Waals, and other forces of nuclear origin, all implying the independence of the orbitals of the individual atoms. Under these assumptions, quantum electrodynamics demands that all molecules acquire a net total magnetic polarity North-South when exposed to an external magnetic field, in dramatic disagreement with reality. The isochemical model of molecular structure resolves this inconsistency because, as indicated in Fig. 4.3, the most stable trajectory for the isoelectronium is *oo*-shaped as it also occurs for the trajectory of planets in binary stars, with each *o*-branch around each nucleus. In this case, the rotation of the two *o*-branches are necessarily opposite to each other, thus resulting in *opposite* magnetic polarities, with the consequential impossibility to reach a *net* molecular magnetic polarity. As we shall see in Chapter 7, the above features have important industrial applications for new clean fuels and energies.

is reduced to the proper selection of the basic nonunitary transform, because the latter will permit dramatically more restrictive screenings.

The derivability of the essentially exact representation from first axioms of hadronic chemistry without adulterations is evident.

Equally evident is the first introduction of an actual, "strongly" attractive interatomic force (where the word "strongly" does not evidently refer to strong interactions in hadron physics), which is absent in current models due to the notorious "weak" nature of exchange and other forces of current used in molecular structures (where the word "weak" does not evidently refer to the weak interactions among leptons).

The representation of the reason why the hydrogen (or water) molecule has only two H-atoms is inherent in the very conception of the isoelectronium. Once the two valence electrons of the H-atoms couple themselves into a singlet quasi-particle state, there is no possibility for a third valence electron to par-
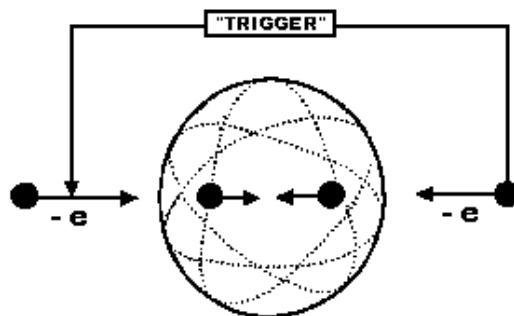
Figure 9.6. A schematic view of the *trigger*, namely, the external means suitable to force electrons with the same charge to penetrate the hadronic barrier (Fig. 9.2), in which attractive hadronic forces overcome the repulsive Coulomb barrier.

ticipate in the bound state, e.g., because we would have an impossible bound state between a fermion (the third electron) and a boson (the isoelectronium).

The achievement of a much faster convergence of the power series, or, equivalently, a dramatic reduction of computer times for the same calculations, is evident from the structure of hadronic chemistry as discussed in Chapter 3.

The avoidance of the prediction of ferromagnetic features (acquisition of a total North-South polarity under an external magnetic field) is due to the nature of the orbit of the isoelectronium, as discussed in details below and in Chapter 8.

In this chapter, we shall study two realizations of the proposed new model of the hydrogen molecule, the first model is a limiting case in which the isoelectronium is assumed to be *stable* (with an infinite lifetime) at ordinary conditions, and the second model in which the isoelectronium is assumed to be *unstable* (with a finite lifetime). The lifetime of the isoelectronium will then be computed in Chapter 6.

The hypothesis of the bonding of electrons at short distances was first introduced by Santilli [7a] for the structure of the π^0 meson as a hadronic bound state of one electron and one positron. Animalu [7b] and Animalu and Santilli [7c] extended the model to the Cooper pair in superconductivity as a hadronic bound state of two identical electrons.

A notion which is important for the very existence of the isoelectronium is that of a *trigger*, namely, *external (conventional) interactions, which cause the identical electrons to move one toward the other and to penetrate the hadronic horizon (Fig. 9.2) against their repulsive Coulomb interactions.* Once

inside the above mentioned horizon, the attractive hadronic forces overcome the repulsive Coulomb interaction, resulting in a bound state.

In the case of the π^0 model as a bound state of an electron and a positron at short distances, there is no need for a trigger because the constituents naturally attract each other. On the contrary, the existence of the Cooper pair does indeed require a trigger, which was identified by Animalu [7b] and Animalu and Santilli [7c] as being provided 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.

It should be indicated that we cannot use the term "electronium" because it would imply a bound state of two identical electrons under *quantum* mechanics, which is known to be impossible. The term "electronium" would also be technically inappropriate because the constituents *are not* ordinary electrons, but rather "isoelectrons," i.e., the image of ordinary particles under *nonunitary* transforms or, more technically, irreducible isounitary representations of the covering of the Poincarè symmetry known as the *Poincarè-Santilli isosymmetry* [3c, 3d, 4a].

We cannot close this conceptual section without a few comments regarding the possibility of treating the isoelectronium via *quantum electrodynamics* (QED), since the latter appears to be the natural discipline for a valence bond of two identical electrons at short distance. This issue is compounded by the general belief of the *unrestricted* exact validity of QED all the way to very small distances of the order of 10^{-24} cm.

It is easy to see that, as it is the case for quantum mechanics, a quantitative treatment of the isoelectronium is beyond the technical capabilities of QED for numerous conceptual and technical reasons. In fact, QED is purely linear, local and potential, while the interactions we are interested in representing are nonlinear, nonlocal and nonpotential.

In any case, it is easy to prove via the use of the Feynman diagrams that QED *cannot* represent any *attraction* between identical electrons in singlet coupling at short distance, as it occurs in the physical reality for the two electrons of the Helium, the Cooper pair, the valence electrons, and other systems. On the contrary, the *isotopies of quantum electrodynamics* (ISOQED) are expected to provide such a representation, but their study here would be vastly beyond the limited scope of this monograph.

The reconciliation between the current belief of the unrestricted exact validity of QED and the bonding of identical electrons is permitted by the fact that all experimental verifications of QED at shorter and shorter distances have been conducted via the use of *higher and higher energies*. On the con-

trary, the experimental verification of QED for the conditions of the isoelectronium require *smaller and smaller energies* which experimental verifications have been absent in the physics of the 20-th century due to the notorious emphasis on high energies.

As a final comment, it should be noted that the limitations of QED for the study of the isoelectronium are purely classical, and rest on *the inability of classical electrodynamics to represent the physical evidence of the attraction of identical spinning charges at sufficiently small distances, evidence which is even visible to the naked eyes, e.g., in ball lighting as created by nature, in microwave ovens or other means.*

As a matter of fact, no classical theory of electromagnetism can possibly be considered as "final" until it achieves the capability of representing the attraction of identical charges under suitable conditions. As a result, no quantum theory of electromagnetism, including QED, can be considered as "final" unless it is based on the preceding classical theory. One of the objectives of classical and operator isochemistry is precisely that of achieving such a missing representation.

9.1.3   The Limit Case of Stable Isoelectronium

We are now equipped to conduct a nonrelativistic study of the isoelectronium (Fig. 9.3) in the limit case of full stability under the assumption that the binding force is of purely hadronic type without potential contributions (Fig. 9.4). This approach is evidently done to test the effectiveness of hadronic chemistry for the numerical studies of the problem considered, since corrections due to potential effects can be easily added.

The reader should be aware upfront that *the above assumptions imply that the isoelectronium has no binding energy*, trivially, because nonpotential forces have no potential energy by conception.

The reader should be aware that the actual hadronic treatment should be conducted within the context of isomathematics, that is, on isoeuclidean and isohilbert spaces defined over isofields. To avoid excessive mathematical complexity, in this section we study the *projection* of this isotopic treatment on conventional spaces over conventional fields. However, it should be stressed that the only correct formulation remains the isotopic one.

As we shall see, the hadronic treatment of the isoelectronium yields an attraction of the type of the Hulten potential which is so strong to "absorb" at short distances all other forces, whether attractive or repulsive. However, the direct interpretation of the Hulten potential as an actual potential would be erroneous, since it solely occurs in the *projection* of the model on conventional spaces, while being completely absent in the technically appropriate treatment on isospaces over isofields. The direct interpretation of the Hulten potential

as an actual potential well of quantum mechanical nature would also be in direct contradiction with the absence of binding energy.

Therefore, the assumption of the projected model as the correct one leads to insidious inconsistencies and misrepresentations, such as the possible interpretation of the isoelectronium via a potential well, which treatment is very familiar in quantum mechanics, but the same treatment has no physical meaning for the isoelectronium. This is due to the fact that, as stressed earlier, a necessary condition to avoid inconsistencies in the interpretation of Pauli's principle is that its interaction *does not* admit a potential energy, thus rendering meaningless, or at best contradictory, conventional potential wells.

Note that the emergence of a "strong" Hulten potential eliminates the issue whether the isoelectronium is due to the dominance of the attractive magnetostatic forces over the repulsive electric ones (Fig. 9.4). This is due to the fact that the Hulten potential, as we shall review shortly in detail, behaves at short distances as *constant/r*, thus absorbing all Coulomb forces, irrespective of whether attractive or not. Moreover, the unified treatment via the Hulten potential presented below eliminates the divergent character of these forces at short distances, thus permitting meaningful numerical results.

We should finally indicate, to avoid inconsistencies, that the study of this section deals with the *limit* case of *a perfectly stable isoelectronium interpreted as a quasi-particle of about 1 fm charge diameter*, while in reality such form of the isoelectronium is unstable. Moreover, in this section we shall not study the expectation that the isoelectronium persists beyond the 1 fm mutual distance of the valence electrons, as necessary to prevent violations of Pauli's principle.

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

$$\left(\frac{p \times p}{m} + \frac{e^2}{r}\right) \times \psi(r) = E \times \psi(r). \tag{9.1.5}$$

To transform this state into the isoelectronium representing the bonding of the H-electron with a valence electron of another atom of generic charge ze, we need first to submit Eq. (9.1.5) to a nonunitary transform characterizing the short range hadronic effects, and then we must add the *trigger*, namely, the Coulomb attraction by the nuclei.

This procedure yields the *isoschrödinger equation for the isoelectronium* (Chapter 1),

$$U \times U^\dagger = \hat{I} = 1/\hat{T} > 0, \tag{9.1.6a}$$

$$\hat{A} = U \times A \times U^\dagger, \quad A = p, \ H, \dots, \tag{9.1.6b}$$

$$U \times (A \times B) \times U^\dagger = \hat{A}\hat{\times}\hat{B} = \hat{A} \times \hat{T} \times \hat{B}, \quad \hat{\psi} = U \times \psi, \tag{9.1.6c}$$

$$\left(\frac{1}{m}\hat{p} \times \hat{T} \times \hat{p} \times \hat{T} + \frac{e^2}{r} \times \hat{T} - \frac{z \times e^2}{r}\right) \times \hat{\psi}(r) = E_0 \times \hat{\psi}(r), \qquad (9.1.6d)$$

$$\hat{p}\hat{\times}\hat{\psi}(r) = -i \times \hat{T} \times \nabla\hat{\psi}(r), \qquad (9.1.6e)$$

where the factor $\hat{T}$ in the first Coulomb term originates from the nonunitary transform of model (9.1.5), while the same factor is absent in the second Coulomb term because the latter is long range, thus being conventional. As a result, in the model here considered the trigger is merely added to the equation.

The angular component of model (9.1.6) is conventional [3], and it is hereon ignored. For the radial component $r = |\mathbf{r}|$, we assume the isounit [7]

$$\hat{I} = e^{N \times \psi/\hat{\psi}} \approx 1 + N \times \psi/\hat{\psi}, \quad N = \int dr^3 \, \hat{\psi}^\dagger(r)_{1\downarrow} \times \hat{\psi}(r)_{2\uparrow}, \qquad (9.1.7a)$$

$$\hat{T} \approx 1 - N \times \psi/\hat{\psi}, \qquad (9.1.7b)$$

$$|\hat{I}| \gg 1, \quad |\hat{T}| \ll 1, \qquad (9.1.7c)$$

$$\lim_{r \gg 1\text{fm}} \hat{I} = 1, \qquad (9.1.7d)$$

where one should note that Eqs. (9.1.7c) and (9.1.7d) are automatically verified by expressions (9.1.7a) and (9.1.7b).

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

$$\psi \approx N \times \exp(-b \times r), \qquad (9.1.8)$$

with N approximately constant at distances near the hadronic horizon of radius

$$r_c = \frac{1}{b}, \qquad (9.1.9)$$

while $\hat{\psi}$ behaves like

$$\hat{\psi} \approx M \times \left(1 - \frac{\exp(-b \times r)}{r}\right), \qquad (9.1.10)$$

with M being also approximately constant under the same range [7a]. We then have

$$\hat{T} \approx 1 - \frac{V_{\text{Hulten}}}{r} = 1 - V_0 \frac{e^{-b \times r}}{(1 - e^{-b \times r})/r}, \qquad (9.1.11)$$

namely, we see the appearance of a Hulten potential in this local approximation. But the Hulten potential behaves at short distances like the Coulomb one,

$$V_{\text{Hulten}}r \approx \frac{1}{b} \approx \frac{V_0}{b} \times \frac{1}{r}. \qquad (9.1.12)$$

As a result, inside the hadronic horizon we can ignore the repulsive (or attractive) Coulomb forces altogether, and write

$$+\frac{e^2}{r}\times\hat{T}-\frac{e^2}{r}\approx+\frac{e^2}{r}\times\left(1-\frac{V_{\text{Hulten}}}{r}\right)-\frac{z\times e^2}{r}=-V\times\frac{e^{-b\times r}}{1-e^{-b\times r}},\quad(9.1.13)$$

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

By assuming in first approximation $|\hat{T}|=\rho\approx 1$, the radial equation of model reduces to the model of π^0 meson [7a] or of the Cooper pair [7b, 7c], although with different values of V and b.

$$\left[\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{d}{dr}\right)+\frac{m}{\rho^2\times\hbar^2}\left(E_0+V\times\frac{e^{-b\times r}}{1-e^{-b\times r}}\right)\right]\times\hat{\psi}(r)=E_0\times\hat{\psi}(r).\quad(9.1.14)$$

The exact solution and related boundary conditions were first computed in Ref. [7a], Sect. 5, and remain fully applicable to the isoelectronium.

The resulting spectrum is the typical one of the Hulten potential,

$$|E_0|=\frac{\rho^2\times\hbar^2\times b^2}{4\times m}\left(\frac{m\times V}{\rho^2\times\hbar^2\times b^2}\times\frac{1}{n}-n\right)^2,\quad(9.1.15)$$

which evidently possesses a *finite* spectrum, as well known.

To reach a numerical solution, we introduce the parametrization as in Ref. [7a],

$$k_1=\frac{1}{\lambda\times b},\quad(9.1.16a)$$

$$k_2=\frac{m\times V}{\rho^2\times\hbar^2\times b^2}.\quad(9.1.16b)$$

We note again that, from boundary conditions, k_2 must be bigger than but close to one, $k_2\approx 1$ [7].

We therefore assume in first nonrelativistic approximation that

$$\frac{m\times V}{\rho^2\times\hbar^2\times b^2}=1.\quad(9.1.17)$$

By assuming that V is of the order of magnitude of the total energy of the isoelectrons at rest as in the preceding models [7],

$$V\approx 2\times\hbar\times\omega\approx 2\times 0.5\text{ MeV}=1\text{ MeV},\quad(9.1.18)$$

and by recalling that $\rho\approx 1$, we reach the following estimate for the *radius of the isoelectronium*

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

$$= \left(\frac{1.054 \times 10^{-27} \text{erg} \cdot \text{sec}}{1.82 \times 10^{-27} \text{ g} \times 1.236 \times 10^{20} \text{ Hz}} \right)^{1/2} = \tag{9.1.19}$$

$$= 6.8432329 \times 10^{-11} \text{cm} = 0.015424288 \text{ bohrs} = 0.006843 \text{ Å},$$

It should be noted that: 1) the above values of r_c and V are only *upper boundary values* in the center-of-mass frame of the isoelectronium, i.e., the largest possible values under the assumptions of this section; 2) the values have been computed under the approximation of null relative kinetic energy of the isoelectrons with individual total energy equal to their rest energy; and 3) the values evidently *decrease* with the addition of the relative kinetic energy of the isoelectrons (because this implies the increase of m in the denominator).

The actual radius of the isoelectronium, when considered to be an quasi-particle as in this section, is also expected to vary with the trigger, that is, with the nuclear charges, as confirmed by the calculations presented in the next sections. This illustrates again the upper boundary character of value (9.1.19).

The value k_1 is then given by

$$k_1 = \frac{V}{2 \times k_2 \times b \times c_0} = 0.19, \quad k_2 \approx 1. \tag{9.1.20}$$

Intriguingly, the above two values for the isoelectronium are quite close to the corresponding values of the π^0 [7a] and of the Cooper pair [7b, 7c] (see also Sect. 1.9),

$$k_1 = 0.34, \quad k_2 = 1 + 8.54 \times 10^{-2}, \tag{9.1.21a}$$

$$k_1 = 1.3 \times \sqrt{z} \times 10^{-4}, \quad k_2 = 1.0 \times \sqrt{z}, \tag{9.1.21b}$$

It is important to see that, at this nonrelativistic approximation, *the binding energy of the isoelectronium is not only unique, but also identically null,*

$$|E_0| = \frac{\rho^2 \times \hbar^2 \times b^2}{4 \times m} \left(\frac{m \times V}{\rho^2 \times \hbar^2 \times b^2} - 1 \right)^2 = \frac{V}{4 \times k_2} \times (k_2 - 1)^2 = 0. \tag{9.1.22}$$

This result is crucial to prevent inconsistencies with Pauli's exclusion principle, which, as indicated earlier, *requires no potently energy between the two electrons for its interpretation in a way consistent with experimental data.*

The notion of *a bound state with only one allowed energy level* (called "hadronic suppression of the atomic spectrum" [7a]) is foreign to conventional quantum mechanics and chemistry, although it is of great importance for hadronic mechanics. In fact, any excitation of the constituents, whether the π^0, the Cooper pair or the isoelectronium, 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.

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 isochemistry. 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 isoelectronium, which can be written in this nonrelativistic approximation [7a]

$$\tau = \frac{\hbar}{4\times\pi\times\hbar^2}|\hat{\psi}(0)|\times\alpha\times E_{\hat{e}}^{\text{Kin}} = 7.16\times10^4\times\frac{k_1}{(k_2-1)^3\times b\times c_0}. \qquad (9.1.23)$$

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

The above derivation characterizes the *limiting assumption of a fully stable isoelectronium in nonrelativistic approximation.* By comparison, the Cooper pair under the same derivation *is not* permanently stable because its binding energy is very small, yet finite [7b], thus implying a large yet finite meanlife. Also by comparison, the π^0 *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.

Another important information of this section is that *the isoelectronium is sufficiently small in size to be treated as a single quasi-particle.* This property will permit rather important simplifications in the isochemical structure of molecules studied in the next sections.

By comparison, the Cooper pair has a size much bigger than that of the isoelectronium [7b, 7c]. This property is fundamental to prevent that the Cooper pair takes the role of the isoelectronium in molecular bonds, i.e., even though possessing the same constituents and similar physical origins, the isoelectronium and the Cooper pair are different, non-interchangeable, hadronic bound states.

The lack of binding energy of the isoelectronium 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 isoelectronium in a molecular structure, as studied in the next sections.

A novelty of isochemistry over quantum chemistry is that the mutual distance (charge diameter) between the two isoelectrons in the isoelectronium could, as a limited case, also be identically null, that is, the two isoelectrons could be 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 isoelectronium, the null value of the relative kinetic energy, and an identically null magnetic field. This is a perfectly diamagnetic state, which evidently al-

lows a better stability of the isochemical bond as compared to a quasi-particle with non-null size.

Note that, if conventionally treated (i.e., represented on conventional spaces over conventional fields), the nonunitary image of model (9.1.5) would yield *noninvariant numerical results* which, as such, are unacceptable (Sect. 1.7). This occurrence mandates the use of the covering isochemistry and related isomathematics which assures the achievement of invariant results.

Note also that the main physical idea of isounit (9.1.7) 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 isounit (9.1.7a) is null, the exponential reduces to I, Eq. (9.1.7d), the nonunitary transform becomes conventionally unitary, and quantum chemistry is recovered identically.

It is also important to see that, under transform (9.1.7a), model (9.1.5) is implemented with interactions which are: *nonlinear*, due to the factor $\psi/\hat{\psi}$ in the exponent; *nonlocal*, because of the volume integral in (9.1.7a); and *nonpotential*, because not represented by a Hamiltonian.

We finally note that the explicit form of the isotopic element $\hat{T}$, Eq. (9.1.7b), emerges in a rather natural way as being *smaller than one* in absolute value, Eq. (9.1.7c), i.e.,

$$|\hat{T}| = |1 - N \times \psi/\hat{\psi}| \ll 1. \tag{9.1.24}$$

As pointed out in Chapter 3, this property alone is sufficient to *guarantee* that all slowly convergent series of quantum chemistry converge faster for isochemistry.

