Scientific Research Publishing

Journal of Modern Physics, 2024, 15, 1313-1336
https://www.scirp.org/journal/jmp
ISSN Online: 2153-120X
ISSN Print: 2153-1196

Surprising New Bohr Models for H_2 and H_2^+

Auguste Meessen

UC Louvain, Louvain-la-Neuve, Belgium
Email: auguste@meessen.net

How to cite this paper: Meessen, A. (2024) Surprising New Bohr Models for H_2 and H_2^+. *Journal of Modern Physics*, **15**, 1313-1336.
https://doi.org/10.4236/jmp.2024.158053

Received: May 8, 2024
Accepted: July 28, 2024
Published: July 31, 2024

Abstract

Niels Bohr constructed the first version of quantum mechanics. It has been called "old quantum mechanics" with a connotation of being obsolete. It is logically consistent, however, and deserves the name of *simple quantum mechanics* (SQM). It differs only from the semiclassical approximation by assuming that the average position and average velocity of an electron can be sharply defined on closed orbits. This assumption does not contradict Heisenberg's uncertainty relations, since the quantization rule means that the electron can be anywhere on this orbit when it allows for stationary waves. This approach was remarkably efficient for one electron in hydrogen atoms and even for the electron pair in hydrogen molecules. However, dissociation of H_2 and determination of the orbit of the single electron in H_2^+ led to problems that remained unsolved for more than 100 years. Their solution, presented here, yields more physical insight and reveals, for instance, that mutual polarization of two hydrogen atoms can yield a metastable state.

Keywords

H_2 Molecules, H_2^+ Molecular Ions, Old Quantum Mechanics, Electron Pairs, Simple Quantum Mechanics

1. Introduction

The basic aim of this article is to clarify the process of constructing new physical theories. That is always necessary when careful observations led to the discovery of facts that cannot be explained by existing theories. Since a new one requires to invent adequate concepts, we will focus attention on this step. It is also useful to realize that progressive structuring of physical theories results from a logical process. The elaboration of quantum mechanics provides an instructive example. It began in 1900, because of Planck's analysis of empirical data concerning EM waves in hot cavities. It revealed that the energy of waves of frequency ν

can only increase or decrease by quanta $h\nu$. However, Max Planck was troubled, since this result contradicted the established idea that physical observables do vary in a continuous way. This was an essential ingredient of Newton's laws of motion and remained valid in Maxwell's theory of EM waves. Could the energy of oscillating charged particles be quantized without modifying the concept of continuous motions?

Planck found an astonishing answer, published in 1906 [1]. The position x and momentum p of this particle can still vary in a continuous way in the course of time, though its energy $E = nh\nu$, where n is a positive integer number. The frequency ν is the natural frequency of oscillation, determined by Newton's laws of motion. It is sufficient that for periodic motions, merely the "action" has to be quantized. This means that the integral

$$\oint p\mathrm{d}x = nh \tag{1}$$

This result was also weird, since the variations of $x(t)$ and $p(t)$ had to be connected to one another during a whole period of oscillation. However, the concept of continuous motions, attributed to the continual existence of material particles, was saved.

Niels Bohr generalized this "quantization rule", because of other empirically discovered facts. In his PHD thesis of 1911, he had examined the validity of Drude's theory [2]. It had been proposed in 1900, immediately after the discovery of the electron, to explain the heigh electrical and thermal conductivity of metals [3]. Drude assumed that they contain a gas of freely moving electrons, but when they are subjected to an electric field, they are randomly scattered by colliding with small positive ions. Their average velocity is then reduced, in agreement with Ohm's law. Thermal gradients led to similar results, but Bohr found that the effects of magnetic fields are not well explained. Since the electrons are then orbiting, Bohr suspected that this could be due to *quantum effects* that Planck had discovered for linear periodic motions. He decided therefore to examine what happens for the single electron in hydrogen atoms. According to Rutherford's discovery of atomic nuclei, this electron should be moving around the proton, but that raised new problems.

The electron would constantly lose energy and that was incompatible with the finite radius of hydrogen atoms. Moreover, there were peculiar spectroscopic observations. Bohr made sense of all these facts, by assuming that the quantization rule (1) is also valid for circular motions. This would yield "stationary states", when radiation can only be emitted or absorbed by transitions between these states. The resulting theory did perfectly account for spectroscopic data. Sommerfeld generalized Bohr's model of hydrogen atoms for elliptical orbits. This led to the discovery of more quantum numbers. However, there are two possible quantization rules for systems that require several canonical coordinates q_i and their conjugate momenta p_i. They could yield

$$\oint p_i\mathrm{d}q_i = n_i h \quad \text{or} \quad \oint \textstyle\sum_i p_i\mathrm{d}q_i = nh \tag{2}$$