9.1.4 Isochemical Model of the Hydrogen Molecule with Stable Isoelectronium

We are now sufficiently equipped to initiate the study of the *isochemical model of the hydrogen molecule*, first submitted by Santilli and Shillady in Ref. [5] (see Figs. 9.3, 9.4 an d 9.5). In this Section we shall begin the study by identifying the equation of structure of the H-molecule under the limit assumption that the isoelectronium is perfectly stable at short distances, namely, that the two valence electrons are permanently trapped inside the hadronic horizon, resulting in the main features derived in the preceding section

$$\text{mass} \approx 1 \text{ MeV}, \quad \text{spin} = 0,$$
$$\text{charge} = 2 \times e, \quad \text{magnetic moment} \approx 0, \tag{9.1.25a}$$

$$\text{radius} = r_c = b^{-1} = 6.8432329 \times 10^{-11} \text{cm} =$$
$$= 0.015424288 \text{ bohrs} = 0.006843 \text{ Å}. \tag{9.1.25b}$$

The more realistic case when the isoelectronium is unstable at such small distances is studied later on in this chapter, where we shall also reach an essentially exact representation of the characteristics of the hydrogen molecule.

The main reason for assuming the isoelectronium to be stable at short distances with characteristics (9.1.25) is that such an approximation permits rather major structural simplifications, most notably, the transition, from the conventional hydrogen molecule (which is a *four-body system*), to the isochemical model of this section (which is a *three-body system*, Fig. 9.3). By recalling that four-body systems do not admit an exact solution, while restricted three-body systems do admit an exact analytic solution, the implications of the approximate model of this section are sufficient to warrant an inspection.

Our foundation is the conventional quantum model of H_2 molecule [1],

$$\left(\frac{1}{2\mu_1} p_1 \times p_1 + \frac{1}{2\mu_2} p_2 \times p_2 + \right. \tag{9.1.26}$$

$$\left. + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\psi\rangle = E \times |\psi\rangle.$$

Our task is that of subjecting the above model to a transform

$$U \times U^\dagger|_{r \approx r_c} = \hat{I} = 1/\hat{T} \neq I, \tag{9.1.27}$$

which is nonunitary only at the short mutual distances

$$r_c = b^{-1} = r_{12} \approx 6.8 \times 10^{-11} \text{cm}, \tag{9.1.28}$$

and becomes unitary at bigger distances,

$$U \times U^\dagger|_{r \leq 10^{-10}\text{cm}} \neq I, \quad I_{r \gg 10^{-10}\text{cm}} = I. \tag{9.1.29}$$

This guarantees that our isochemical model coincides with the conventional model everywhere except for small contributions at small distances.

Assumption (9.1.29) also guarantees that *the conventional energy level of the individual hydrogen atoms are not altered.* In other words, assumption (9.1.29) realizes the main conception of this monograph, the exact character of quantum mechanics for the structure of *one* hydrogen atom, and its insufficiency for *two* hydrogen atoms bounded into the hydrogen molecule (Chapter 1).

The Hilbert space of systems (9.1.26) can be factorized in the familiar form (in which each term is duly symmetrized or antisymmetrized) as in Refs. [1]

$$|\psi\rangle = |\psi_{12}\rangle \times |\psi_{1a}\rangle \times |\psi_{1b}\rangle \times |\psi_{2a}\rangle \times |\psi_{2b}\rangle \times |\psi_R\rangle, \tag{9.1.30a}$$

$$\mathcal{H}_{\text{Tot}} = \mathcal{H}_{12} \times \mathcal{H}_{1a} \times \mathcal{H}_{1b} \times \mathcal{H}_{2a} \times \mathcal{H}_{2b} \times \mathcal{H}_R. \tag{9.1.30b}$$

The nonunitary 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

$$U(r_{12}) \times U^\dagger(r_{12}) = \hat{I} = \exp\left[\frac{\psi(r_{12})}{\hat{\psi}(r_{12})}\int dr_{12}\hat{\psi}^\dagger(r_{12})_{1\downarrow} \times \hat{\psi}(r_{12})_{2\uparrow}\right], \quad (9.1.31)$$

where the ψ's represent conventional wavefunctions and the $\hat{\psi}$'s represent isowavefunctions.

As an alternative yielding the same results, one can transform short-range terms (isochemistry), and add un-transformed long-range terms (quantum chemistry), resulting in the radial equation

$$\left(-\frac{\hbar^2}{2 \times \mu_1}\hat{T} \times \nabla_1 \times \hat{T} \times \nabla_1 - \frac{\hbar^2}{2 \times \mu_2}\hat{T} \times \nabla_2 \times \hat{T} \times \nabla_2 + \right.$$

$$\left. +\frac{e^2}{r_{12}} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (9.1.32)$$

By recalling that the Hulten potential behaves at small distances like the Coulomb one, Eq. (9.1.32) becomes

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2 - V \times \frac{e^{-r_{12}\times b}}{1 - e^{-r_{12}\times b}} - \right.$$

$$\left. -\frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \quad (9.1.33)$$

The above equation does indeed achieve our objectives. In fact, it exhibits a *new explicitly attractive force between the neutral atoms of the hydrogen molecule, which force is absent in conventional quantum chemistry.* The equation also explains the reasons why the H_2 molecule admits only *two* H-atoms. As we shall see in the remaining sections, Eq. (9.1.33) also permits essentially exact representations of the binding energy and other molecular characteristics, yields much faster convergence of series with much reduced computer times, and resolves other insufficiencies of conventional models.

9.1.5   Exactly Solvable, Three-Body, Isochemical Model of the Hydrogen Molecule

Our isochemical model of the hydrogen molecule, Eqs. (9.1.33), can be subjected to an additional simplification, which is impossible for quantum chemistry. In our isotopic model, the two isoelectrons are bonded together into a single state we have called isoelectronium. In particular, the charge radius of the latter is sufficiently small to permit the values (see Fig. 9.3)

$$r_{12} \lesssim r_{1a}, \text{ and } r_{1b}, \quad r_{12} \approx 0, \quad (9.1.34a)$$

$$r_{1a} \approx r_{2a} = r_a, \quad r_{1b} \approx r_{2b} = r_b. \tag{9.1.34b}$$

Moreover, the H-nuclei are about 2,000 times heavier than the isoelectronium. Therefore, our model (9.1.33) can be reduced to a *restricted three body problem* similar to that possible for the conventional H_2^+ *ion* [1], but *not* for the conventional H_2 molecule.

Such a restricted model essentially consists of two H-protons at rest at a fixed mutual distance plus the isoelectronium moving around them in the *oo*-shaped orbit of Fig. 9.4, according to the structural equation

$$\left(-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_1^2 - V \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \right.$$

$$\left. -\frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \tag{9.1.35}$$

Under the latter approximation, the model permits, for the first time, the achievement of an *exacts solution for the structure of the H_2 molecule*, as it is the case for the H_2^+ ion or for all restricted three-body problems. This solution will be studied in Chapter 6 via variational methods. The exact analytic solution has not been studied at this writing, and its study is here solicited by interested colleagues. At this introductory level we only limit ourselves to a few comments.

Note that *the above exact solution of the hydrogen molecule is only possible for the case of the isoelectronium fully stable at short mutual distances*. In fact, for the case of the mutual distance of the valence electrons no longer restricted to 1 fm, the model is a full *four-body structure*, which, as such, admits no exact solution.

Note also that model (9.1.35) is the isochemical model of the H_2 molecule inside the hadronic horizon. The matching representation *outside* the hadronic horizon is presented in the next section.

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, each admitting an exact solution, with possible extension to molecular chains, and evident extensions to other molecules.

Readers interested in studying model (9.1.35) should keep in mind that *the rest energy of the isoelectronium is unknown at this writing, thus being a free parameter suitable for fitting experimental data*. More specifically, in Eq. (9.1.35) we have *assumed* from Sect. 9.3 that

$$m_{\text{isoelectronium}} = 2 \times m_{\text{electron}}. \tag{9.1.36}$$

However, the results of Sect. 9.3 are approximate. In particular, they hold under *the assumption that the isoelectronium has no internal binding energy.* Such an assumption was made for the specific purpose of proving that non-potential forces represented with the isounit can indeed yield a bound state. In particular, the assumption was suggested by the need to represent Pauli's exclusion principle without the introduction of a potential.

However, such a view may be solely valid at molecular distances of valence electrons, and not necessarily at short distances. As a result, the isoelectronium may indeed have an internal binding energy, that is, it can have internal forces derivable from a potential in addition to the nonpotential forces without binding energy of hadronic chemistry, as outlined in Fig. 9.4.

This is due to the fact that the structure of the isoelectronium implies *three* acting forces: *one repulsive* Coulomb force due to the same changes, plus *two attractive* forces due to the two pairs of opposite magnetic polarities in singlet configuration. The latter two attractive forces may overcome the repulsion due to the change beginning at distances of the order of one Fermi, resulting in a conceivable net attractive force derivable from a potential.

Under the latter conditions, the isoelectronium would indeed have a *negative* binding energy, resulting in the unknown value

$$m_{\text{isoelectronium}} < 2 \times m_{\text{electron}}. \tag{9.1.37}$$

The understanding is that the case $m_{\text{isoelectronium}} > 2 \times m_{\text{electron}}$ is impossible.

The unknown character of the isoelectronium mass alters considerably the perspective of restricted model (9.1.35). As we shall see in Chapter 6, it is possible to prove via variational and other methods that *model* (9.1.35) *under assumption* (9.1.36) *does not admit exact solutions accurately representing the binding energy of the hydrogen molecule.* However, under the use of the isoelectronium mass free for fitting experimental data, the situation may be different.

Another information which should not be assumed to be exact is the *size of the isoelectronium*, Eq. (9.1.19). In fact, as stressed in Sect. 9.3, such a value too must be assumed to be an *upper boundary value.* In model (9.1.35) the isoelectronium is assumed to be point-like. However, the model can be first extended via Eq. (9.1.35) for a stable isoelectronium with a *fixed* unknown radius

$$r_c = b^{-1} \le 6.8 \times 10^{-11} \text{cm}. \tag{9.1.38}$$

A second extension of model (9.1.35) should also be taken into consideration, that in which

$$r_c = b^{-1} \ge 6.8 \times 10^{-11} \text{cm}, \tag{9.1.39}$$

because, as stressed in Sects. 9.2 and 9.3, any assumption that the isoelectronium ceases to exist at distances bigger than 10^{-11} cm would imply a violation of Pauli's exclusion principle.

As a matter of fact, the assumed mass (9.1.36) is more in line with assumption (9.1.39), than with assumption (9.1.38), again, to prevent the existence at large mutual distances of the valence electrons of attractive internal potential forces with a binding energy which would alter conventional atomic structures.

Even though, admittedly, *the size of the isoelectronium is variable in the physical reality*, its average into a constant value may have meaning, of course, as a first approximation.

A third quantity of model (9.1.35) deserving inspection is the experimental value of the bond length, which is generally referred to the distance between the two nuclei R. In principle, such a distance is expected to be altered by a fully stable isoelectronium. Therefore, a solution of model (9.1.35) in which R is fitted from the experimental data is indeed meaningful, of course, as a first approximation.

In conclusion, in both, the four-body model (9.1.33) and the restricted three-body model (9.1.35), we have *three quantities which, in principle, can be assumed to be unknown and, therefore, should be derived from the fit of experimental data: 1) the mass of the isoelectronium; 2) the size of the isoelectronium; and 3) the bond length.*

There is no doubt that an exact analytic solution of model (9.35) suitable to represent the binding energy of the hydrogen is permitted by the above three free fits with intriguing implications for all H-bonds whose study is left to interested researchers.

9.1.6 Isochemical Model of the Hydrogen Molecule with Unstable Isoelectronium

In this section we review the study of Ref. [5] on the solution of the restricted isochemical model of the hydrogen molecule, Eq. (9.1.35) and Fig. 9.3, via conventional variational methods used in chemistry, under the assumption that the isoelectronium has characteristics (9.3.21). As we shall see, these studies have achieved an essentially exact representation of experimental data on the hydrogen molecule, including its binding energy and bond length, for the first time from exact first principles without ad hoc adulterations.

For historical papers in chemistry connected to our model, see Refs. [6]. Representative, more recent papers with technical connections to our study as outlined below are given by Refs. [8 – 38].

The possibilities that the mass of the isoelectronium be smaller than $2\times$mass of electron and its radius be bigger than 6.8×10^{-11} cm will not be considered in this section.

For this purpose we first note that the solution of the full model with the Hulten potential $e^{-rb}/(1 - e^{-rb})$ where $r_c = b^{-1}$ is the size of the isoelectronium, implies rather considerable technical difficulties. Therefore, we shall study model (9.1.35) under an *approximation* of the Hulten potential given by

one Gaussian of the type

$$\frac{e^{-rb}}{1 - e^{-rb}} \approx \frac{1 - Ae^{-br}}{r},$$
(9.1.40)

with A a constant identified below.

It is known that a linear combination of sufficient number of Gaussians can approximate any function. Therefore, the achievement of an essentially exact representation of molecular data via approximation (9.1.40) will evidently persist under the full use of the Hulten potential.

Recall from Sect. 9.3 that the *stable* character of the isoelectronium is crucially dependent on the use of the attractive Hulten potential, which "absorbs" repulsive Coulomb forces at short distances resulting in attraction. Therefore, the weakening of the Hulten potential into the above Gaussian form has the direct consequence of turning the isoelectronium into an *unstable* state.

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

It should be indicated that the terms "unstable isoelectronium" should be referred as the period of time in which the two valence electrons remain within the hadronic horizon of 6.8×10^{-11} cm. The same terms *should not* be interpreted to the fact that the isoelectronium does not exist outside the hadronic horizon, because the latter view implies a number of inconsistencies, such as possible violation of Pauli's exclusion principle, acquisition by molecules of ferromagnetic character, *etc.*

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 (9.1.40). The question whether the isoelectronium is stable or unstable evidently depends on the amount of instability and its confrontation with experimental data, e.g., on magnetic susceptibility. As such, the issue will be addressed theoretically and experimentally in a future paper.

Under the above assumption, our first step is the study of model (9.1.35) in an exemplified Coulomb form characterized by the following equation, hereon expressed in atomic units (a.u.)

$$H \times \Psi = \left(-\frac{1}{2} \nabla^2 - \frac{2}{r_a} - \frac{2}{r_b} + \frac{1}{R} \right) \times \Psi,$$
(9.1.41)

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

The standard method for solving the above equation is the following. The variational calculation is set up in matrix algebra form in a nonorthogonal

basis set S 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 and S are Hermitean matrices. E is a diagonal matrix with the energy eigenvalues

$$HC = ESC; \quad \text{define } C = S^{-\frac{1}{2}}C', \text{ then } HS^{-\frac{1}{2}}C' = ES^{-\frac{1}{2}}C', \quad (9.1.42a)$$

$$(S^{-\frac{1}{2}}HS^{+\frac{1}{2}}C') = H'C' = E(S^{-\frac{1}{2}}SS^{-\frac{1}{2}})C' = EC', \quad (9.1.42b)$$

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

Here the basis is formed from contracted basis sets Φ, which are fixed linear combinations of Gaussian spheres χ fitted to real shapes of spherical harmonic functions. The eigenvector column in C gives the basis coefficients of the molecular orbitals according to the expression

$$\Psi_i = \sum_{c_{i,j}} (j : \Psi_j = \sum_{a_{j,k}} \Psi_k; \ \chi = \left(\frac{2\alpha}{\pi}\right)^{3/4} \exp[-(\alpha - A)^2] = /\alpha, A). \quad (9.1.43)$$

The problem of how to form a sharp cusp on a $1s$ orbital is solved to a practical extent by using up to six Gaussians; here we use the very best "least-energy" 1s orbital from Pople's group [18]. In this problem the s-, p-, d- and f-orbitals are polarization functions that merely serve to evaluate the effect of other angular components on the $1s$ orbitals which are the main terms of the $1s$-sigma bond in H_2.

Gaussian orbitals can easily be scaled to screened nuclear charge values by multiplying the Gaussian exponents by the square of the scaling factor (in effect, shrinking the space of the H-atom model) followed by renormalization of the linear combination of Gaussians. In this work the scaling constant of the $1s$ orbitals was optimized to 1.191 and the 2-, 3- and 4-shell orbitals optimized as scaled shells rather than optimizing each orbital individually.

As the orbitals were optimized using parabolic fitting to three energy values as a function of the scaling value, it became apparent that the bond length of the three-body model is much shorter than the usual value of 1.4011 Bohr (= 0.74143 Angströms). Thus, the bond length was re-optimized after optimization of the scaling for each principle shell. The scaling constants and the orbital contractions are Angströms at an energy of -7.61509174 Hartrees (= -207.2051232 eV) where the achievement of an exact representation of the binding energy is studied in detail.

Although a large basis set of $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, $4s$, $4p$, and $4f$ orbitals was used, this variational energy is probably higher than the exact solution of

the type used by Bates, Ledsham and Stewart [12]. However, the energy of the 6-gaussian ($6G$) Least-Energy $1s$ function [18] is -0.499946 Hartrees for the H atom so the energy quoted here should be within 0.001 Hartrees of the exact solution.

While it is expected that a collapsed isoelectronium pair would be even more unstable than a collapsed positronium quasi-particle due to the repulsive interaction of the electrons, this three-body model of H_2 predicts over 6 Hartrees added molecular stability and a substantial decrease in bond length. The $E(1)$ value of the electronium-pair of some -11.473164 Hartrees is lower than the total energy of the molecule due to the repulsion of the proton-nuclei from the $1/R$ term of the Hamiltonian.

9.1.7 Gaussian Approximation of the Isochemical Model of the Hydrogen Molecule as a Four-Body System

As indicated earlier, it is possible that the valence electrons bond themselves into the isoelectronium not in a permanent fashion, but rather in a statistical fashion, with only a percentage of their time in a bonded state, in which case the restricted three-body model is evidently insufficient. In this section we review the studies of Ref. [5] on the full four-body isochemical model of H_2, which model also permits the achievement of an exact representation of the binding energy from first principles without adulterations (see Fig. 9.7).

A considerable effort has been made since the time of Hylleraas [20] in the 1930's to find a way to calculate the last 2% of the binding energy of molecules. Boys [22] derived a form of "configuration interaction" which offered exact variational solutions, but this proved to be very slowly convergent and only applicable to small molecules. Moller-Plesset perturbation developed by Pople *et. al.* [23] is popular today, but studies up to eighth order have been shown not to converge after huge expense in computer time. Linked-cluster diagrams by Bartlett *et. al.* [24]) multiconfiguration-self-consistent-field (MC-SCF) calculations by Schaefer *et. al.* [25] and Goldstone-Bruekner-Feynman diagrammatic perturbation by Kelly [26] have all been shown to require very large computer resources, are limited to small molecules and sometimes fail to give even negative binding energies as shown by Goddard [27] for Cr_2.

All these slow and expensive methods seem to share one common feature, the use of high energy empty "virtual" orbitals from a ground state calculation, usually of Hartree-Fock-Roothaan type, to improve the representation of the ground state.

One might ask how it is possible to lower the energy by using higher energy wavefunctions. The fact that some energy lowering is found suggests electron
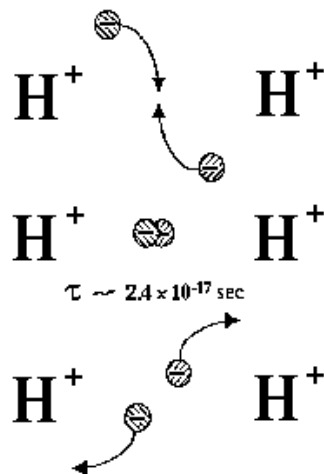
Figure 9.7. A schematic view of the *isochemical model of the hydrogen molecule with unstable isoelectronium* due to the weakening of the Hulten potential and consequential relaxation of the infinite lifetime, as a view complementary to that of Fig. 9.4 with stable isoelectronium. In this case the notion of isoelectronium essentially represents a tendency of pairs of valence electrons to correlate-bond in singlet states at short distances. The use of isochemistry, rather than conventional chemistry, is necessary because even this weaker form of the isoelectronium, as well as all screenings of the Coulomb potential at large, are nonunitary images of conventional Coulomb settings, as established in Chapter 1. Therefore, all these models require a representation on isospaces over isofields for their invariant formulation. In the text, we present the projection of such an invariant formulation on conventional spaces over conventional fields for simplicity.

dynamics is indeed complicated, and the rate of convergence of this method is quite slow.

The method adopted here is to use the usual Hartree-Fock-Roothaan self-consistent-field equations [1] (which also has some formal flaws such as the self-interaction terms [27]), and question the form of the Coulomb interaction of the electron.

Note that reducing the values of the Coulomb integrals will lower the energy by reducing the electron-electron repulsion while reducing the exchange terms will raise the energy, but the $1/2$ factor reduces the effect of the exchange terms. Thus, a reduction of the value of the integrals will lower the energy. Note that Goddard [27] has already recommended reducing the atomic self-energy by subtracting 1.39 eV from Hartree-Fock exchange integrals in the

cases of Cr_2 and Mo_2. In this way, we reach the expressions

$$FC = ESC; \quad F_{i,j} = H_{i,j} + \sum_{k,l} P_{k,l}[(i,j|k,l) - \frac{1}{2}(i,k|j,l)], \qquad (9.1.44a)$$

$$(i,j|k,l) = \iint \chi_i(1)\chi_j(1)\frac{1}{r_{12}}\chi_k(2)\chi_l(2)\,d\tau_1 d\tau_2, \qquad (9.1.44b)$$

$$P_{i,j} = 2\sum_n c_{n,i}c_{n,j} \quad \text{(sum n only over occupied orbitals)}. \qquad (9.1.44c)$$

The 1995 paper on Cooper pairs by Santilli and Animalu [7c] invokes the non-local hadronic attractive force first identified in the π^0-meson [7a] as applied to singlet-paired electrons which form a boson particle. After using a non-local isotopic nonlinear transformation, the hadronic attraction was transformed back to real-space and modeled resulting into an attractive force which overcomes the repulsive Coulomb force. In turn, the latter occurrence constitutes the physical-chemical origin in the use of a suitably screened Coulomb potential for the binding energy.

Examination of the original 1978 paper on positronium collapse by Santilli [7a], reveals that the Hulten potential is not necessarily a unique representation of the hadronic force; since a linear combination of similar potentials could be used to represent the same hadronic bound state, provided that they characterize an attractive force among the electrons capable of overcoming their Coulomb repulsion.

This work assumes that until matrix elements of a two-Gaussian-screened-Coulomb potential can be used to approximate the real-space form of the hadronic attraction. This form has the important property that it can be merged with the general case of the four-center Coulomb or exchange integral derived by Shavitt [16] using the famous Gaussian transform technique.

$$\frac{1}{r_{12}} = \sqrt{\frac{1}{\pi}} \int_0^\infty s^{-\frac{1}{2}} \exp[-sr_{12}^2]ds, \qquad (9.1.45a)$$

$$1 + \frac{p+q}{pq}s = \frac{1}{1-t^2}. \qquad (9.1.45b)$$

For future reference, note that this transform already has a pole at the lower limit where $s = 0$. This pole was removed at the last step by a change in variable, given as Eqs. (9.1.45). Shavitt was able (as a former graduate student of S.F. Boys) to show that the Gaussian transform technique reproduced the formula previously derived by Boys [6] in 1950 using electrostatic arguments. The Gaussian-lobe basis SCF programs by Shillady [8, 28] and others.

It is important to note that the formula is completely general in orientation of four Gaussian sphere lobe-orbitals as well as the distance between two electrons. As modified for description of correlation of two electrons, *such a general formula can describe angular correlation as well as distance interaction.* Thus, matrix Coulomb repulsion to model the real-space form of the hadronic attraction of two electrons.

Well-founded admiration for Shavitt's work in deriving the Coulomb interaction was rekindled as his derivation was checked. This work added the Gaussian screening as $\exp[-r^2]/r$ so that the special properties of Gaussians could be used, especially the property that polar coordinates readily separate into factorable x, y, z components. The goal is to evaluate the two-electron four-center matrix elements of the Gaussian-screened-Coulomb potential as shown below,

$$Y(r) = \frac{1 - 2\exp[-\alpha r^2]}{r}. \tag{9.1.46}$$

Intriguingly, the Gaussian exponent carried through the original derivation of the Coulomb interaction by resorting to a well known auxiliary function F_0 which has been studied by Shillady [8, 28] and others. Since both $s^{\frac{1}{2}}$ and $(s + \alpha)^{\frac{1}{2}}$ occur in the denominator of the screened-Coulomb form, two poles occur in the integral. A change of variable absorbs the term

$$1 + \frac{p + q}{pq}(s + \alpha) = \frac{1}{1 - t^2}, \tag{9.1.47}$$

while the pole due to $(s + \alpha)^{-1/2}$ shifts the other pole at $s^{-\frac{1}{2}}$ to the lower limit of the integral. A smooth spike is evident at the lower value of the integration using a 70 point Simpson's Rule Integration (two ranges are used with 20 points more closely spaced near the pole and 50 points for the remaining range.)

The above work was carried out using 64 bit double precision arithmetic which provides 14 significant figures. A simple offset (δ) of 1.0×10^{-15} has provided useful results with this simple offset to avoid numerical overflow. While this pole is a problem in need of a continuous function to integrate, numerical integration seems to handle this well to 14 significant figures, particularly since the routines used for the Coulomb integrals are known to be accurate only to 12 significant figures [28].

The area under the pole-spike is estimated as a narrow triangle upon a rectangle 1.0×10^{-15} wide with the height of the triangle set at 1.79940×10^{13} times the height of the point set 1.0×10^{-15} into the range of integration (the first Simpson point).

The present code for this screened-Coulomb integral is presently slower than the corresponding function used for the Coulomb integrals due to the 70 point

Simpson integration [28], but the integrand is nearly flat after the spike at $s = 0.0$ so that portion of the integrand can be evaluated more rapidly with fewer points. The simple offset of the lower limit by 1.0×10^{-15} is adequate for this monograph.

$$\left(aA(1), bB(1) \left| \frac{\exp(-\alpha(r_{12})^2)}{r_{12}} \right| cC(2), dD(2) \right) = \qquad (9.1.48a)$$

$$= \frac{2\pi^{5/2}}{pq\sqrt{p+q}} e^{[ab/(a+b)]\overline{AB}^2 - [cd/(c+d)]\overline{CD}^2} \times$$

$$\times \int_\rho^1 e^{-[pq/(p+q)]\overline{PQ}^2 t^2} \left(\frac{[pq/(p+q)]t^2}{[pq/(p+q)]t^2 + \alpha(t^2-1)} \right)^{1/2} dt, \qquad (9.1.48b)$$

$$\rho = \delta + \frac{\alpha\sqrt{p+q}}{pq+(p+q)\alpha}, \quad p = (a+b), \quad q = c+d, \quad \delta = 1.0 \times 10^{-15}, \quad (9.1.48c)$$

$$\text{pole} = (1.79940 \times 10^{13}) e^{-[pq/(p+q)]\overline{PQ}^2 \rho^2}. \qquad (9.1.48d)$$

The new integral was incorporated into the same routine used to evaluate the usual Hartree-Fock-Roothaan SCF scheme except F_0 was supplemented by the new auxiliary function (9.1.46). The H_2 molecule was treated using the same fixed-nuclei method with a bond distance of 1.4011 Bohrs. A simple basis set of just one Least-Energy $6G$-$1s$ orbital [18] centered on each H-nucleus was used to test the new program "Santilli-Animalu-Shillady-Lobe" (SASLOBE), which is set to handle up to 512 contracted orbitals.

It must be stated that the energies given are now parametrically dependent on the Gaussian-screening constant as $E(\alpha)$. The energy is variationally bound to be above the true energy in a narrow range around the optimum value. It is extremely important to note that the energy is lowered using the new attractive hadronic term, but the optimum value is difficult to locate and "variational collapse" occurs when r_c is extended or reduced away from a shallow minimum in the energy.

In order to minimize the number of parameters in the model (only one, the Coulomb screening constant A) two equations were imposed on the Gaussian-function. First, the function was required to be equal to zero at some radial cutoff value r_c which is assumed to be the inverse of the b-variable of Sect. 9.1.5,

$$b = \frac{1}{r_c} = A\frac{\exp[-\alpha r_c^2]}{r_c}, \quad A = \exp[+\alpha r_c^2]. \qquad (9.1.49)$$

Second, this radial cutoff value was used as sigma of the inverted Gaussian (radius at half-height),

$$A\exp\left[-\frac{\ln 2}{r_c^2} r_c^2 \right] = \frac{A}{2}, \quad \alpha = \frac{\ln 2}{r_c}, \quad A = 2. \qquad (9.1.50)$$

The upper boundary of the radius of the isoelectronium has been estimated in Sect. 9.3 to be about 0.6843×10^{-10} cm, which corresponds to 0.012931401 Bohrs. This radius does lower the Hartree-Fock-Roothaan energy noticeably for H_2, and further optimization of the pole-spike produced an SCF energy of -1.17446875 Hartrees with a cutoff radius of 0.0118447 Bohrs or 1.18447×10^{-10} cm using the minimum $1s$ basis. In conclusion, the fitted value of $b \equiv 1/r_c$ is reasonably close to the estimate value for the H_2 molecule. The minimum basis was later extended to $6G$-$1s$, $1G$-$2s$, $1G$-$2p$ for pole calibration.

Details of the exact representation of the binding energy via the above second method are presented in Appendix 9.B.

9.1.8 Summary of the Results

In order to demonstrate the advantage of the isochemical model using a Gaussian-screened-Coulomb attraction between electrons, a standard Boys-Reeves [22] calculation was carried out in Ref. [2]. This included all single- and double-excitations CISD from the ground state Hartree-Fock-Roothaan SCF orbitals for a 99×99 "codetor" [6] 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 $1G$-$2s$, $2G$-$2p$, $1G$-$3s$, $1G$-$3p$, $3G$-$3d$, Thd $1G$-$4sp$ (tetrahedral array of four Gaussian spheres), and $4G$-$4f$ orbitals scaled to hydrogenic values as previously optimized [17].

The additional basis functions provide opportunity to excite electrons to higher orbitals as is the standard technique in configuration interaction, somewhat contrary to the main hypothesis of this work, which is that there is an attractive hadronic force between electron pairs inside the r_c critical radius. The results of the above calculations are summarized in Table 9.1.

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 (i.e., -7.0×10^{-7} Hartrees), indicates the 99-configuration representation is close to the lower energy bound using this basis set while the isochemistry calculation produced the exact energy with a comparatively much smaller basis set.

Since SASLOBE has only a n^7 routine for the necessary integral transformation instead of the most efficient n^5 algorithm ($\simeq n$ is the number of basis functions), the SASLOBE C.I. runs are somewhat slow and required about 20 hours 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

Table 9.1.   Summary of results for the hydrogen molecule.

Species	H_2	H_2 [a]	H_2
Basis screening			
$1s$	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^b	*
$4sp$	0.25	12.18	*
$4f$	0.25	12.18	*
Variational energy (a.u.)	*	-7.61509174	*
SCF energy (a.u.)	-1.12822497	*	-1.13291228
CI energy (a.u.)	-1.14231305	*	*
CINO energy (a.u.)	-1.14241312	*	*
SAS energy (a.u.)	*	*	-1.174444
Exact energy (a.u.) [30]	-1.174474	*	-1.174474
Bond length (bohr)	1.4011	0.2592	1.4011
Isoelectronium radius (bohr)	*	*	0.01124995

[a] Three-body Hamiltonian (5.1).
[b] The negative $3d$ scaling indicates five equivalent three-sphere scaled to 16.20 rather than "canonical" $3d$ shapes.

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 calculations in hadronic chemistry are, conservatively, at least 1,000 times faster than a C.I. calculation, an occurrence fully similar to the corresponding case in hadronic *vs.* quantum mechanics.

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 isochemistry 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 isochemical model of the H_2 molecule to other molecules is conceptually straightforward. In particular, the notion of isoelectronium essentially restricts all possible bonds to the established ones, as it is the case for the water molecule (see next chapter).

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.

Table 9.2.   Isoelectronium results for selected molecules.

Species	H_2	H_2O	HF
SCF-energy (DH) (a.u.)	-1.132800^a	-76.051524	-100.057186
Hartree-Fock^d (a.u.)			-100.07185^d
Iso-energy (a.u.)	-1.174441^c	-76.398229^c	-100.459500^c
Horizon R_c (Å)	0.00671	0.00038	0.00030
QMC energy^{d,e} (a.u.)	-1.17447	-76.430020^e	-100.44296^d
Exact non-rel. (a.u.)	-1.174474^f		-100.4595^d
Corellation (%)	99.9^b	91.6^b	103.8
SCF-dipole (D)	0.0	1.996828	1.946698
Iso-dipole (D)	0.0	1.847437	1.841378
Exp. dipole (D)	0.0	1.85^g	1.82^g
Time^h (min:s)	0:15.49	10:08.31	6:28.48

(DH$^+$) Dunning-Huzinaga (10S/6P), [6,2,1,1,1/4,1,1]+H_2P_1+3D1.
^{a}LEAO-6G1S + optimized GLO-2S and GLO-2P.
^{b}Relative to the basis set used here, not quite HF-limit.
^{c}Iso-energy calibrated to give exact energy for HF.
^{d}Hartree-Fock and QMC energies from Luchow and Anderson [33].
^{e}QMC energies from Hammond *et al.* [30].
^{f}First 7 sig. fig. from Kolos and Wolniewicz [34].
^{g}Data from Chemical Rubber Handbook, 61st ed., p. E60.
^{h}Run times on an O2 Silicon Graphics workstation (100 MFLOPS max.).

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 (QMC) energy of Luchow and Anderson [33], which requires hours on a much larger computer, as compared to less than 10 minutes for this work. In fact, the run times for HF were about 8 CPU minutes on a 100 MFLOP Silicon Graphics O2 workstation.

The principal value of the pole (9.1.48d) 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 isoelectronium. 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 9.2.

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

9.1.9   Concluding Remarks

The fundamental notion of the new model of molecular bonds studied in this chapter [5] is the bonding at short distances of pairs of valence electrons from two different atoms into a singlet quasi-particle state we have called *isoelectronium*, which travels as an individual particle on an oo-shaped orbit around the two respective nuclei.

The isoelectronium and related methodology are then characterized by a covering of contemporary chemistry called *isochemistry*, which is the branch of the more general *hadronic chemistry* specifically constructed to represent closed-isolated systems with linear and nonlinear, local and nonlocal, and potential as well as nonpotential internal forces.

A main assumption is that linear, local, and potential interactions are sufficient for atomic structures since the atomic distances are much bigger than the size of the wavepackets of the electrons. However, in the transition to molecular structures we have the additional presence of nonlinear, nonlocal, and nonpotential effects due to the deep penetration of the wavepackets of valence electrons, which is essentially absent in atomic structures (Fig. 1.7).

The attractive short-range interactions needed to overcome the repulsive Coulomb force in the isoelectronium structure originate precisely from nonlinear, nonlocal, and nonhamiltonian effects in deep wave-overlappings; they are described by *hadronic mechanics* [3b]; and their invariant formulation is permitted by the recently achieved broadening of conventional mathematics called *isomathematics*.

Specific experimental studies are needed to confirm the existence of the isoelectronium, 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, a feature we have called the "*trigger*."

Nonrelativistic studies yield a radius of the isoelectronium of 0.69×10^{-10} cm. This "horizon" is particularly important for isochemical applications and developments because outside the horizon the electrons repel one-another while inside the horizon there is a hadronic attraction.

The same nonrelativistic studies also predict that, as a limit case, the isoelectronium is stable within a molecule, although partially stable configurations also yield acceptable results. The question of the stability vs. instability of the isoelectronium inside the hadronic horizon must therefore also be left to experimental resolutions.

The understanding is that, when the restriction to the hadronic horizon is lifted, and molecular dimensions are admitted for the inter-electron distance, the isoelectronium must be stable, otherwise violations of Pauli's exclusion

principle could occur. In this sense, the isoelectronium is a direct representation of Pauli's exclusion principle.

The foundations of the isoelectronium can be seen in a paper by Santilli [7a] of 1978 on the structure of the π^0-meson as a bound state of one electron and one positron. The latter model also illustrates the capability of hadronic mechanics vs. quantum mechanics. In fact, quantum mechanics *cannot* represent the π^0 as the indicated bound state of one electron and one positron because of numerous inconsistencies, such as: the inability to represent the rest energy of the π^0, which would require a "positive" binding energy, since the sum of the rest energies of the constituents is much smaller than the rest energy of the bound state; the impossibility to represent the charge radius of the π^0, which can only be that of the positronium for quantum mechanics; the lack of representation of the meanlife of the π^0; and other insufficiencies.

By comparison, *all* the above insufficiencies are resolved by hadronic mechanics, which permits the first quantitative, numerical representation of *all* characteristics of the π^0 as a bound state of one electron and one positron at short distances, including its spontaneous decay with the lowest mode $\pi^0 \rightarrow e^- + e^+$, which results in being the hadronic tunnel effect of the constituents [7a].

In particular, the indicated model of the π^0 contains the first identification of the attractive character of nonlinear, nonlocal, and nonhamiltonian interactions due to deep wave-overlappings in singlet coupling (and their repulsive character in triplet coupling).

The isoelectronium also sees its foundations in subsequent studies by Animalu [7b] of 1994 and Animalu and Santilli [7c] of 1995 on the construction of *hadronic superconductivity* for a quantitative representation of the structure of the Cooper pair. We have in this case an occurrence similar to the preceding one for the structure of the π^0. In fact, quantum mechanics can indeed represent superconductivity, but only via an *ensemble of Cooper pairs*, all assumed to be point-like. In particular, quantum mechanics simply cannot represent the structure of *one* Cooper pair, due to the divergent character of the Coulomb repulsion between the identical electrons of the pair.

Again Animalu-Santilli hadronic superconductivity did indeed resolve this insufficiency and permitted, for the first time, the achievement of a structure model of *one* Cooper pair in remarkable agreement with experimental data. Hadronic superconductivity also shows predictive capacities simply absent in quantum mechanics, such as *the prediction of a new electric current mostly given by the motion of electron pairs, rather than the conventional electric current composed of individual electrons* (patent pending). Such a new hadronic current implies an evident reduction of the electric resistance due to the essentially null magnetic moment of the pair, as compared to the large magnetic

moment of individual electrons, and its interactions with atomic electrons when moving within a conductor.

Note finally that the preceding hadronic model of the π^0 and of the Cooper pair are ultimately due to the capability of hadronic mechanics to eliminate divergencies at short distances, which is technically realized via the isotopies of the unit and related associative products of quantum mechanics

$$I \rightarrow \hat{I} = 1/\hat{T}, \tag{9.1.51a}$$

$$|\hat{I}| \gg 1, \quad |\hat{T}| \ll 1, \tag{9.1.51b}$$

$$A \times B \rightarrow A \times \hat{T} \times B, \tag{9.1.51c}$$

under which divergent or slowly convergent series can be evidently turned into rapidly convergent forms.

The tendency of identical valence electrons to bond into the isoelectronium is additionally confirmed by other evidence, such as ball lighting, which are composed by a very large number of electrons bonded together into a small region.

In summary, incontrovertible experimental evidence establishes that *electrons have the capability of bonding themselves at short distances contrary to their Coulomb repulsion.* Quantum mechanics simply cannot provide a scientific study of this physical reality. Hadronic mechanics resolved this impasse, by first identifying the conditions needed to achieve attraction, called "trigger," and then permitting quantitative numerical study of the bond.

The isoelectronium results in having deep connections with a variety of studies in chemistry conducted throughout the 20-th century [6, 8 – 38], and actually provides the physical-chemical foundations for these studies as well as their appropriate mathematical formulation for the invariance of the results.

In summary, *the isochemical model of molecular bonds submitted by Santilli and Shillady [5] is supported by the following conceptual, theoretical and experimental evidence:*

1) The isoelectronium introduces a new *attractive* force among the *neutral* atoms of a molecular structure which is absent in quantum chemistry and permits a quantitative understanding of the *strength* and *stability* of molecular bonds.

2) The isoelectronium permits an immediate interpretation of the reasons why the H_2 and H_2O molecules only admit *two* H-atoms.

3) The isoelectronium permits the achievement of a representation of the binding energy of the hydrogen molecule which is accurate to the *seventh digit*, thus allowing meaningful thermodynamical calculations.

4) The isoelectronium provides an explanation of the long known, yet little understood Pauli's exclusion principle, according to which electrons correlate

themselves in singlet when on the same orbital without any exchange of energy, thus via a process essentially outside the representational capabilities of quantum mechanics and chemistry.

5) The isoelectronium is consistent with the known existence of superconducting electron-pairs which bond themselves so strongly to tunnel together through a potential barrier.

6) The isoelectronium provides a quantitative model for the explanation of electron correlations. Instead of a complicated "dance of electrons" described by positive energy excitations, the isochemistry 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 isoelectronium is consistent with the "Coulomb hole" studied by Boyd and Yee [35] as found from subtracting accurate explicitly-correlated wavefunctions from self-consistent-field wavefunctions. In our studies the "Coulomb hole" is re-interpreted as a "hadronic attraction".

8) The isoelectronium is also in agreement with the "bipolaron" calculated for anion vacancies in KCl by Fois, Selloni, Parinello and Car [36] and bipolaron spectra reported by Xia and Bloomfield [37].

9) The isoelectronium permits an increase of the speed in computer calculations conservatively estimated at least 1,000-fold, and prevents the inconsistent prediction that all molecules are ferromagnetic (see Chapter 7).

Moreover, *another remarkable result of this study is that the value of the radius of the isoelectronium, 0.69×10^{-10} cm, computed via dynamical equations in Sect. 9.3 has been fully confirmed by the independent calculations conducted in Sects. 9.1.6 and 9.1.7 via the Gaussian-lobe basis set, yielding 0.00671 Å.*

We should also mention *preliminary yet direct experimental verifications of the isoelectronium offered by the ongoing experiments on photoproduction of the valence electrons in the helium indicating that electrons are emitted in pairs* [38]. The studies of this monograph warrant the systematic conduction of these experiments *specifically for the hydrogen molecule*, and the experimental finalization as to whether electrons are emitted in an isolated form or in pairs, including relative percentages of both emissions. If conducted below the threshold of disintegration of the isoelectronium, the proposed experiments can evidently provide final proof of the existence of the isoelectronium.

We should finally note that *the representation of the binding energy and other characteristics of the hydrogen molecule exact to the seventh digit first achieved in Ref. [5] constitutes the strongest experimental evidence to date on the insufficiency of quantum mechanics and the validity of the covering hadronic mechanics for the representation of nonlinear, nonlocal, and nonpotential, thus nonhamiltonian and nonunitary effects due to deep overlappings*

of the "extended wavepackets" of electrons with a "point-like charge structure."

It is evident that all the above results provide scientific credibility for the isoelectronium, the related isochemical model of molecular bonds, and the underlying hadronic chemistry, sufficient to warrant systematic theoretical and experimental studies.

As shown in Chapter 7, a significant feature of the proposed novel isochemistry is not only the capability to provide accurate representations of experimental data in shorter computer times, but also the capability to predict and quantitatively treat *new industrial applications.*

9.2   ISOCHEMICAL MODEL OF THE WATER MOLECULE

9.2.1   Introduction

Water is an extremely important compound on Planet Earth in a biological as well as geophysical sense. As a consequence, comprehensive studies on water have been conducted since the beginning of quantitative science with outstanding scientific achievements (see, e.g., Ref. [1]). Nevertheless, despite all these efforts, a number of fundamental issues on the structure of the water molecule remain still open, such as:

1) The total electrostatic force among the atomic constituents of a water molecule is null in semiclassical approximation, while the currently used forces (exchange, van der Waals and other forces [40]) are known from nuclear physics to be "weak," thus insufficient to fully explain the "strong" bond among the constituents (where the words "weak" and "strong" do not refer hereon to the corresponding interactions in particle physics). In different words, the representation of the nuclear structure required the introduction of the "strong nuclear force" because of the insufficient strength of the exchange, van der Waals and other forces. It appears that current models on the water molecule lack the equivalent of the "strong nuclear force" to achieve a full representation of molecular structures.

2) Quantum chemistry has not provided a rigorous explanation of the reason why the water molecules only has *two* hydrogen atoms. This is an evident consequence of the assumption of exchange and other nuclear-type forces which were built in nuclear physics for an *arbitrary number of constituents*, a feature which evidently persists in its entirety in molecular structures.

3) Quantum chemistry has been unable to achieve an exact representation of the binding energy of the water molecule under the rigorous implementation of its basic axioms, such as the Coulomb law. In fact, there is a historical 2% still missing despite efforts conducted throughout the 20-th century.

4) More accurate representations have been recently achieved although via the use of Gaussian screenings of the Coulomb law, which, however, are outside the class of equivalence of quantum chemistry, since they are *nonunitarily* connected to the Coulomb law.

5) Quantum chemistry cannot provide a meaningful representation of thermodynamical properties related to water. In fact, the value of 2% missing in the representation of binding energy corresponds to about 950 Kcal/mole while an ordinary thermodynamical reaction takes about 50 Kcal/mole. The use of quantum chemistry in thermodynamical calculations would, therefore, imply an error of the order of 20 times the value considered.

6) Quantum chemistry has been unable to reach an exact representation of the electric and magnetic dipole and multipole moments of the water molecule to such an extent that, sometimes, the models result in having even the *wrong sign* (see, e.g., Ref. [42a], p. 22). This insufficiency is generally assumed to be due to the incompleteness of the assumed basis, although one should not keep adding terms without deeper analysis.

7) Computer usages in quantum chemical calculations require excessively long periods of time. This occurrence, which is due to the slow convergence of conventional quantum series, has persisted to this day, despite the availability of more powerful computers.

8) Quantum chemistry has been unable to explain the "correlation energy" which is advocated for the missing percentages of the binding energies. Orbital theories work well at qualitative and semi-empirical levels, but they remain afflicted by yet unresolved problems, such as the currently used correlation among many electrons as compared to the evidence that the *correlation solely occurs for electron pairs.*

9) Quantum chemistry predicts that the water molecule is ferromagnetic, in dramatic disagreement with experimental evidence. This prediction is a consequence quantum electrodynamics, which establishes that, under an external magnetic field, the orbits of valence electrons must be polarized in such a way as to offer a magnetic polarity opposite to that of the external homogeneous field. As it is well known, the individual atoms of a water molecule preserve their individuality in the current model of chemical bonds. As a result, quantum electrodynamics predicts that all valence electrons of the individual atoms of a water molecule acquire the same magnetic polarization under a sufficiently strong external magnetic field, resulting in a total net magnetic polarity North-South.

Particularly insidious are variational methods because they give the impression of achieving exact representations within the context of quantum chemistry, while this can be easily proved *not* to be the case. To begin, representations of 100% of the experimental data occur with the introduction of a number of *empirical parameters* which lack a physical or chemical meaning.

Moreover, it is easy to prove that *variational solutions cannot be the solution of quantum chemical equations*, trivially, because the former provide 100% representations, while the latter do not. In reality, the arbitrary parameters introduced in variational and other calculations are a measure of the *deviation from the basic axioms of quantum chemistry*.

When passing from the structure of one water molecule to more general molecular structures the number of open, basic, unsolved issues increases. For instance, it is generally admitted that quantum chemistry has been unable to provide a systematic theory of the liquid state in general, let alone that of liquid water in particular [40].

Also, chemical reactions in general are *irreversible*, while the axiomatic structure of quantum chemistry is *strictly reversible* because the theory is strictly Hamiltonian and all known potential forces are reversible. This results in an irreconcilable incompatibility between the very axiomatic structure of quantum chemistry and chemical reactions in general, and those involving water in particular. In fact, an axiomatically consistent representation of irreversibility is expected to imply effects which are simply inconceivable for quantum chemistry, evidently because they are outside its structure.

When passing to water as a constituent of biological entities, the limitations of quantum chemistry reach their climax. In fact, biological structures (such as a cell) are not only irreversible (because they grow, age and die), but have such a complex structure to require multi-valued theories (also known in mathematics as hyperstructures). The expectation that quantum chemistry, with its reversible and single-valued structure, can effectively represent biological systems and their evolution is beyond the boundaries of science.

In view of the above numerous and basic limitations, in the preceding works [41] Santilli and other scientists have constructed a covering of quantum mechanics under the name of *hadronic mechanics*. By conception and construction, quantum and hadronic mechanics coincide everywhere, except inside a small sphere of radius of the order of 1 fm ($= 10^{-13}$ cm) called *hadronic horizon*, in which interior (only) the broader theory holds.

Hadronic mechanics results in being a form of "completion" of quantum mechanics much along the historical Einstein-Podolsky-Rosen argument, although achieved via the addition of contact, nonhamiltonian, nonlinear, nonlocal, and nonpotential forces due to deep overlappings of the wavepackets of particles.

On more technical grounds, hadronic mechanics is based on *new mathematics*, called *iso-, geno- and hyper-mathematics* [41c] (see Chapter 2) for the characterization of reversible, irreversible, and multivalued systems, respectively, possessing features not representable via the Hamiltonian.

These new mathematics are characterized by a progressive generalization of the trivial unit I of quantum mechanics into generalized units $\hat{I}$ of Her-

mitean single-valued, nonhermitean single-value, and nonhermitean multi-valued character, respectively, first proposed by Santilli in 1978 (see Refs. [41]),

$$I \to \hat{I} = \hat{I}^\dagger, \quad I \to \hat{I} \neq \hat{I}^\dagger, \quad I \to \{\hat{I}\} = \{\hat{I}_1, \hat{I}_2, \hat{I}_3, ...\} \neq \{\hat{I}\}^\dagger. \qquad (9.2.1)$$

The new mathematics then emerge from the reconstruction of the conventional mathematics of quantum mechanics in such a way as to admit $\hat{I}$, rather than I, as the correct left and right unit at *all* levels.

The iso-, geno-, and hyper-mathematics characterize corresponding branches of hadronic mechanics, called *iso-, geno-, and hyper-mechanics*, which have been constructed for the corresponding representation of:

1) closed-isolated, reversible, single-valued systems with Hamiltonian and nonhamiltonian internal forces;

2) open-nonconservative, irreversible, single valued systems with unrestricted interactions with an external system; and

3) open-nonconservative, irreversible, multi-valued systems of arbitrary structure.

Subsequently, Animalu and Santilli [43] constructed *hadronic superconductivity*, with corresponding iso-, geno-, and hyper-branches (Sect. 9.1.9) for the representation of the *structure* (rather than an ensemble) of the Cooper pairs, in a way remarkably in agreement with experimental data.

In 1999, Santilli and Shillady [43a] constructed *hadronic chemistry* (Chapter 3) with corresponding branches called *iso-, geno-, and hyperchemistry*. Since molecules are considered as isolated from the rest of the universe, and are reversible in time, they are studied via *isochemistry*.

Santilli and Shillady [43a] also constructed *a new isochemical model of the hydrogen molecule* (Chapter 4) based on the assumption that *pairs of valence electrons from different atoms couple themselves into a singlet quasi-particle state called isoelectronium.*

As shown in Chapter 4, the new model was proved to resolve at least the major insufficiencies of the quantum chemical model of the hydrogen molecule, such as: explain why the molecule has only two H-atoms; represent the binding energy to the seventh digit; achieve computer calculations which converge at least 1,000 times faster than those of quantum chemistry; and permit other advances.

The main scope of this chapter is that of studying the *new isochemical model of the water molecule* first submitted by Santilli and Shillady in Ref. [43b] via a suitable expansion of the results obtained for the hydrogen molecule.

The main assumption is that, when the valence electrons of the water molecule correlate-bond themselves into singlet pairs in accordance with Pauli's exclusion principle, there is the emergence of *new interactions structurally be-*

yond any hope of representation by quantum mechanics and chemistry, trivially, because they are nonhamiltonian.

In particular, the new interactions are strongly attractive, thus introducing, for the first time, a molecular bond sufficiently "strong" to represent reality. These and other features of the model, such as the sole possible correlation-bond being in pairs, will resolve all insufficiencies 1)–9) indicated earlier, as we shall see.

To provide introductory guidelines, let us recall that the main function of the isounit $\hat{I}$ (hereon assumed to be Hermitean, single-valued and positive-definite) is that of representing all interactions, characteristics and effects outside the representational capabilities of a Hamiltonian. This includes the representation of contact, nonpotential and nonhamiltonian interactions in deep overlapping of the wavepackets of valence electrons.

By recalling that, whether conventional or generalized, the unit is the fundamental invariant of any theory, the representation of the new interactions via the generalized unit assures invariance, that is, the prediction of the same numbers for the same quantities under the same conditions but at different times.

Representation of nonhamiltonian effects via quantities other than the generalized unit are encouraged, *provided that they achieve the indicated invariance*, as a necessary condition to avoid the catastrophic inconsistencies of Sect. 9.1.7.

The most fundamental mathematical, physical, and chemical notion of the new model of structure of the water molecule studied in this Chapter is, therefore, the generalization of the trivial unit $+1$ of current models into the isounit.

On pragmatic grounds, isochemistry can be easily constructed via a step-by-step application of the nonunitary transform

$$\hat{I} = 1/\hat{T} = U \times U^\dagger > 0, \tag{9.2.2}$$

to *all* aspects of quantum chemistry (Sect. 9.1.4). In particular, we shall assume that the above isounit recovers the conventional unit outside the hadronic horizon, and its average value is much bigger than 1,

$$\lim_{r \gg 1\,\text{fm}} \hat{I} = I. \tag{9.2.3a}$$

$$|\hat{I}| \gg 1. \tag{9.2.3b}$$

Assumption (9.2.3a) will assure the compatibility of a generalized discipline for the bonding of valence electrons, while preserving conventional quantum mechanics identically for the structure of the individual atoms composing the water molecule. Assumption (9.2.3b) will assure a much faster convergence of perturbative expansions, and other features.

In summary, the new isochemical model of the water molecule [43b] studied in this chapter can be constructed via the following steps:

1) Select a nonunitary transforms according to rules (9.2.2) and (9.2.3) which is representative of contact, nonlinear, nonlocal, and nonpotential effects in deep wave-overlapping, essentially similar to that used for the hydrogen molecule [43a] of the preceding Chapter;

2) Submitting to the selected nonunitary transform the totality of the notions, equations, and operations of the conventional quantum chemical model of the water molecule; and

3) Reconstructing the entire mathematics of the conventional model in such a way as to admit $\hat{I}$, rather than I, as the correct left and right unit at *all* levels, with no known exceptions. This lifting is necessary to avoid the catastrophic inconsistencies of Sect. 1.7 (e.g., to achieve invariance), thus requiring the isotopic lifting of numbers and fields, Cartesian and trigonometric functions, ordinary and partial differential equations, *etc.*

The axiomatically correct isochemical model of the water molecule is that formulated on isospaces over isofields. However, on pragmatic grounds, one can study its *projection* on ordinary spaces over ordinary numbers, *provided* that the results are interpreted with care.

For instance, in the indicated projection there is the general emergence of a *potential*, which, as such, may lead to imply that the model carries a *potential energy* and/or it can be treated via a conventional *potential well*. Such interpretations are correct if and only if the potential is well defined on isospaces over isofields. On the contrary, if said potential solely emerges in the projection, then it has a purely mathematical meaning without any associated energy.

The best illustration of the above seemingly contradictory occurrences was that for the isoelectronium of Sect. 9.3, whose structure did indeed exhibit the appearance of the *Hulten potential*, yet the quasi-particle had *no binding energy*. The reason is that binding energies are indeed well defined on isospaces over isofields via the isoschrödinger's equation and related isoeigenvalues, while the Hulten potential does not exist on isospaces, and solely occurs in the projection of the isoschrödinger's equation on ordinary Hilbert spaces.

To illustrate this important point, consider the isotopies of the conventional Schrödinger's equation via the nonunitary transform indicated above,

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

$$(9.2.4)$$

with corresponding liftings of numbers and Hilbert spaces,

$$U \times n \times U^\dagger = n \times (U \times U^\dagger) = n \times \hat{I}, \quad \hat{n} \in \hat{R}, \qquad (9.2.5a)$$

$$U \times \langle\psi| \times |\psi\rangle \times U^\dagger = \langle\hat\psi| \times \hat{T} \times |\hat\psi\rangle \times (U \times U^\dagger) = \langle\hat\psi| \times |\hat\psi\rangle \times \hat{I} \in \hat{\mathcal{C}}. \qquad (9.2.5b)$$

As one can see, binding energies $\hat{E} = E \times \hat{I}$ are fully defined on isohilbert spaces $\hat{\mathcal{H}}$ over isofields $\hat{R}$, and actually acquire the conventional value E following the simplification $\hat{E} \times \hat{T} \times |\hat\psi\rangle = (E/\hat{T}) \times \hat{T} \times |\hat\psi\rangle = E \times |\hat\psi\rangle$.

However, *the Hulten potential does not exist on isospaces over isofields*, trivially, because it does not exist in the Hamiltonian $\hat{H}$ which is fully conventional.

The Hulten potential of the isoelectronium of Sect. 9.3 emerge only when we project the real system, that on isohilbert spaces with equation $\hat{H} \times |\hat\psi\rangle = E \times |\hat\psi\rangle$, on conventional Hilbert spaces. As such, one should not expect that the Hulten potential necessarily carries an actual binding energy.

The reader should equally exercise caution for other aspects, and generally abstain from formulating opinions for hadronic chemistry essentially dependent on quantum chemical concepts and notions.

9.2.2 Main Characteristics of the Water Molecule

Water is a mixture of several different molecules in different percentages and molecular weights. In fact, we know *three* different isotopes of the hydrogen, ^1H, ^2H and ^3H, and *six* different isotopes of the oxygen ranging from ^{14}O to ^{19}O. In this monograph, we shall solely study the molecule $^1H_2-^{16}O$, and denote it $H_2O = H\text{-}O\text{-}H$ where the symbol "$-$" is referred to the molecular bond. Such a water molecule will be studied hereon under the following conditions: 1) at absolute zero degrees $^\circ K$; 2) in the absence of any rotational, vibrational, translational, or other motions; and 3) with all atoms in their ground state (see Ref. [40] for all details contained in this section).

The electrons of the individual H-atoms are assumed to be in the ground state $1s$. Of the eight electrons of the oxygen, two electrons with opposite spin orientation are in the lowest $1s$ state which is tightly bound to the nucleus; two electrons are in the next possible state $2s$; and the remaining four electrons are in the $2p$ state.

By using a three-dimensional reference frame with the $y\text{-}z$ plane containing the nuclei of the H and O-atoms with origin in the latter, the $1s$ and $2s$ electrons have a spherical distribution while the $2p$ electrons are in orbitals perpendicular to the yz plane denoted $2p_x$; the remaining two electrons have orbitals perpendicular to the xz and xy planes denoted $2p_y$ and $2p_z$, respectively.

Also, the energy of formation of the water molecule from hydrogen and oxygen is -9.511 eV; the binding energy is -10.086 eV; the sum of the ground
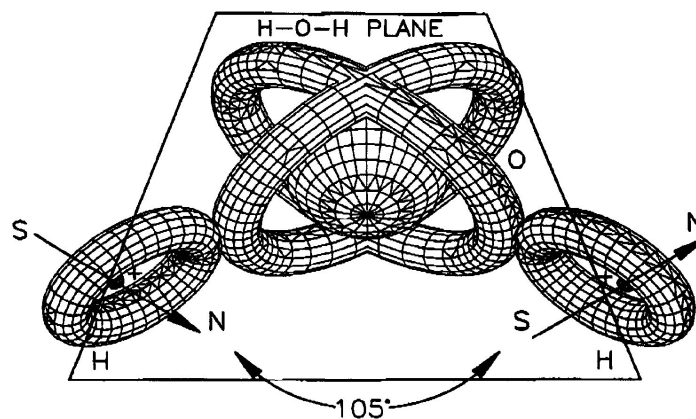
Figure 9.8. A conceptual rendering of the conventional water molecule with its typical electric polarization. Note the consequential predominance of a positive charge in the two hydrogen atoms that is responsible in part for the angle of 105° between the two HO radicals.

state energies of the three separate atoms is $-2,070.46$ eV; the total molecular energy at $0°$K is $-2,080.55$ eV as a result of kinetic energy $+2,080.6$ and potential energy $-4,411.4$; the nuclear repulsion energy is $+250.2$ eV; the total electrostatic energy is $-2,330.8$ eV; the dissociation energy of O-H is 5.11 eV and that of H alone is 4.40 eV.

Again at $0°$K and for all atoms in their ground states, the bond length of the H-O dimer is 0.95718×10^{-8} cm, while the two dimers H-O and O-H form a characteristic angle of $104.523°$. Therefore, by no means the scripture H-O-H denotes that the water has a linear structure because of the indicated characteristic angles in between the two dimers H-O and O-H.

It is evident that when the individual atoms are in their excited states, the bond length and the characteristic angle change. In fact, increases of up to $8.5°$ have been measured for the characteristic H-O-H angle for excited states. The same characteristic angle is expected to be altered by the application of sufficiently strong electric and magnetic fields, although we are unaware of accurate measurements under the indicated conditions.

The water molecule possesses an electric dipole moment of 1.83×10^{-8} e.s.u. cm and a mean quadrupole moment of -5.6×10^{-26} e.s.u. cm. It should be recalled that the very existence of a non-null value of electric dipole and quadruple moments excludes the linear structure of the water H-O-H in ordinary isolated conditions (that with a characteristic angle of $180°$).

Water is a *diamagnetic* substance with a magnetic polarization (also called susceptibility) of $(2.46, 0.77$ and $1.42) \times 10^{-6}$ e.m.u./mole for the corresponding three space-dimension xx, yy and zz, respectively.

In first approximation, the water molecule can be represented via two individual H-O dimers with wavefunction of the molecular orbitals (m.o.'s),

$$\psi_1 = \lambda \phi(\mathrm{H}', 1s) + \mu \phi(\mathrm{O}, 2p_z), \qquad (9.2.6a)$$

$$\psi_2 = \lambda \phi(\mathrm{H}'', 1s) + \mu \phi(\mathrm{O}, 2p_y), \qquad (9.2.6b)$$

where λ and μ are parameters.

However, the above simple model predicts a characteristic angle of $90°$. As a consequence, the model is generally modified with a mixture of electrons from the $2p$ and $2s$ states also called *hybridization*. The occurrence confirms that any model of the water with charge distributions of the valence electrons in the H-O-H plane is insufficient to represent the experimental data. In turn, this mixing creates the known two *lobes* on the side of the oxygen atom, away from the hydrogen atoms, above and below the molecular plane. This results in models of the type

$$\psi_1 = \lambda[\cos \varepsilon \psi(\mathrm{O}, 2s) + \sin \varepsilon \phi((\mathrm{O}, 2p)] + \mu \phi(\mathrm{H}', 1s), \qquad (9.2.7a)$$

$$\psi_2 = \lambda[\cos \varepsilon \psi(\mathrm{O}, 2s) + \sin \varepsilon \phi((\mathrm{O}, 2p)] + \mu \phi(\mathrm{H}'', 1s), \qquad (9.2.7b)$$

where ε is the hybridization parameter with generic value of the order of $\cos \varepsilon = 0.093$ confirming that the valence electrons are mainly from $2p$ states.

It should be indicated that the exact configuration, location and function of the two lone-pair electron lobes are unsettled at this writing, since they are evidently dependent on the selected theoretical model. Also, the individual electric and/or magnetic dipoles of the lobes cannot be measured (only their total values is measurable), thus implying lack of direct experimental evidence on the individual lobes.

We should also recall that the individual H-O and O-H bonds are not independent from each other, as confirmed by the different values of the dissociation energies.

Water is both an acid and a base due to dissociation of H_2O into H^+ and $O\text{-}H^-$ to the extent that the product of the concentrations $[H^+][O\text{-}H^-]$ sets up an equilibrium whose constant value is 1.0×10^{-14}, which is the well known pH scale of the equations

$$\mathrm{pH} = -\log_{10}[\mathrm{H}^+], \quad \mathrm{pOH} = 14 - \mathrm{pH}. \qquad (9.2.8)$$

In neutral water the ion concentrations are $[\mathrm{H}^+] = [\mathrm{O\text{-}H}^-] = 1.004 \times 10^{-7}$ mole/liter.

Water is quite polar with a dipole moment of 1.84 to 1.834 Debye and a bulk dielectric constant of 80 at 20 °C. This implies that pure water is not a good conductor, with a direct current conductivity of only 5.7×10^{-8} ohm^{-1}·cm^{-1}.

However, it is well known that small amounts of strong acids such as HCl or H_2SO_4 can make water highly conducting due to the ease with which H^+ can attach to H_2O to form H_3O^+ which then offers a *domino effect* for one H^+ to successively "bump" an H^+ off the other side of H_3O^+ and so produce a very effective conduction mechanism [44]. In fact it is well known that in aqueous solutions the transport numbers for the anions and cations are not equal, because up to 70% of the current is carried by H^+. Although OH^- typically carries much less current than H^+ in aqueous conduction of electricity (due to its larger size and lack of the domino-effect cited earlier for H^+), once a current flow is initiated additional ions are created due to collisions in solution.

An important aspect is the known existence of an equilibrium between H-O-O-H and HO^- around pH 11.63 [45] with a voltage dependence of 1.363 ± 0.0293 pH as given by M. Pourbaix for aqueous equilibria involving H^+, $O-H^-$, H^-, H-O-O-H and $H-O^-$. Thus, there is no doubt of the existence of small amounts of H-O-O-H in water at high pH.

In a high current process the flow of H^+ will be much greater than that of OH^- so that as H_2O is electrolyzed to $2H_2$ and $1O_2$, local concentrations/fluctuations will slightly favor higher pH (local depletion of H^+) and hence favor the existence of H-O-O-H.

We should finally mention the inability of quantum chemistry to achieve a scientific-quantitative representation (or at least an understanding) of the *different types of water when exposed to magnetic fields*, as established by the evidence, e.g., that plants grow faster when irrigated with water exposed to one type of magnetic field, while they die rapidly when exposed to a different type of magnetic field. In fact, quantum chemistry admits only *one* type of water, H_2O.

It is easy to see that this additional insufficiency of quantum chemistry is a direct consequence of the current use of exchange, van der Waals and other forces of nuclear origin under which the individual H and O atoms in the H_2O molecule preserve their individuality, thus resulting in one single configuration.

On the contrary, isochemistry introduces a real, strong bond for the valence electrons via the notion of isoelectronium. In this latter case different types of water, that is, water molecules with different physical characteristics, are indeed readily possible, as we shall see.

9.2.3 Exactly Solvable Model of the Water Molecule with Stable Isoelectronium

In the preceding Chapter 3 [43a], we have introduced the main hypothesis of the *isochemical molecular model*, according to which two electrons from two

different atoms bond themselves into a singlet quasi-stable and quasi-particle state called *isoelectronium*, which describes an *oo*-shaped orbit around the nuclei, as it is the case for planets in certain binary stars (Fig. 9.3). The main characteristics of the isoelectronium in first nonrelativistic approximation are calculated in Sect. 9.3 and resulted in being:

$$\text{charge} - 2e, \quad \text{spin } 0, \quad \text{magnetic dipole moment } 0,$$
$$\text{mass } 1.022 \text{ MeV}, \quad \text{radius} = r_c = b^{-1} \approx$$
$$\approx (\hbar^2/m \times V)^{1/2} = (\hbar/m \times \omega)^{1/2} = 6.8432329 \times 10^{-11} \text{cm} =$$
$$= 0.015424288 \text{ bohrs} = 0.006843 \text{ Å}.$$

$$(9.2.9)$$

In the above nonrelativistic approximation, the meanlife resulted in being infinite (full stability, with the understanding that relativistic corrections are expected to render such a meanlife finite (partial stability). All conventional forces of current use in chemistry (exchange, van der Waals and other forces) then hold when the valence electrons are at mutual distances bigger than the hadronic horizon.

In this Chapter, we study the *isochemical model of the water molecule* H_2O=H-O-H first introduced by Santilli and Shillady [43b], under the assumption that the molecule is considered at °C and in the absence of any rotational, oscillation or other motion. The main hypothesis is that each electron from the two H-atoms couples in singlet with one $2p$ electron from the O-atom, resulting in *two isoelectronia*, one per each H-O dimer as in Fig. 9.8.

In this Section we shall study a hadronic/isoschrödinger equation for the water molecule under the above assumptions, which equation evidently approximate, yet *exactly solvable* for the first time to our knowledge. We shall then show that the model is extendable to all other dimers comprising one hydrogen atom, such as H-C.

For this purpose, we approximate the H-O-H molecule as being composed of two intersecting identical dimers H-O with evidently only one oxygen atom. This requires a first correction due to the lack of independence of said dimers reviewed in Sect. 9.2. Moreover, in each H-O dimer we shall assume that the oxygen appears to the isoelectronium as having only one net positive charge $+e$ located in the nucleus. This evidently requires a second correction which essentially represents the screening of the various electrons of the oxygen. Additional corrections are also in order along conventional lines [40].

A study of these corrections has indicated that they can all be represented via one single Gaussian screening of the Coulomb law of the type [43b]

$$\frac{+e}{r} \rightarrow \frac{+e(1 \pm e^{-\alpha r^2})}{r}, \quad (9.2.10)$$
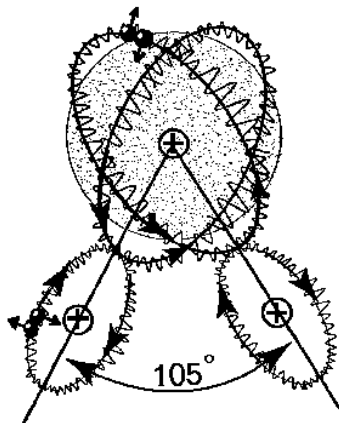
Figure 9.9. A schematic view of the proposed *isochemical model of the water molecule* here depicted at absolute zero degrees temperature and in the absence of any motion for the case of fully stable isoelectronium. It should be stressed that *at ordinary temperature rotational motions recover the conventional space distribution*, thus recovering the conventional "Mickey Mouse" configuration of the water. Also, the model is presented in terms of the *orbits* of the valence electrons (rather than in terms of *density distributions*). The fundamental assumption is that the two valence electrons, one per each pair of atoms, correlate themselves into two bonded singlet states at short distance we have called *isoelectronia*, one per each dimer H-O, which states are assumed to be mostly stable (see the text for the mostly unstable case). The water molecule is then reducible to two intersecting H-O dimers with a common O-atom. The only orbits yielding a stable water molecule are those in which each isoelectronium describes a *oo*-shaped orbit around the respective two nuclei of the H- and O-atoms. The isoelectronia are then responsible for the *attractive force* between the atoms. The *binding energy* is instead characterized by the *oo*-shaped orbits of the isoelectronia around the respective two nuclei, conceptually represented in this figure via a standing wave for a particle of spin 0 and charge $-2e$. Note that, in the absence of molecular motions, the orbits of the two isoelectronia are perpendicular to the H-O-H plane, thus confirming a characteristic of the water molecule reviewed in Sect. 9.2. Conventional exchange, van der Waals and other forces remain admitted by the model when the isoelectronia are mostly unstable. The model permits a representation of: 1) the "strong" value of the molecular bond; 2) the reason why the H_2O molecule has only two hydrogen atoms and one oxygen atom; 3) a representation of the binding energy, electric and magnetic moments accurate to several digits; and other advances studied in the text. The above model of the H-O dimer is then extendable to other H-based dimers, such as H-C.

where α is a positive parameters to be determined from experimental data, the sign "$-$" applies for the screened O-nucleus as seen from an *electron* (because of the *repulsion* caused by the electron clouds of the oxygen), while the sign "$+$" applies for the screened O-nucleus as seen from the H-*nucleus* (because of the *attraction* this time caused by said electron clouds).

The resulting model is structurally equivalent to the isochemical model of the hydrogen molecule of Chapter 3 [43a], except for the modifications indicated about, and can be outlined as follows.

By denoting with the sub-indices 1 and a the hydrogen, 2 and b the oxygen, prior to the indicated screening and in the absence of all hadronic effects, the conventional Schrödinger equation of the H-O dimer with the oxygen assumed to have only one elementary charge $+e$ in the nucleus is given by

$$\left(\frac{1}{2\mu_1}p_1 \times p_1 + \frac{1}{2\mu_2}p_2 \times p_2-\right.$$

$$\left.-\frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{r_R} + \frac{e^2}{r_{12}}\right) \times |\psi\rangle = E \times |\psi\rangle, \quad (9.2.11)$$

As it was the case for the H_2-molecule, our task is that of subjecting the above model to a transform, which is nonunitary only at the short mutual distances $r_c = b^{-1} = r_{12}$ of the two valence electrons (here assumed to be hadronic horizon), and becomes unitary at bigger distances $\hat{I}_{r \leq 10^{-10}\text{cm}} \neq I$, $I_{r \gg 10^{-10}\text{cm}} = I$.

We assume that the state and related Hilbert space of systems (9.2.11) can be factorized in the familiar form (in which each term is duly symmetrized or antisymmetrized)

$$|\psi\rangle = |\psi_{12}\rangle \times |\psi_{1a}\rangle \times |\psi_{1b}\rangle \times |\psi_{2a}\rangle \times |\psi_{2b}\rangle \times |\psi_R\rangle, \quad (9.2.12a)$$

$$\mathcal{H}_{\text{Tot}} = \mathcal{H}_{12} \times \mathcal{H}_{1a} \times \mathcal{H}_{1b} \times \mathcal{H}_{2a} \times \mathcal{H}_{2b} \times \mathcal{H}_R. \quad (9.2.12b)$$

The nonunitary transform we are looking for shall act only on the r_{12} variable characterizing the isoelectronium while leaving all other variables unchanged. The simplest possible solution is given by

$$U(r_{12}) \times U^{\dagger}(r_{12}) = \hat{I} = e^{[\psi(r_{12})/\hat{\psi}(r_{12})] \int d\mathbf{r}_{12}\hat{\psi}^{\dagger}(r_{12})_{1\downarrow} \times \hat{\psi}(r_{12})_{2\uparrow}}, \quad (9.2.13)$$

where the ψ's represents conventional wavefunction and the $\hat{\psi}$'s represent isowavefunctions, for which we have, again the fundamental condition of fast convergence

$$|\hat{T}| = |(U \times U^{\dagger})^{-1}| \ll 1. \quad (9.2.14)$$

We now construct the isochemical model by transforming short-range terms (isochemistry) and adding un-transformed long range ones (chemistry), thus resulting in the radial equation

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \times \hat{T} \times \nabla_1 \times \hat{T} \times \nabla_1 - \frac{\hbar^2}{2 \times \mu_2} \times \hat{T} \times \nabla_2 \times \hat{T} \times \nabla_2+\right.$$

$$\left.+\frac{e^2}{r_{12}} \times \hat{T} - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R}\right) \times |\hat{\psi}\rangle = E|\hat{\psi}\rangle. \quad (9.2.15)$$

By recalling that the Hulten potential behaves at small distances like the Coulomb one, Eq. (9.2.15) becomes

$$\left(-\frac{\hbar^2}{2 \times \mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2 \times \mu_2} \times \nabla_2^2 - V \times \frac{e^{-r_{12} \times b}}{1 - e^{-r_{12} \times b}} - \right.$$

$$\left. -\frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \qquad (9.2.16)$$

The above model can be subjected to an important simplification. In first approximation under the assumption herein considered, the H-O dimer (9.2.16) can be reduced to a *restricted three body problem* similar to that possible for the conventional H_2^+ *ion* [41], but *not* for the conventional H_2 molecule, according to the equation

$$\left(-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_1^2 - V \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \right.$$

$$\left. -\frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{e^2}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle. \qquad (9.2.17)$$

The indicated corrections due to the screening of the various electrons in the oxygen and other corrections are needed in the "sensing" of the O-nucleus by the isoelectronium as well as by the H-nucleus, yielding in this way our final model

$$\left(-\frac{\hbar^2}{2\mu_1} \times \nabla_1^2 - \frac{\hbar^2}{2\mu_2} \times \nabla_2^2 - V \times \frac{e^{-r_{12}b}}{1 - e^{-r_{12}b}} - \right.$$

$$\left. -\frac{2e^2}{r_a} - \frac{2e^2(1 - e^{-\alpha r_b})}{r_b} + \frac{e^2(1 + e^{-\alpha R})}{R} \right) \times |\hat{\psi}\rangle = E \times |\hat{\psi}\rangle, \qquad (9.2.18)$$

where: α is a positive parameter; E is half of the binding energy of the water molecule; and, as it was the case for model (9.1.35), the mass of the isoelectronium, the internuclear distance, and the size of the isoelectronium can be fitted from the value of the binding energy and other data.

Under the latter approximation, the model admits an exact analytic solution, for the first time to our knowledge, which solution however exists only for the case of the *fully stable isoelectronium*. In fact, for the unstable isoelectronium, the model becomes a *four-body structure*, which as such admits no exact solution.

Besides being exactly solvable, model (9.2.18) exhibits a *new explicitly attractive "strong" force among the neutral atoms of the H-O dimer*, which is absent in conventional quantum chemistry; the equation also explains the reasons why the water molecule admits only *two* H-atoms.

As we shall see in the remaining sections, the model permits an essentially exact representation of the binding energy, electric and magnetic moments; the model yields much faster convergence of series with much reduced computer times, and resolves other insufficiencies of conventional models.

Finally, the model is evidently extendable with simple adjustment to an exact solution of other dimers involving the hydrogen, such as H-C. In addition, it permits the identification of electric and magnetic polarizations, which are not predictable with quantum chemistry (Chapter 8).

9.2.4 Gaussian Approximation of the Isochemical Model of the Water Molecule with Unstable Isoelectronium

The solution of the exactly solvable model (9.2.18) are not available at this writing, and its study is here encouraged. In this section, we review the studies of Ref. [43b] on a Gaussian *approximation* of the isochemical model of the water molecules, with the Hulten potential approximated to a certain Gaussian form.

It should be indicated from the onset that such an approximation implies an evident weakening of the Hulten attraction among the two isoelectrons of the isoelectronium, which, in turn, implies the instability of the isoelectronium itself, thus reaching a model which is somewhat intermediate between the full isochemical model and the conventional quantum chemical model of the water.

Despite this approximate character, the results of this section are significant because they show the capability of isochemistry to achieve an essentially exact representation of the binding energy, electric and magnetic moments and other characteristics of the water molecule.

The results of this study can be outlined as follows. Since HOOH will be slightly more allowed under the assumed conditions, collisions of HO^- with neutral H_2O and the internal repulsion within the anion could favor the release of a quasiparticle with charge $-2e$ to form OH^+. Collisions of OH^+ with OH^- will then further enhance the concentration of HOOH, and transport of $-2e$ will contribute to the current.

The question here is whether under extreme cases of forced conduction a singlet-pair of electrons (isoelectronium), can be "triggered" (Fig. 9.6) within a water molecule to form and release a $-2e$ charged isoelectronium particle which will provide an additional conduction mechanism analogous to Cooper-pairs of electrons in superconducting solids.

Since the energy depth of the V_0 parameter in the isoelectronium Hulten potential of the original 1978 derivation by Santilli [42] is not known, nor how closely the Gaussian representation fits the Hulten form, we can only match the radius of the two potentials and calculate the energy differences caused by the "sticky-electrons" model in which a transient form of isoelectronium

can occur (the Gaussian potential well may not be deep enough to ensure a permanent bound state for the isoelectronium).

The "sticky-electron" model is a parametric model which includes the magnetic dipole attraction between singlet-paired electrons, as well as the nonlocal merging of the wave-packets of each electron at short distance. The radius of the Gaussian screening is then determined empirically by fitting the calculated energy as nearly as possible to the most accurate energy values available.

As used here, it should be emphasized that the off-axis positions of the Gaussian-lobe basis sets [46-48] ensure that angular correlation is included as well as radial dependence, and can include the magnetic dipole attraction of opposite electron spins as well as merger of wavepackets.

One radial screening parameter used with off-axis basis sets parametrically covers all forms of short range attraction which may include angular dependence. Thus the present model can give us an approximate energy difference required to release an electron-pair from OH^-.

$$OH^- \rightarrow OH^+ + (2e)^{-2}. \tag{9.2.19}$$

It will be seen below that the energy difference between OH^- and OH^+ as calculated, allowing a transient form of isoelectronium, is well within the voltage accessible using capacitive discharge through water. Such a mechanism which would allow $-2e$ particles to flow through water would not be superconductivity as conventionally understood, since the freely moving molecules and ions are not constrained to lattice positions as in solids, so that resistive I^2R heating will still occur.

This is mainly due to the fact that conduction in liquids occurs by mobility of both anions and cations along with size differences, polarizability differences and special mechanisms such as the hydrogen-bonding "domino effect" for H^+ transport. In solid-state conduction, only the electrons move by ignoring in-place phonon oscillations because the atoms do not travel from one electrode to the other.

Despite the indicated lack of superconducting character, it should be indicated that yet, the essentially null magnetic moment of the $-2e$ particle would imply indeed a reduction of the resistivity.

The apparent motion of positively charges "holes" is also due to motion of electrons while the atoms merely oscillate about mean lattice positions. In solutions there is a two-way traffic with positive and negative ions travelling in opposite directions and with differing velocities, thus leading to resistive heat even up to the vaporization of the water as well as a high probability of ion collisions.
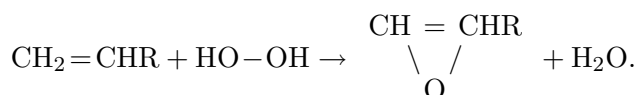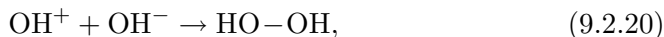
It should be noted that in recent work Ashoori *et. al.* [49] have measured migration of paired-electrons to quantum dot wells in GaAs, while Boyd and Yee [50] have observed "bipolaron" electron pairs in alkali halide lattice

vacancies. Calculations leading to unexpected bipolarons in crystal lattice vacancies have also been observed by using the method of Car and Parinello [51]. These findings in solids lend support to the concept of an electron pair as an individual particle, called by the authors isoelectronium.

The calculations given here do not prove the presence of isoelectronium particles in high current aqueous electrical conduction; they only indicate the energy threshold necessary to form the isoelectronium within the conducting solution by double-ionization of OH^-.

It is not easy to envision an experiment that would be able to analyze components of a given current, due to multiple ion species in terms of the amount of current due to $-2e$ particles, and none is proposed here. However, there may be a chemical test for such a mechanism. Once OH^- is doubly-ionized to form OH^+, collisions with $-2e$ particles would regenerate OH^- ions just as collisions of H^+ with OH^- will reform H_2O, and no new species will be evident.

However, if OH^- collides with OH^+ a new chemical species HO-OH will be formed that may last long enough in the liquid to behave as a strong oxidizing agent. Thus, organic compounds with double bonds (alkenes), which have negligible conductance, could be added to water undergoing a high current flow to cause hydroxylation of such compounds [52], (i.e., conversion of alkenes to epoxide, which are then readily hydrolyzed in the presence of H^+ to diols). Enhanced concentrations of epoxides and diols would be indirect evidence of double ionization of OH^-, according to the expressions

$$OH^+ + OH^- \rightarrow HO-OH, \tag{9.2.20}$$

$$CH_2{=}CHR + HO-OH \rightarrow \overset{\displaystyle CH = CHR}{\underset{\displaystyle O}{\diagdown \diagup}} + H_2O.$$

If the isoelectronium can be detected indirectly by a chemical method, this would in itself be an important inference on the existence of a two-electrons, spin-zero particle. More importantly, "isochemical reactions" could be driven by high conduction "liquid plasma" environments where the isoelectronium is at an enhanced concentration.

Another case of interest is that of aqueous mixtures of insoluble organic compounds forming a separate oil layer over water in an intense magnetic field of several Tesla. At normal thermal energy of room temperature $kT \cong RT$ per mole the main energy form would be random Brownian motion.

However, in the presence of a strong magnetic field HO^+ and HO^- would be constrained to favor circular motions in the magnetic field by the "cyclotron effect," but there is no obvious source of HO^+.

Since two ions of opposite sign charges would be favored to collide by both electrical attraction and by opposite path curvature in a magnetic field, there

is an enhancement that when created as a normal result of H^+, OH^-, H^-, H_2O_2, HO_2^-, H_2O equilibrium system studied by Pourbaix [45], any natural concentration of HOOH would be augmented by collision of H^+ with HOO^-.

In addition there is some slight chance that H^+ would collide with OH^- with sufficient excess energy to produce OH^+ and H^-. Thus the presence of an intense magnetic field would cause positive and negative ions to collide more easily while travelling in opposite rotational arcs in such a way as to enhance the concentration of HOOH,

$$H^+ + HOO^- \rightarrow HOOH, \qquad (9.2.21a)$$

$$H^+ + OH^- \rightarrow H^- + OH^+, \qquad (9.2.21b)$$

$$OH^+ + OH^- \rightarrow HOOH, \qquad (9.2.21c)$$
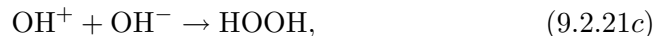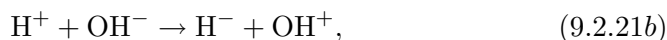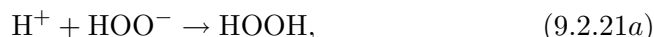
which could then epoxidate alkenes and upon hydrolysis would lead to diols.

A direct measure of this effect would be to determine the enhanced solubility of alkenes in water. The alkenes are only slightly soluble in water ("oil and water do not mix") but alkenes converted to diols will have a measurably greater solubility in water due to the attached OH-groups. Again. If such enhanced solubility of alkenes in water can be caused by intense magnetic fields, this would be indirect evidence of the existence of an electron-pair particle with charge $-2e$.

In the description of the calculations below the key to the above possibility is that it is easy to calculate the energy of OH^- when one subtracts a small amount from the two-electron repulsion terms in the usual HFR-SCF treatment, due to the attraction of singlet-paired electrons at close range within 1.0 picometer.

In the recent *Handbook of Computational Quantum Chemistry* by Cook, Ref. [53], p. 438, it is noted that solutions to the HFR-SCF scheme may not always exist for anions. However, in the method used here convergence of the HFR-SCF method was normal for an SCF process, because the so called "self-energy" error of the Hartree-Fock method [54] (in which each electron repels all electrons including itself) is largely cancelled by the new attractive terms used here. In effect, this description of OH^- is possible because of the easy convergence of the "correlated-SCF process."

9.2.5 The Method

The model adopted in Ref. [43b] is to use the usual Hartree-Fock-Roothan self-consistent-field equations [55] (which also has some formal flaws such as the self-interaction terms [54]) and lift in a nonunitary way the form of the Coulomb interaction of the electrons.

Note that reducing the values of the Coulomb integrals will lower the energy by reducing the electron-electron repulsion while reducing the exchange terms

will raise the energy, but the factor 1/2 reduces the effect of the exchange terms. Thus a reduction of the value of the integrals will lower the energy.

Note that Goodgame and Goddard [54] have already recommended reducing the atomic self-energy by subtracting 1.39 eV from Hartree-Fock exchange integrals in the cases of Cr_2 and Mo_2.

$$FC = ESC; \quad F_{i,j} = H_{i,j} + \sum_{k,l} P_{k,l}[(i,j|k,l) - 1/2(i,k|j,l)], \qquad (9.2.22a)$$

$$(i,j|k,l) = \int\int \chi_i(l)\chi_j(l)\frac{1}{r_{12}}\chi_k(2)\chi_l(2)d\tau_1 d\tau_2, \qquad (9.2.22b)$$

$$P_{i,j} = 2\sum_n c_{n,i}c_{n,j} \quad \text{(sum } n \text{ only over occupied orbitals)}. \qquad (9.2.22c)$$

The 1995 paper on electron-electron pairs by Animalu and Santilli [42b] invokes the non-local hadronic attractive force evident in the π^0-meson by Santilli [42a] applied to a pair of singlet-paired electrons which form a boson quasi-particle. However, the "collapsed positronium" rapidly decays since the particle-antiparticle annihilation takes place in less than a picosecond.

In the electron-electron case it is believed that there may be a stable quasi-particle singlet bond we have called the isoelectronium. After using a non-local isotopic nonlinear transformation, the hadronic attraction was projected into real-space, and modeled with a Hulten potential.

Considerable effort was made to evaluate the matrix elements for the Hulten potential without success. Examination of the original 1978 paper on positronium collapse by Santilli [6a] revealed that the Hulten potential is not necessarily a unique representation of the hadronic force. In fact, a linear combination of similar potentials could be used to represent the Hulten potential if matrix elements of such other potentials could be evaluated.

The depth of the screened Gaussian approximation is determined by requiring that the width at half height of the Gaussian is equal to the b value of the Hulten horizon (the radius at which the Coulomb repulsion is annulled by other attractive forces). Thus, the screened Gaussian potential probably has a depth which is too shallow although the V_0 depth parameter for the Hulten potential is not known at present.

This work assumes that until matrix elements of a two-electron interaction for singlet-pairs can be found for the Hulten potential, a Gaussian-screened-Coulomb potential can be used to describe the real-space form of the hadronic attraction and as a parameter fitted to experimental energies the screening exponent probably includes other effects such as the magnetic dipole interaction of two electrons with opposite spin-magnetic-moments. This form has the important property that it can be merged with the general case of the

four-center Coulomb or exchange integral derived by Shavitt [56] using the famous Gaussian transform technique.

The Gaussian transform two-electron integral for four Gaussian spheres has been used in a number of Gaussian-lobe basis SCF programs written by Shillady [57, 58] and others. It is important to note that the formula is completely general in orientation of four Gaussian sphere lobe-orbitals as well as the distance between two electrons.

As modified for a description of the correlation of two electrons, such a general formula can describe angular correlation as well as distance interaction. Thus matrix elements of a screened-Coulomb interaction were subtracted from the usual $1/r$ Coulomb repulsion to model the real-space form of the hadronic attraction of two electrons. The work outlined in this section, first presented in Ref. [43b], added the Gaussian screening as $\exp[-\alpha r^2]/r$ so that the special properties of Gaussians could be used, especially the properties that the product of two Gaussians form another Gaussian (times a re-centering factor), and that polar coordinates readily separate into factorable x, y, z components.

The goal was to evaluate the two-electron four-center matrix elements of the Gaussian-screened Coulomb potential in the expression

$$Y(r) = \frac{1 - 2\exp[-\alpha r^2]}{r}. \tag{9.2.23}$$

Amazingly, the Gaussian-Gaussian exponent and carried through the original derivation until the last step when integration over "s" is required. α is usually a very high number, this work used 0.13441885×10^7. At this point the usual Coulomb interaction resorts to a well known auxiliary function F_0 which has been studied by Shillady [57] and others.

Since both $s^{1/2}$ and $(s + \alpha)^{1/2}$ occur in the denominator of the screened-Coulomb form, two poles occur in the integral. A change of variable absorbs the pole due to $(s + \alpha)^{-1/2}$ and shifts the other pole due to $s^{-1/2}$ to the lower limit of the integral. A smooth spike is evident at the lower limit of the numerical integration using a 70 point Simpson's Rule integration (two ranges are used with 20 points more closely spaced near the pole and 50 points for the remaining range).

This work was carried out using 64 bit double precision arithmetic, which provides 14 significant figures. A simple offset δ of 1.0×10^{-15} has provided useful results with this simple offset to avoid numerical overflow.

While this pole is formally a problem in needing a continuous function to integrate, numerical integration seems to handle these Coulomb integrals are known to be accurate only to 12 significant figures. The area under the pole-spike is estimated as a narrow triangle upon a rectangle 1.0×10^{-15} wide with the height of the triangle set at 3.43207×10^8 times the height of the point set 1.0×10^{-15} into the range of integration (the first Simpson point).

The present code for this screened-Coulomb integral is presently slower that the corresponding F_0 function [56] used for the Coulomb integrals due to the 70 point Simpson integration, but the integrand is nearly flat after the spike at $s = 0.0$ so that portion of the integrand can be evaluated more rapidly with fewer points. For results presented here, the simple offset of the lower limit by 1.0×10^{-15} is adequate for this monograph. Further details on the auxiliary integral can be found in a previous paper on the H_2 molecule [59].

Work in progress indicates it may be possible to express the new auxiliary integral to an analytical expression involving the $erf(x)$ function (see Chapter 6), but until further checks are completed this work used the Simpson integration. Note the integral is a result of a simplification of a twelve-fold integration over the volume elements of two electrons, and has been reduced to a one-dimensional integration multiplied by appropriate factors.

9.2.6   The Main Results

The geometry given for H_2O by Dunning [60] was used to carry out the usual HFR-SCF calculation after an additional $3d$ orbital mimic [58] was optimized in Ref. [43b] for the O atom and ($2s$,$2p$) orbitals were added for the H atoms. The exponent for the O$3d$ orbitals was optimized to three significant figures and the (O$3d$,H$2s$,H$2p$) exponents were (2.498, 0.500, 1.000). These polarization orbitals were added to the Dunning-Huzinaga ($10s6p$) [59] basis with the H$1s$ orbitals scaled to 1.2 which produced a lower energy than that of a 6-31G^{**} basis using the GAMESS program. The bond length of OH$^+$ was Angströms.

The same bond length was used for OH$^-$ since the anion calculation using the usual HFR-SCF process was not feasible, and, in any case, the bond length is only slightly longer than that in water. The horizon cutoff value of 0.00038 Angströms optimized for H_2O was also used for OH$^+$ and OH$^-$.

The spike in the numerical integral routine was optimized by fitting the R_c cut-off value so as to obtain as near as possible the non-relativistic energy of the HF molecule as determined from Quantum Monte Carlo calculations [60]. The dipole moments for the ions are not very useful since ion dipoles are origin dependent, but they were calculated using the center-of-mass as the origin.

As we see in Table 9.3, the difference in energy between OH$^-$ and OH$^+$ is 0.497621 Hartrees (13.54 eV) according to the Correlated-SCF calculations. It is clear from the standard SCF energy value for H_2O that this basis is very good, but not quite at the Hartree-Fock limit of energy. In addition, the fitting of the numerical integration spike so as to most nearly reproduce the total energy of HF is not exact.

These two artifacts introduce an energy uncertainty of about 0.0115 Hartrees, but this is less uncertainty than that of the Quantum Monte Carlo (QMC) energy of Luchow and Anderson [61]. Note that the Iso-Dipoles for H_2O and HF

Table 9.3. Isoelectronium results for selected molecules [43b].

	OH$^+$	OH$^-$	H$_2$O	HF
SCF-Energy^a	-74.860377	-75.396624	-76.058000	-100.060379
Hartree-Fock^b				-100.07185^b
Iso-Energy^c	-75.056678	-75.554299	-76.388340	-100.448029
Horizon R_c (Å)	0.00038	0.00038	0.00038	0.00030
QMC Energy^{b,d}	-76.430020^d			-100.44296^b
Exact non-rel.				-100.4595
Iso-Dipole (D)	5.552581	8.638473	1.847437	1.8413778
Exper. Dipole			1.84	1.82

^{a} Dunning-Huzinaga (10s/6p), (6,2,1,1,1/4,1,1)+H2s1+H2p1+3d1.
^{b} Iso-Energy calibrated to give maximum correlation for HF.
^{c} Hartree-Fock and QMC energies from Luchow and Anderson [61].
^{d} QMC energies from Hammond, Lester and Reynolds [60].

are very close to the experimental values which indicates that the calculated wavefunctions are of high quality.

Since the ionization energy of a neutral H atom is 13.60 eV and the energy difference of 13.54 eV would convert OH$^-$ to OH$^+$, a threshold of about 13.7 eV should maintain H$^+$ in solution as well as transfer $(2e)^{-2}$ through an aqueous solution to or from the OH$^-$/OH$^+$ system.

These calculations indicate that there may be an enhancement of current flow with a potential above 13.7 volts across an aqueous cell and that the enhanced concentration of HOOH may be measurable above a potential of 13.7 volts. It is worth repeating that this estimate is possible largely due to the easy convergence of the Correlated-SCF process for a negative ion species; a process which is formally not defined under the usual Hartree-Fock-Roothan process [53], and most quantum chemists are familiar with the difficulty in treating negative ions using the standard Hartree-Fock-Roothaan method.

Admitting that the Correlated-SCF equations are a parametrized approximation to the Santilli derivation of the Hulten potential [42a] for a bound electron-pair, the method has the advantage of easy incorporation into an existing Hartree-Fock-Roothaan Gaussian basis program merely by subtracting a small "correlation integral" from the usual two-electron integrals.

With some thought, one should realize that fitting the single parameter (Gaussian screening exponent, α) to experimental energies, and/or Quantum Monte Carlo results will incorporate another attraction in the form of a magnetic dipole interaction between the spin moments of paired electrons. Including the magnetic dipole interaction and substituting a Gaussian form for the

Hulten exponential potential leaves only a simulation of the bound electron-pair Isoelectronium. Thus, these results are for a model in which the usual HFR-SCF method is corrected for at least two attractive interactions of electrons causing them to approach each other as if they were "sticky"; hence the term "sticky-electron-pair model."

9.2.7   Conclusions

In Chapter 3, we have presented a covering of quantum chemistry under the name of *hadronic chemistry*. In Chapter 4, we have applied the new discipline to the construction of a new model of molecular structures based on the bonding of a pair of valence electrons from different atoms into a singlet quasi-particle state called *isoelectronium*.

We have then applied the model to the structure of the hydrogen molecule, by achieving results manifestly not possible with quantum chemistry, such as: a representation of the binding energy and other features of the hydrogen molecule accurate to the *seventh digit*; an explanation of the reason why the hydrogen molecule has only *two* hydrogen atoms; a reduction of computer usage at least 1,000 fold; and other advances.

In this chapter, we have applied the isochemical model of molecular bonds to the water and other molecules with similar results. In fact, *the isochemical model of the water and other molecules is supported by the following conceptual, theoretical and experimental evidence:*

1) It introduces a new strong binding force (which is absent in current models) capable of explaining the strength and stability of molecules;

2) It explains the reason why the water molecule has only *two* hydrogen atoms and one oxygen;

3) It permits a representation of the binding energy of the water and other molecules, which are accurate to *several digits*;

4) It represents electric and dipole moments and other features of the water and other molecules, also accurate to *several digits*;

5) It permits a reduction of computer usages in calculations at least 1,000 fold; as well as it permits other achievements similar to those obtained for the hydrogen molecule.

Moreover, as it happened for the hydrogen molecule in Chapter 4, *the value of the radius of the isoelectronium, Eqs. (9.2.9) computed via dynamical equations has been fully confirmed by independent calculations for the water and other molecules conducted via the Gaussian-lobe basis set.*

The emission of electron pairs in superconductivity has been emphasized in Chapter 3. In Chapter 4 we also indicated *preliminary, yet direct experimental verifications of the isochemical model of molecular bonds offered by the on-going experiments on photoproduction of the valence electrons in the helium indicating that electrons are emitted in pairs* [62]. The systematic repetition of

these experiments *specifically for water* is here recommended. The statistical percentages of electron pairs over the total number of emitted electrons would then establish whether the isoelectronium is fully or only partially stable.

We should finally note that *the representation of the binding energy, electric and magnetic moments and other characteristics of the water and other molecules exact to the several digits, as first achieved in Refs. [43] constitutes the strongest experimental evidence to date on the insufficiency of quantum mechanics and the validity of the covering hadronic mechanics for the representation of nonlinear, nonlocal and nonpotential-nonunitary effects, due to deep overlappings of the "extended wavepackets" of electrons with a point-like charge structure.*

The new isochemical model of the water molecule outlined in this chapter has a number of intriguing new applications. For instance, the correlated-SCF method is used to easily obtain an energy for the OH- anion in water, while the OH^+ ion is easily treated in either the standard or modified method. The difference in energy between the 8-electron OH^+ system and the 10-electron OH^- system is found to be 13.54 eV. This represents the energy needed to remove $(2e)^{-2}$ from OH^-. This indicates there may be a threshold for current flow in terms of $(2e)^{-2}$ as a quasi-particle in aqueous media at 13.6 eV. This voltage will also maintain H^+ in solution to some extent. Organic alkenes in solution should undergo epoxidation followed by solvolysis to diols under the conditions of abundant $(2e)^{-2}$.

Another interesting result is that the natural trace amounts of HOOH in water may be increased in water by merely placing the sample in an intense magnetic field. Positive and negative ions will traverse short arc segment paths driven by simple thermal Brownian motion in a way which will lead to an increase in collisions of oppositely charged ions. In particular, OH^- and OH^+ may undergo collisions more frequently leading to an increase in HOOH.

This additional HOOH should then be available to react with alkenes to form epoxides which will then hydrolyze in water to form diols. Such diols would be much more soluble in water than the original alkenes. This leads to the important possibility that merely exposing water-insoluble alkenes to water in a magnetic field will lead to a chemical reaction of the alkenes to form modified compounds which are more soluble in water. In other words, organic oils containing some double bonds may be made somewhat more soluble in water just by mechanical emulsification of the oils in water in an environment of a high magnetic field.

Thus, mixtures of oils and water could be mechanically agitated in a magnetic field of several Tesla to produce new oils which are chemically similar to the original oils (assuming a large organic structure) but more soluble in water after exposure to the magnetic field (see Chapter 8 for details).

Similarly, it is easy to see that, while the conventional quantum chemical model of the water molecule predicts one and only configuration, our isochemical model predicts various physically inequivalent configurations depending on the relative orientation of the two *oo*-shaped orbits and other properties, which are under separate study.

The industrial significance of the studies outlined in this chapter will be presented in Chapters 7 and 8.

9.3 VARIATIONAL CALCULATIONS OF ISOCHEMICAL MODELS

9.3.1 Introduction

In Ref. [64a] outlined in Chapter 4, Santilli and Shillady introduced a restricted isochemical three-body model of the hydrogen molecule admitting an exact solution, and a full four-body isochemical model of the hydrogen molecule which no longer admits an exact solution.

In Ref. [64b] outlined in Chapter 5, Santilli and Shillady introduced two corresponding isochemical models of the water and other molecules, one based on a restricted three-body model of the HO dimer admitting exact solutions, and a second fully isochemical four-body model.

As also reviewed in Chapters 4 and 5, Shillady's SASLOBE variational method [64] showed the capability of the isochemical models to reach an essentially exact representation of experimental data on the hydrogen, water and other molecules, as well as resolving other shortcomings or inconsistencies of conventional quantum chemical molecular models.

A greatly detailed, independent verification of models [64a,64b] was conducted by A.K. Aringazin and M.G. Kucherenko [65a] via exact solution and by A.K. Aringazin [65b] via Ritz's variational method, by confirming all numerical results of Refs. [64].

In this chapter we outline Refs. [65] since they achieve new important insights and results on isochemistry of rather general character, and possible application to a variety of other molecules and applications of isochemistry.

9.3.2 Aringazin-Kucherenko Study of the Restricted, Three-Body Isochemical Model of the Hydrogen Molecule

In this section we outline the studies by Aringazin and Kucherenko [65a] of Santilli-Shillady exactly solvable, restricted three-body isochemical model of the H_2 molecule [64a], Eq. (9.1.35), $r_{12} \simeq 0$, i.e.,

$$-\frac{\hbar^2}{2M}\nabla^2_{ab}\psi + \left(-\frac{2e^2}{r_a} - \frac{2e^2}{r_b} + \frac{2e^2}{R}\right)\psi = E\psi. \qquad (9.3.1)$$

As the reader will recall from Chapter 4, model (9.3.1) constitutes a limit case in which the two valence electrons are assumed to be permanently bonded together into the stable singlet quasi-particle state with features (9.1.25), i.e.,

$$\text{mass} \simeq 1 \text{ MeV}, \quad \text{spin} = 0, \quad \text{charge} = 2e, \quad \text{magnetic moment} \simeq 0,$$

$$\text{radius} = r_c = b^{-1} = 6.8432329 \times 10^{-11} \text{ cm} = \qquad (9.3.2)$$

$$= 0.015424288 \text{ bohrs} = 0.006843 \text{ Å},$$

which we have called *isoelectronium.*

The assumption of stationary nuclei (or, equivalently, nuclei with infinite inertia), then turns the four-body hydrogen molecule H_2 into a restricted three-body system which, as such, admits exact solution.

The reader should also recall that, the assumption of the rest energy of the isoelectronium as given by twice the electron mass is merely an upper boundary occurring when the internal forces are of purely nonpotential type. In reality, a total attractive force of purely potential type is possible because the magnetostatic attraction is bigger than the electrostatic repulsion as illustrated in Fig. 9.4. It is evident that the latter bond implies a negative binding energy resulting in a value of the isoelectronium mass

$$M_{\text{isoelectronium}} < 2m_{\text{electron}}, \qquad (9.3.3)$$

which is unknown, and should be derived from fitting experimental data.

As one can see, the above restricted isochemical model of the H_2 molecule is similar to the conventional restricted three-body H_2^+ ion. To avoid confusion, we shall denote the three-body isochemical model with the "hat", $\hat{H}_2$, and the conventional (four-body) model without the "hat," H_2.

More specifically, studies [65a] were conducted under the following conditions:
1) the isoelectronium is stable;
2) the effective size of the isoelectronium is ignorable, in comparison to internuclear distance of H_2;
3) the two nuclei of H_2 are at rest;
4) the rest energy of the isoelectronium is assumed to be unknown and to be determined by the fit of the binding energy of the molecule;
5) the internuclear distance R of H_2 is also assumed to be unknown and to be fitted from the stability condition of the solution, and then compared with its experimental value.

A main result of Ref. [65a] is that the restricted three-body Santilli-Shillady model $\hat{H}_2$ is capable to fit the experimental binding energy for the following value of the isoelectronium mass,

$$M = 0.308381m_e, \qquad (9.3.4)$$

although its stability condition is reached for the following internuclear distance

$$R = 1.675828 \text{ a.u.}, \tag{9.3.5}$$

which is about 19.6% bigger than the conventional experimental value $R[H_2] = 1.4011$ a.u. $= 0.742$ Å.

These results confirm that the isochemical model (9.3.1) is indeed valid, but only in first approximation, in accordance with the intent of the original proposal [64a].

In Born-Oppenheimer approximation, i.e., at fixed nuclei, the equation for the H_2^+ ion-type system for a particle of mass M and charge q is given by

$$\nabla^2 \psi + 2M \left(E + \frac{q}{r_a} + \frac{q}{r_b} \right) \psi = 0. \tag{9.3.6}$$

In spheroidal coordinates,

$$x = \frac{r_a + r_b}{R}, \quad 1 \leq x \leq \infty; \quad y = \frac{r_a - r_b}{R}, \quad -1 \leq y \leq 1; \quad 0 \leq \varphi \leq 2\pi, \tag{9.3.7}$$

where R is the separation distance between the two nuclei a and b, we have

$$\nabla^2 = \frac{4}{R^2(x^2 - y^2)} \left(\frac{\partial}{\partial x}(x^2 - 1)\frac{\partial}{\partial x} + \frac{\partial}{\partial y}(1 - y^2)\frac{\partial}{\partial y} \right) + \tag{9.3.8}$$

$$+ \frac{1}{R^2(x^2 - 1)(1 - y^2)} \frac{\partial^2}{\partial \varphi^2}.$$

Eq. (9.3.1) then becomes

$$\left[\frac{\partial}{\partial x}(x^2 - 1)\frac{\partial}{\partial x} + \frac{\partial}{\partial y}(1 - y^2)\frac{\partial}{\partial y} + \frac{x^2 - y^2}{4(x^2 - 1)(1 - y^2)} \frac{\partial^2}{\partial \varphi^2} + \right. \tag{9.3.9}$$

$$\left. + \frac{MER^2}{2}(x^2 - y^2) + 2MqRx \right] \psi = 0,$$

where

$$\frac{1}{r_a} + \frac{1}{r_b} = \frac{4}{R} \frac{x}{x^2 - y^2}. \tag{9.3.10}$$

The use of the expression

$$\psi = f(x)g(y)e^{im\varphi}, \tag{9.3.11}$$

then allows the separation

$$\frac{d}{dx} \left((x^2 - 1)\frac{d}{dx}f \right) - \left(\lambda - 2MqRx - \frac{MER^2}{2}x^2 + \frac{m^2}{x^2 - 1} \right) f = 0,$$

$$\frac{d}{dy}\left((1-y^2)\frac{d}{dy}g\right) + \left(\lambda - \frac{MER^2}{2}y^2 - \frac{m^2}{1-y^2}\right)g = 0, \tag{9.3.12}$$

where λ is the separation constant. The exact solutions for $f(x)$ and $g(y)$ are given by the angular and radial Coulomb spheroidal functions (CSF) containing infinite recurrence relations.

Aringazin and Kucherenko [65a] calculated the energy levels via the use of recurrence relations of the type

$$Q_{k+1} = Q_k \bar{\kappa}_{N-k} - Q_{k-1}\bar{\rho}_{N-k}\bar{\delta}_{N-k+1}, \quad Q_{-1} = 0, \quad Q_0 = 1, \tag{9.3.13}$$

where the coefficients are

$$\rho_s = \frac{(s+2m+1)[b-2p(s+m+1)]}{2(s+m)+3},$$

$$\kappa_s = (s+m)(s+m+1) - \lambda, \tag{9.3.14}$$

$$\delta_s = \frac{s[b+2p(s+m)]}{2(s+m)-1}.$$

Ref. [65a] then used the value $N = 16$ for the power degree approximation of both the radial and angular components. The two polynomials have 16 roots for λ from which only one root is appropriate due for its asymptotic behavior at $R \to 0$. Numerical solution of the equation,

$$\lambda^{(x)}(p,a) = \lambda^{(y)}(p,b), \tag{9.3.15}$$

gives the list of values of the electronic ground state energy,

$$E(R) = E_{1s\sigma}(R), \tag{9.3.16}$$

which corresponds to $1s\sigma_g$ term of the H_2^+ ion-like system, as a function of the distance R between the nuclei. Note that the term "exact solution" refers to the fact that by taking greater values of N, for example $N = 50$, one can achieve higher accuracy, up to a desired one (for example, twelve decimals).

Also, the scaling method based on the Schrödinger equation has been developed which enables one to relate the final $E(R)$ dependence of different H_2^+ ion-like systems to each other.

Table 9.4 presents result of the calculations of the *minimal total energy* and the corresponding *optimal distance*, at various values of the isoelectronium mass parameter

$$M = \eta m_e, \tag{9.3.17}$$

where $M = \eta$, in atomic units.

Table 9.4. The minimal total energy E_{min} and the optimal internuclear distance R_{opt} of Santilli-Shillady restricted three-body isochemical model $\hat{H}_2$ as functions of the mass M of the isoelectronium[a].

M, a.u.	E_{min}, a.u.	R_{opt}, a.u.	M, a.u.	E_{min}, a.u.	R_{opt}, a.u.
0.10	-0.380852	5.167928	0.32	-1.218726	1.614977
0.15	-0.571278	3.445291	0.33	-1.256811	1.566041
0.20	-0.761704	2.583964	0.34	-1.294896	1.519981
0.25	-0.952130	2.067171	0.35	-1.332982	1.476553
0.26	-0.990215	1.987664	0.40	-1.523408	1.291982
0.27	-1.028300	1.914050	0.45	-1.713834	1.148428
0.28	-1.066385	1.845688	0.50	-1.904260	1.033585
0.29	-1.104470	1.782044	0.75	-2.856390	0.689058
0.30	-1.142556	1.722645	1.00	-3.808520	0.516792
0.307	-1.169215	1.683367	1.25	-4.760650	0.413434
0.308	-1.173024	1.677899	1.50	-5.712780	0.344529
0.308381	-1.174475	1.675828	1.75	-6.664910	0.295310
0.309	-1.176832	1.672471	2.00	-7.617040	0.258396
0.31	-1.180641	1.667073			

[a] See also Figs. 9.10 and 9.11.

Table 9.5. Summary of main data and results on the ground state energy E and the internuclear distance R.

	E, a.u.	R, a.u.
H_2^+ ion, exact theory, N=16 [65a]	-0.6026346	1.9971579
H_2^+ ion, experiment [66]	-0.6017	2.00
3-body $\hat{H}_2$, M=$2m_e$, exact theory [65a]	-7.617041	0.258399
3-body $\hat{H}_2$, M=$2m_e$, var. theory [64a]	-7.61509174	0.2592
3-body $\hat{H}_2$, M=$0.381m_e$, exact theory [65a]	-1.174475	1.675828
4-body H_2, r_c=0.01125 a.u., V_g var. theory [64a]	-1.174474	1.4011
4-body H_2, r_c=0.01154 a.u., V_e var. theory [65b]	-1.144	1.4011
4-body H_2, r_c=0.08330 a.u., V_e var. theory [65b]	-1.173	1.3184
H_2, experiment	-1.174474	1.4011

Aringazin and Kucherenko [65a] computed some 27 tables, each with the identification of the minimum of the total energy, together with the corresponding optimal distance R. Then, they collected all the obtained energy minima and optimal distances in Table 9.4.
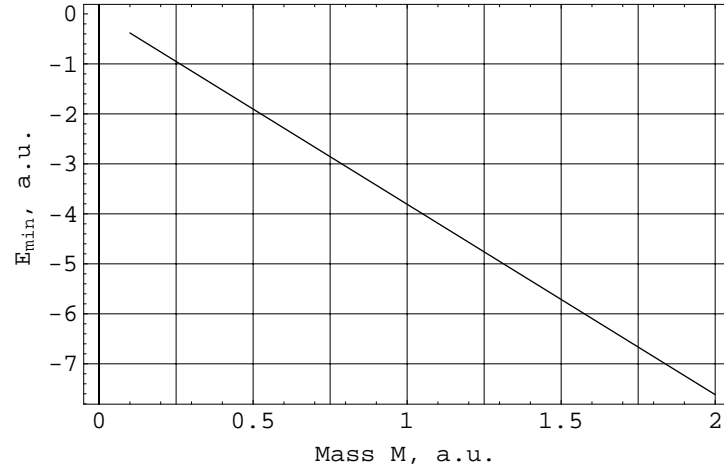
Figure 9.10. The minimal total energy $E_{min}(M)$ of the $\hat{H}_2$ system as a function of the isoelectronium mass M.
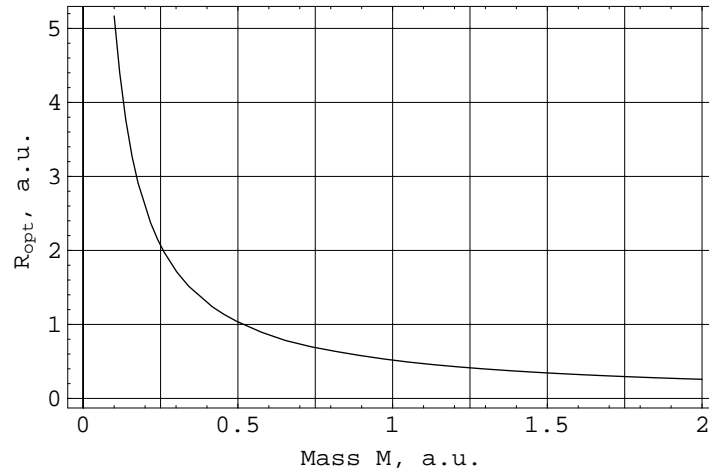

Figure 9.11. The optimal internuclear distance $R_{opt}(M)$ of the $\hat{H}_2$ system as a function of the isoelectronium mass M.

With the fourth order interpolation/extrapolation, the graphical representations of Table 9.4 (see Figs. 9.10 and 9.11) show that the minimal total energy behaves as

$$E_{min}(M) \simeq -3.808M, \tag{9.3.18}$$

and the optimal distance behaves as

$$R_{opt}(M) \simeq 0.517/M. \tag{9.3.19}$$

One can see that at $M = 2m_e$ we have

$$E_{min}(M) = -7.617041 \text{ a.u.}, \quad R_{opt}(M) = 0.258399 \text{ a.u.}, \tag{9.3.20}$$

which recover the values obtained in Ref. [64a]

$$E_{min} = -7.61509174 \text{ a.u.}, \quad R_{opt} = 0.2592 \text{ a.u.}, \tag{9.3.21}$$

to a remarkable accuracy.

The conclusion by Aringazin and Kucherenko is that the Santilli-Shillady restricted three-body isochemical model of the hydrogen molecule is indeed valid as suggested, that is, as in first approximation. The main data and results on E_{min} and R_{opt} are collected in Table 9.5.

An important conclusion of Ref. [65a] is, therefore, that *the two valence electrons of the hydrogen molecule cannot be permanently bound inside the hadronic horizon with radius of one Fermi.*

The clear understanding, stressed in Chapter 4, is that the isoelectronium must continue to exist beyond the hadronic horizon, otherwise, in its absence, we would have a violation of Pauli's exclusion principle.

9.3.3   Aringazin Variational Study of the Four-Body Isochemical Model of the Hydrogen Molecule

In the subsequent Ref. [65b] Aringazin applied Ritz variational method to Santilli-Shillady four-body isochemical model of molecule of the hydrogen molecule (9.1.33), i.e.

$$\left(-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 - V_0\frac{e^{-r_{12}/r_c}}{1 - e^{-r_{12}/r_c}} + \frac{e^2}{r_{12}} - \right. \tag{9.3.22}$$

$$\left. -\frac{e^2}{r_{1a}} - \frac{e^2}{r_{2a}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2b}} + \frac{e^2}{R} \right)|\psi\rangle = E|\psi\rangle,$$

without restriction that the isoelectronium has the permanent dimension of about one Fermi.

In particular, Aringazin's objective was to identify the ground state energy and bond length of the H_2 molecule, in Born-Oppenheimer approximation, via a Gaussian screening of the Coulomb potential, V_g, the exponential screening of the Coulomb potential,

$$V_e = -\frac{Ae^{-r_{12}/r_c}}{r_{12}}, \tag{9.3.23}$$

as well as the original Hulten potential V_h of the model (9.3.22). The resulting analysis is quite sophisticated, and cannot be reviewed herein the necessary detail. Readers seriously interested in this verification of the new isochemical model of the hydrogen molecule are suggested to study Aringazin's original memoir [65b].

The Coulomb and exchange integrals were calculated only for V_e while for V_g and V_h Aringazin achieved analytical results only for the Coulomb integrals because of the absence of Gegenbauer-type expansions for the latter potentials.

A conclusion is that *the Ritz's variational treatment of model (9.2.45) with the potential (9.3.23) 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 [64a] via the SASLOBE variational approach to Gaussian V_g-type model.* The main data and results on the ground state energy E_{min} and internuclear distance R_{opt} are collected in Table 9.5.

Note that in the variational approach of Ref. [65b] Aringazin used a *discrete* variation of the hadronic horizon r_c and approximate exchange integral (9.3.24) that resulted in approximate fittings of the energy and distance, as shown in Table 9.5.

In addition, Ref. [65b] computed the weight of the isoelectronium phase which results to be of the order of 1% to 6% that for the case of V_e model. However, we note that this is it not the result corresponding to the original Santilli-Shillady model, which is based on the Hulten potential V_h.

An interesting result is that in order to prevent divergency of the Coulomb integral for V_h *the correlation length parameter r_c should run discrete values* due to Eq. (9.3.25). This condition has been used in the V_e model, although it is not a necessary one within the framework of this model.

As recalled earlier, Aringazin [*loc. cit.*] assumes that the isoelectronium undergoes an increase of length beyond the hadronic horizon, and the resulting two electrons are separated by sufficiently large distance. This leads us to problem of how to compute *the effective life-time of isoelectronium.*

To estimate the order of magnitude of such a life-time, Aringazin uses the ordinary formula for radioactive α-decay since the total potential $V(r)$ is of the same shape as that here considered, with very sharp decrease at $r < r_{max}$ and Coulomb repulsion at $r > r_{max}$, where r_{max} corresponds to a maximum of the potential.

This quasiclassical model is a crude approximation because in reality the electrons do not leave the molecule. Moreover, the two asymptotic regimes act simultaneously, with some distribution of probability, and it would be more justified to treat the frequency of the decay process (i.e., the tunneling outside the hadronic horizon), rather than the life-time of the isoelectronium.

However, due to the assumption of the small size of isoelectronium in comparison to the molecule size, we can study an elementary process of decay

separately, and use the notion of life-time. The results of Aringazin's calculations are presented in Table 9.6.

Table 9.6. Summary of Aringazin's calculations [65b] on the lifetime of the isoelectronium, where E is relative kinetic energy of the electrons, at large distance, $r \gg r_{max}$, in the center of mass system.

Energy E, a.u.	eV	Lifetime, $D_0 \cdot sec$
2	54.4	$2.6 \cdot 10^{-18}$
1	27.2	$1.6 \cdot 10^{-17}$
0.5	13.6	$2.2 \cdot 10^{-16}$
0.037	1	$5.1 \cdot 10^{-6}$
0.018	0.5	4.0
0.0018	0.1	$3.1 \cdot 10^{+25}$

In Ritz's variational approach, the main problem is to calculate analytically the so-called *molecular integrals*. The variational molecular energy in which we are interested, is expressed in terms of these integrals. These integrals arise when using some wave function, usually a simple hydrogen-like ground state wave function, as an infinite separation asymptotic solution, in the Schrödinger equation for the diatomic molecule. The main idea of Ritz's approach is to introduce parameters into the wave function, and vary them together with the separation parameter R, to achieve a minimum of the total molecular energy, which is treated as the resulting ground state energy.

In the case under study, Aringazin [*loc. cit.*] uses two parameters, γ and ρ, where γ enters hydrogen-like ground state wave function

$$\psi(r) = \sqrt{\frac{\gamma^3}{\pi}} \, e^{-\gamma r}, \qquad (9.3.26)$$

and $\rho = \gamma R$ measures internuclear distance. These parameters should be varied *analytically or numerically* in the final expression of the molecular energy, after the calculation is made for the associated molecular integrals.

However, the four-body Santilli-Shillady model H_2 suggests an additional Hulten potential interaction between the electrons, which potential contains two parameters V_0 and r_c, where V_0 is a general factor, and r_c is a correlation length parameter characterizing the hadronic horizon. Thus, four parameters should be varied, γ, ρ, V_0, and r_c.

The introducing of Hulten potential leads to a modification of some molecular integrals, namely, of the Coulomb and exchange integrals. The other molecular integrals remain the same as in the case of the usual model of H_2,
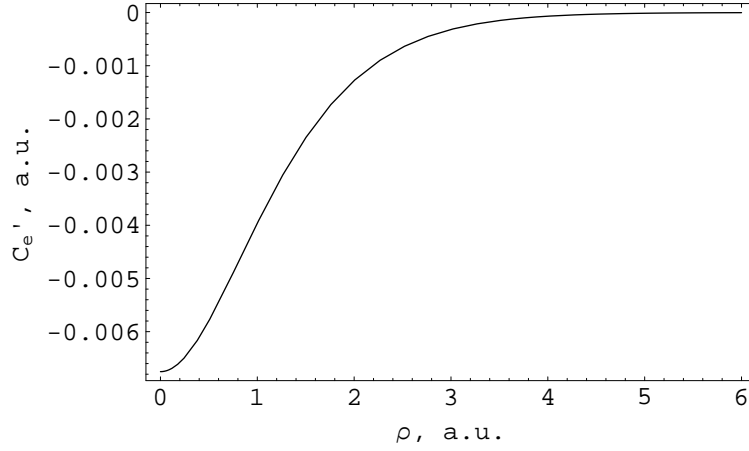
Figure 9.12. The Coulomb integral C'_e as a function of ρ, at $\lambda = 1/37$, where $\rho = \gamma R$, R is the internuclear distance, $\lambda = 2\gamma r_c$, and r_c is the hadronic horizon.
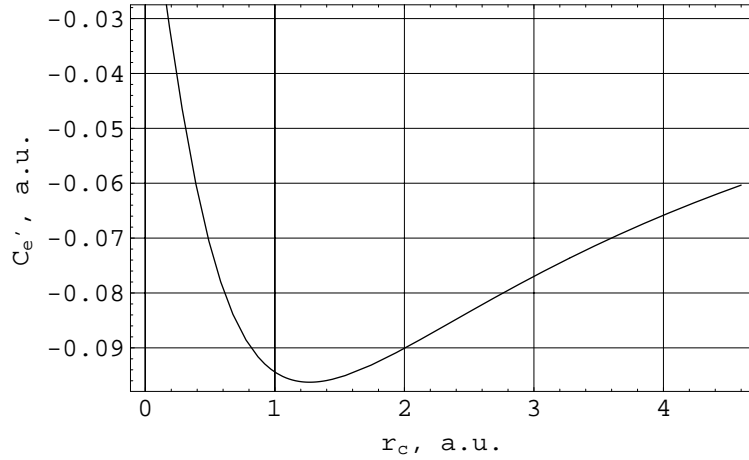
Figure 9.13. The Coulomb integral C'_e as a function of r_c, at $\rho = 1.67$. For $r_c > 0.2$ a.u., the regularized values are presented.

with well-known analytic results. Normally, the Coulomb integral, which can be computed in bispherical coordinates, is much easier to resolve than the exchange integral, which is computed in bispheroidal coordinates.

Calculations of the Coulomb integral for Hulten potential V_h appeared to be quite nontrivial [2b]. Namely, in the used bispherical coordinates, several special functions, such as polylogarithmic function, Riemann zeta-function, digamma function, and Lerch function, appeared during the calculation.

In order to proceed with the Santilli-Shillady approach, Aringazin [65b] invoked two different *simplified* potentials, the exponential screened Coulomb potential V_e, and the Gaussian screened Coulomb potential V_g, instead of the Hulten potential V_h. The former potentials both approximate well the Hulten potential at short and long range asymptotics, and each contains two parameters denoted A and r_c.

In order to reproduce the short range asymptotics of the Hulten potential, the parameter A should have the value $A = V_0 r_c$, for both potentials. The Coulomb integrals for these two potentials have been calculated *exactly* owing to the fact that they are much simpler than the Hulten potential.

In particular, we note that the final exact expression of the Coulomb integral for V_g contains only one special function, the error function $\mathrm{erf}(z)$, while for V_e it contains no special functions at all. In this way, Aringazin [65b] reaches the exact expression

$$C'_e = -\frac{A\lambda^2}{8(1-\lambda^2)^4} \frac{\gamma e^{-2\rho}}{\rho} \left[-(\rho + 2\rho^2 + \frac{4}{3}\rho^3) + 3\lambda^2(5\rho + 10\rho^2 + 4\rho^3) - \right.$$

$$\left. -\lambda^4(15\rho + 14\rho^2 + 4\rho^3) + \lambda^6(8 + 11\rho + 6\rho^2 + \frac{4}{3}\rho^3 - 8e^{2\rho - \frac{2\rho}{\lambda}}) \right], \quad (9.3.27)$$

where $\lambda = 2\gamma r_c$. This Coulomb integral is plotted in Figs. 9.12 and 9.13.

The most difficult part of calculations [65b] is the exchange integral. Usually, to calculate it one has to use bispheroidal coordinates, and needs in an expansion of the potential in some orthogonal polynomials, such as Legendre polynomials in bispheroidal coordinates. In Ref. [65b], only the exponential screened potential V_e is known to have such an expansion but it is formulated, however, in terms of bispherical coordinates (so called Gegenbauer expansion). Accordingly, the exchange integral E'_e for V_e at *null* internuclear separation, $R = 0$ (in which case one can use bispherical coordinates) was calculated exactly. After that, the R-dependence using the standard result for the exchange integral for Coulomb potential E'_C (celebrated Sugiura's result) was partially recovered,

$$E'_e \simeq \frac{A\lambda^2}{(1+\lambda)^4} \left(\frac{1}{8} + \frac{1}{2}\lambda + \frac{5}{8}\lambda^2 \right) \frac{8}{5} E'_C, \quad (9.3.28)$$

where $\lambda = 2\gamma r_c$ (see Fig. 9.14). Thus, only some approximate expression of the exchange integral for the case of V_e has been achieved. In this way, all subsequent results apply to the approximate V_e-based model.
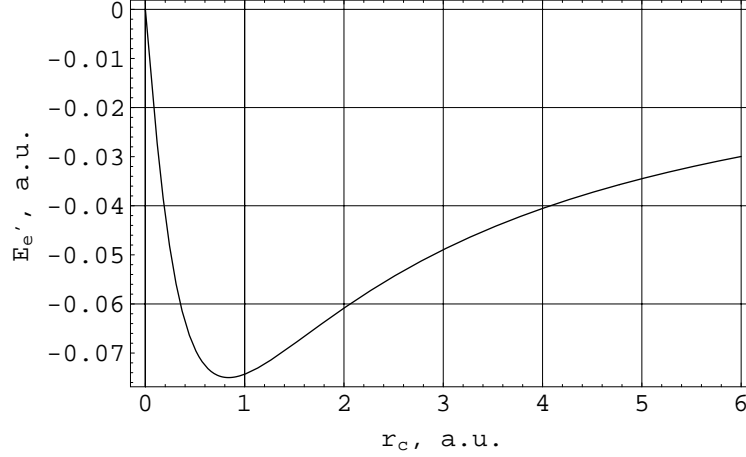
Figure 9.14. The exchange integral E'_e as a function of r_c, at $\rho = 1.67$.
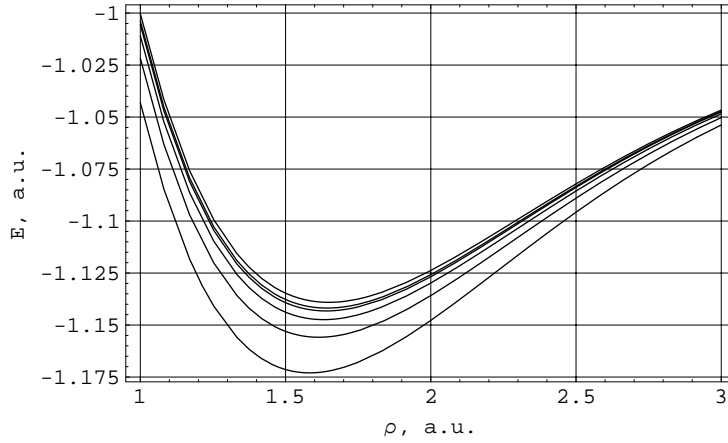
Figure 9.15. The total energy $E = E_{mol}$ as a function of ρ, at $\lambda = 1/60$, $1/40$, $1/20$, $1/10$, $1/5$. The lowest plot corresponds to $\lambda = 1/5$.

Inserting the so-obtained V_e-based Coulomb and exchange integrals into the total molecular energy expression, the final analytical expression containing four parameters, γ, ρ, A, and r_c, was obtained. From a separate consideration of the Hulten potential case, the existence of a bound state of two electrons (which is the proper isoelectronium) leads to the following relationship between

the parameters for the case of one energy level of the electron-electron system, $V_0 = \hbar^2/(2mr_c^2)$. Thus, using the relation $A = V_0 r_c$ Aringazin has $A = 1/r_c \equiv 2\gamma/\lambda$, in atomic units ($\hbar = m_e = c = 1$).

Note that Aringazin [65b] introduces the *one-level isoelectronium* characterized by the fact that the condition,

$$\lambda^{-1} = \text{ integer numbers} > 0, \qquad (9.3.29)$$

follows from the analysis of the Coulomb integral for Hulten potential.

With the above set up, minimization of the total molecular energy of the V_e-based model can be made. Numerical analysis shows that the λ-dependence does not reveal any minimum in the interval of interest,

$$4 \leq \lambda^{-1} \leq 60, \qquad (9.3.30)$$

while there is a minimum of the energy for some values of γ and ρ, at fixed λ.

Therefore, 56 tables have been calculated to identify the energy minima and optimal distances for different values of λ, in the interval (9.3.30).

Aringazin's results are collected in Tables 9.7, 9.8, and Fig. 9.15. One can see that the binding energy decreases with the increase of the parameter r_c, which corresponds to an effective radius of the isoelectronium.

In conclusion, the calculation by Aringazin [65b] reviewed in this Chapter have not identified the meanlife of the isoelectronium assumed as a quasiparticle of charge radius r_c of about 1 fm. As one can see in Table 9.7, the predicted meanlife varies over a rather large range of values.

The achievement of an accurate meanlife of the isoelectronium of 1 fm charge radius can be reached only after reaching a more accurate knowledge of its rest energy. As the reader will recall from Chapter 4, the value of 1 MeV should be solely considered as an upper boundary value of the rest energy of the isoelectronium, since it holds only in the absence of internal potential forces while the latter cannot be excluded. Therefore, the actual value of the rest energy of the isoelectronium is today basically unknown.

The reader should also recall that the terms "meanlife of the isoelectronium when of charge radius of about 1 fm" are referring to the duration of time spent by two valence electrons at a mutual distance of 1 fm which is expected to be small. The understanding explained in Chapter 3 is that, *when the restriction of the charge radius to 1 fm is removed, and orbital mutual distances are admitted, the isoelectronium must have an infinite life (for the unperturbed molecule), because any finite meanlife under the latter conditions would imply the admission of two electrons with identical features in the same orbit, and a consequential violation of Pauli's exclusion principle.*

An interesting result of the Ritz variational approach to the Hulten potential studied by Aringazin [65b] is that *the charge radius of the isoelectronium r_c*

Table 9.7. The total minimal energy E_{min} and the optimal internuclear distance R_{opt} as functions of the correlation length r_c for the exponential screened Coulomb potential V_e.

λ^{-1}	r_c, a.u.	R_{opt}, a.u.	E_{min}, a.u.
4	0.10337035071618050	1.297162129235449	-1.181516949656805
5	0.08329699109108888	1.318393698326879	-1.172984902150024
6	0.06975270534273319	1.333205576478603	-1.167271240301846
7	0.05999677404817234	1.344092354783681	-1.163188554065554
8	0.05263465942162049	1.352417789644028	-1.160130284706318
9	0.04688158804756491	1.358984317233049	-1.157755960428922
10	0.04226204990365446	1.364292909163710	-1.155860292450436
11	0.03847110142927672	1.368671725082009	-1.154312372623724
12	0.03530417706681329	1.372344384866235	-1.153024886026671
13	0.03261892720535206	1.375468373051375	-1.151937408039373
14	0.03031323689615631	1.378157728092548	-1.151006817317425
15	0.02831194904031777	1.380497017045902	-1.150201529091051
16	0.02655851947236431	1.382550255552670	-1.149497886394651
17	0.02500959113834722	1.384366780045693	-1.148877823925501
18	0.02363136168905809	1.385985219224291	-1.148327310762828
19	0.02239708901865092	1.387436244558651	-1.147835285349041
20	0.02128533948435381	1.388744515712491	-1.147392910500336
21	0.02027873303335994	1.389930082626193	-1.146993041730378
22	0.01936302821907175	1.391009413196452	-1.146629840949675
23	0.01852644434336641	1.391996158084790	-1.146298491232105
24	0.01775915199935013	1.392901727808297	-1.145994983116511
25	0.01705288514774330	1.393735733699196	-1.145715952370148
26	0.01640064219648127	1.394506328745493	-1.145458555325045
27	0.01579645313764336	1.395220473843219	-1.145220372020229
28	0.01523519631632570	1.395884147817973	-1.144999330178493
29	0.01471245291356761	1.396502514589167	-1.144793644973560
30	0.01422439038752817	1.397080057337240	-1.144601770891686

entering the Hulten potential and the variational energy, should run discrete set of values during the variation.

In other words, this means 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.*

This result was completely unexpected and may indicate a kind of "hadronic fine structure" of the isoelectronium whose origin and meaning are unknown at this writing. It should be indicated that such a "hadronic fine structure" of the isoelectronium is solely referred to the case when r_c is restricted to be about 1 fm or less. The problem whether such a "hadronic fine structure"

Table 9.8. A continuation of Table 9.8.

λ^{-1}	r_c, a.u.	R_{opt}, a.u.	E_{min}, a.u.
31	0.01376766836566138	1.397620687025853	-1.144422362947838
32	0.01333936209977966	1.398127830817745	-1.144254245203342
33	0.01293689977547854	1.398604504597664	-1.144096385030938
34	0.01255801083612469	1.399053372836414	-1.143947871939897
35	0.01220068312791624	1.399476798299823	-1.143807900045981
36	0.01186312715793131	1.399876883556063	-1.143675753475045
37	0.01154374612489787	1.400255505817128	-1.143550794143290
39	0.01095393745919852	1.400954915288619	-1.143320213707519
40	0.01068107105944273	1.401278573036792	-1.143213620508321
41	0.01042146833640030	1.401586548200467	-1.143112256673494
42	0.01017418516195214	1.401879953246168	-1.143015746732479
43	0.00993836493541500	1.402159797887369	-1.142923750307661
44	0.00971322867044429	1.402427000676349	-1.142835958109381
45	0.00949806639934841	1.402682399061957	-1.142752088467028
46	0.00929222969498477	1.402926758144872	-1.142671884314343
47	0.00909512514431396	1.403160778323019	-1.142595110561057
48	0.00890620863525624	1.403385101987775	-1.142521551794315
49	0.00872498034101540	1.403600319405678	-1.142451010262626
50	0.00855098030451296	1.403806973898863	-1.142383304102633
51	0.00838378454080327	1.404005566419838	-1.142318265775268
52	0.00822300158793934	1.404196559601683	-1.142255740683024
53	0.00806826944722482	1.404380381352424	-1.142195585944305
54	0.00791925286251402	1.404557428052374	-1.142137669304475
55	0.00777564089552400	1.404728067404676	-1.142081868166104
56	0.00763714476025456	1.404892640982100	-1.142028068723488
57	0.00750349588477794	1.405051466507240	-1.141976165188595
58	0.00737444417302681	1.405204839898059	-1.141926059097351
59	0.00724975644291090	1.405353037106507	-1.141877658686723
60	0.00712921502024112	1.405496315774223	-1.141830878334298

persists for values of r_c up to orbital distances is also unknown at this writing. It should be also indicated that this remarkable property is specific to the Hulten potential V_h, while it is *absent* in the V_e, or V_g models.

Moreover, Aringazin [65b] has achieved an estimation of *the weight of the isoelectronium phase* for the case of V_e model which appears to be of the order of 1% to 6%. This weight has been estimated from the energy contribution related to the exponentially screened potential V_e, in comparison to the contribution related to the usual Coulomb interelectron repulsive potential.

Finally, an important result of the Ritz variational four-body model studied by Aringazin [65b] is its fit to the experimental data of both the binding energy

E and the bond length R of the hydrogen molecule thus providing an excellent independent confirmation of the results obtained by Santilli and Shillady [64].

Appendix 9.A
Isochemical Calculations for the Three-Body H_2 Molecule

This appendix contains a summary of the computer calculations conducted in Ref. [5] for the restricted three-body model of the hydrogen molecule according to isochemistry, Eq. (9.1.35), showing an exact representation of the binding energy. The calculations are based on the isoelectronium as per characteristics (9.1.25).

```
Gaussian-Lobe Program for Large Molecules
     set up by D. Shillady and S. Baldwin
          Richmond Virginia 1978-1997
            3 BODY H2 (Electronium)
```

ipear = 1, dt = 0.0, tk = 0.0, imd = 0, ntime = 60, mul = 1, iqd = 0, icor = 3, mdtim = 0, idb = 0.

ELECTRONIUM-PAIR CALCULATION

Atomic Core				Nuclear		Coordinates
		X		Y		Z
1.		0.000000		0.000000		0.000000
	Z1s =	6.103	Z2s =	24.350	Z2p =	24.350
	Z3s =	16.230	Z3p =	16.230	Z3d =	-16.200
	Z4p =	12.180	Z4f =	12.180		
1.		0.000000		0.000000		0.259200
	Z1s =	6.103	Z2s =	24.350	Z2p =	24.350
	Z4p =	12.180	Z4f =	12.18O	Z3d =	-16.200

Basis Size = 50 and Number of Spheres = 142 for 2 Electrons.

Distance Matrix in Angströms:

	H	H
H	0.00000	0.13716
H	0.13716	0.00000

A-B-C Arcs in Degrees for 2 Atoms.
The Center of Mass is at Xm = 0.000000, Ym = 0.000000, Zm = 0.129600.

One-Electron Energy Levels:

E(1) =	-11.473116428176	E(26) =	28.974399759209
E(2) =	-4.103304982059	E(27) =	28.974400079775
E(3) =	-1.621066945385	E(28) =	31.002613061833
E(4) =	-1.621066909587	E(29) =	31.002614578175
E(5) =	0.735166320188	E(30) =	35.201145239721
E(6) =	3.760295564718	E(31) =	38.003259639003
E(7) =	3.760295673022	E(32) =	44.948398097510
E(8) =	4.206194459198	E(33) =	44.94839B118458
E(9) =	4.813241859203	E(34) =	52.259825531212
E(10) =	11.2330B0571453	E(35) =	57.732587951875
E(11) =	15.70B645318078	E(36) =	57.732589021798
E(12) =	15.708645469273	E(37) =	68.743644612501
E(13) =	18.535761604401	E(38) =	68.743644649428
E(14) =	18.535761951543	E(39) =	73.195648957615
E(15) =	19.329445299735	E(40) =	79.303486379907
E(16) =	19.329445306194	E(41) =	85.865499885249
E(17) =	19.644048052034	E(42) =	85.865531919077
E(18) =	24.002368034839	E(43) =	127.196518644932
E(19) =	24.002368621986	E(45) =	130.602186113463
E(20) =	24.076849036707	E(46) =	130.602190550265
E(21) =	24.076853269415	E(47) =	137.484863078186
E(22) =	24.574406183060	E(48) =	158.452350229845
E(23) =	26.836031180463	E(49) =	205.158233049979
E(25) =	27.860752485358	E(50) =	446.152984041077

epair Energy = -7.615091736818.

Appendix 9.B
Isochemical Calculations for the Four-Body H_2 Molecule

In this appendix we present a summary of the computer calculations conducted in Ref. [5] for the four-body model of the hydrogen molecule, Eq. (9.1.33), according to isochemistry by using only $6G$-$1s$ orbitals for brevity. The calculations are also based on the characteristics of the isoelectronium in Eqs. (9.1.25). Note, again, the exact representation of the binding energy at -1.174447 Hartrees.

```
        Gaussian-Lobe Program for Large Molecules
            set up by D. Shillady and S. Baldwin
               Virginia Commonwealth University
                      Richmond Virginia
                         1978-1997
                   Test of SASLOBE on H2
```

SANTILLI-RADIUS = 0.01184470000000.
Cutoff = (A/r)*(exp(-alp*r*r)), A = 0.20E+01, alp = 0.49405731E+04.

Atomic Core						
				Nuclear		Coordinates
		X		Y		Z
1.		0.000000		0.000000		0.000000
	Z1s =	1.200	Z2s =	0.000	Z2p =	0.000
	Z3s =	0.000	Z3p =	0.000	Z3d =	0.000
	Z4p =	0.000	Z4f =	0.000		
1.		0.000000		0.000000		1.401100
	Z1s =	1.200	Z2s =	0.000	Z2p =	0.000
	Z3s =	0.000	Z3p =	0.000	Z3d =	0.000
	Z4p =	0.000	Z4f =	0.000		

Basis Size = 2 and Number of Spheres = 12 for 2 Electrons.

Distance Matrix in Angströms:

	H	H
H	0.00000	0.74143
H	0.74143	0.00000

The center of Mass is at: Xm = 0.000000, Ym = 0.000000, Zm = 0.700550.

Spherical Gaussian Basis Set:

No. 1	alpha =	0.944598E+03 at X = 0.0000 Y = 0.0000 Z = 0.0000 a.u.
No. 2	alpha =	0.934768E+02 at X = 0.0000 Y = 0.0000 Z = 0.0000 a.u.
No. 3	alpha =	0.798123E+01 at X = 0.0000 Y = 0.0000 Z = 0.0000 a.u.
No. 4	alpha =	0.519961E+01 at X = 0.0000 Y = 0.0000 Z = 0.0000 a.u.
No. 5	alpha =	0.235477E+00 at X = 0.0000 Y = 0.0000 Z = 0.0000 a.u.
No. 6	alpha =	0.954756E+00 at X = 0.0000 Y = 0.0000 Z = 0.0000 a.u.
No. 7	alpha =	0.1944598E+03 at X = 0.0000 Y = 0.0000 Z = 1.4011 a.u.
No. 8	alpha =	0.7934768E+02 at X = 0.0000 Y = 0.0000 Z = 1.4011 a.u.
No. 9	alpha =	0.40798123E+01 at X = 0.0000 Y = 0.0000 Z = 1.4011 a.u.
No. 10	alpha =	0.11519961E+01 at X = 0.0000 Y = 0.0000 Z = 1.4011 a.u.
No. 11	alpha =	0.37235477E+00 at X = 0.0000 Y = 0.0000 2 = 1.4011 a.u.
No. 12	alpha =	0.12954756E+00 at X = 0.0000 Y = 0.0000 Z = 1.4011 a.u.

Contracted Orbital No. 1:
0.051420*(1), 0.094904*(2), 0.154071*(3), 0.203148*(4), 0.169063*(5), 0.045667*(6).
Contracted Orbital No.2:
0.051420*(7), 0.094904*(8), 0.154071*(9), 0.203148*(10), 0.169063*(11),
0.045667*(12).

***** Nuclear Repulsion Energy in au = 0.71372493041182. *****

Overlap Matrix:

#		at-orb	1	2
1	H	1s	1.000	0.674
2	H	1s	0.674	1.000

S(-1/2) Matrix:

#		at-orb	1	2
1	H	1s	1.263	-0.490
2	H	1s	-0.490	1.263

H-Core Matrix:

#		at-orb	1	2
1	H	1s	-1.127	-0.965
2	H	1s	-0.965	-1.127

Initial-Guess-Eigenvectors by Column:

#		at-orb	1	2
1	H	1s	0.546	1.239
2	H	1s	0.546	-1.239

One-Electron Energy Levels: E(1) = -1.249428797385, E(2) = -0.499825553916.

(1,1/1,1) =	0.75003658795676
minus (1,1/1,1) =	0.08506647783478
total (1,1/1,1) =	0.66497011012199
(1,1/1,2) =	0.44259146066210
minus (1,1/1,2) =	0.02960554295227
total (1,1/1,2) =	0.41298591770983
(1,1/2,2) =	0.55987025041920
minus (1,1/2,2) =	0.01857331166211
total (1,1/2,2) =	0.54129693875709
(1,2/1,2) =	0.30238141375547
minus (1,2/1,2) =	0.01938180841827
total (1,2/1,2) =	0.28299960533720
(1,2/2,2) =	0.44259146066210
minus (1,2/2,2) =	0.02960554295227
total (1,2/2,2) =	0.41298591770983
(2,2/2,2) =	0.75003658795676
minus (2,2/2,2) =	0.08506647783478
total (2,2/2,2) =	0.66497011012199

Block No. 1 Transferred to Disk/Memory. The Two-Electron Integrals Have Been Computed.

Electronic Energy = -1.88819368266525 a.u., Dif. = 1.8881936827,

Electronic Energy = -1.88819368266525 a.u., Dif. = 0.0000000000.

Energy Second Derivative = 0.00000000000000.

e1a =	-2.499	e1b =	-2.499		
e2a =	0.611	e2b =	0.611	e2ab =	0.611

Iteration No. = 2, alpha = 0.950000.

Electronic Energy = -1.88819368266525 a.u., Dif. = 0.0000000000.

Total Energy = -1.17446875 a.u.

One-Electron Energy Levels: E(1) = -0.638764885280, E(2) = 0.561205833046

Reference State Orbitals for 1 Filled Orbitals by Column:

#	at-orb		1	2
1	H	1s	0.546	1.239
2	H	1s	0.546	-1.239

Dipole Moment Components in Debyes:

Dx = 0.0000000, Dy = 0.0000000, Dz = 0.0000000.

Resultant Dipole Moment in Debyes = 0.0000000.

Computed Atom Charges: Q(1) = 0.000, Q(2)= 0.000.

Orbital Charges: 1.000000, 1.000000.

Milliken Overlap Populations:

#	at-orb		1	2
1	H	1s	0.597	0.403
2	H	1s	0.403	0.597

Total Overlap Populations by Atom:

	H	H
H	0.597222	0.402778
H	0.402778	0.597222

Orthogonalized Molecular Orbitals by Column:

#	at-orb		1	2
1	H	1s	0.422	2.172
2	H	1s	0.422	-2.172

Wiberg-Trindie Bond Indices:

#	at-orb		1	2
1	H	1s	0.127	0.127
2	H	1s	0.127	0.127

Wiberg-Trindie Total Bond Indices by Atoms:

	H	H
H	0.127217	0.127217
H	0.127217	0.127217

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