The first relation was independently proposed in 1915 by Wilson [4] and Sommerfeld [5]. Ishiwara considered the second one [6]. Einstein noted also the existence of an ambiguity [7], but these remarks were eclipsed by the success of Sommerfeld's theory. Louis de Broglie proposed a radically new idea in his doctoral thesis of l924. It justified Bohr's quantization rule, but resulted also from trying to understand experimental results. He had studied history, but became interested in quantum physics because of his brother Maurice [8]. He was a physicist and made experiments on the scattering of X-rays by electrons. These processes involved waves and particles. Louis de Broglie thought that they were always related to one another. A material particle had thus an "associated wave". Its wavelength λ and frequency ν are determined by the momentum p and the energy E of the particle, so that

$$p = h/\lambda \quad \text{and} \quad E = h\nu \tag{3}$$

These relations generalized what was known for photons, but applied only to freely moving material particles. Their trajectories are rectilinear, of course, while Bohr's model of hydrogen atoms is applied to circular motions. However, the radius and orbital velocity were constant. This fact may have encouraged de Broglie to assume that (3) is also valid for circular motions. Anyway, Bohr's quantization rule could be interpreted as being equivalent to the requirement that circular orbits have to allow for stationary waves ($2\pi r = n\lambda$). This explanation led Erwin Schrödinger to another idea.

He realized that if an electron has an associated wave, it cannot only be defined on particular orbits. It has also to exist in space and time, outside these orbits. Instead of determining possible orbits, he tried thus to discover the needed wave equation. How could that be achieved? According to de Broglie's reasoning, a single particle that is freely moving along a given x-axis should be associated with a plane wave that varies in space and time so that

$$\psi(x,t) = A\mathrm{e}^{i(kx-\omega t)} \quad \text{when} \quad p = \frac{h}{\lambda} = \hbar k \quad \text{and} \quad E = h\nu = \hbar\omega$$

Thus, $-i\hbar\frac{\partial\psi}{\partial x} = p\psi$ and $i\hbar\frac{\partial\psi}{\partial t} = E\psi$.

These relations define "local values" of p and E by means of the function $\psi(x,t)$. Schrödinger assumed that the components of the momentum vector $\boldsymbol{p}$ of any material particle at a given point in space and its instantaneous energy E are always defined by first-order derivatives of its wave function, even when the particle is subjected to forces. Assuming that these local values are also related to one another as in classical mechanics, he got a differential equation that could be solved for hydrogen atoms. This theory was published in 1926 and constituted the foundation of wave-mechanics [9]. Since this equation did yield a conservation law, similar to the continuum equation for fluids, Schrödinger thought that the wave equation describes "matter waves". When Max Born did solve Schrödinger's equation for electron scattering by a point-like particle [10], it appeared that $\rho(\boldsymbol{r},t) = \left|\psi(\boldsymbol{r},t)\right|^2$ is the probability density that the electron is detectable at the point $\boldsymbol{r}$ and the instant t. This statistical interpretation of the wave function revealed that physical processes can be random.

In the meantime, Werner Heisenberg had followed another path. He considered that we are unable to observe how electrons are moving inside atoms. We do only have spectroscopic data concerning frequencies and intensities of emitted or absorbed light. This led to another definition of possible positions and velocities. Being represented by arrays with two indexes, they were matrixes. Motions at atomic scales were thus described in a rather abstract way [11]. This "matrix mechanics" was published in 1925, but turned out to be equivalent to wave mechanics. Because of a discussion with Einstein, who considered that electron orbits should really exist, Heisenberg tried to find out if they are observable or not. This led to the ground breaking discovery that precise simultaneous knowledge of the position and velocity of an electron is limited by the value of Planck's constant h. These *uncertainty relations* [12] led us to propose a generalization of fundamental importance.

It is not sufficient that the definition of local values of momenta and energies by first-order derivatives does lead to the field equation of relativistic quantum mechanics. Since there are two universal constants (h and c) that impose restrictions on possible results of measurements, there could exist a third one. Actually, we do merely *believe* that space and time are continuous. This was initially suggested by considering that space and time are analogous to continuous media, but we can only define space and time by possible results of measurements. It has therefore been assumed that it should be possible to measure always smaller and smaller space-time intervals without ever reaching a finite limit. That allows to express physical laws by means of differential equations, but there could exist a finite limit for the smallest distance. The value (a) of this "quantum of length" could be extremely small, but it has to be a universal constant.

It is then still possible to define local values of $\boldsymbol{p}$ and instantaneous values of E, but all differential equations have to be replaced by finite-difference equations. We verified that this theory of *space-time quantization* (STQ) is logical consistent and does explain basic mysteries of elementary particle physics [13]. Since second-order finite differences can result from combining two different first-order finite differences, there appear new degrees of freedom, indeed. They account for the fact that elementary particle can be distinguished from one another by means of a set of quantum numbers. Moreover, it is known that the "standard model" of elementary particle physics is incomplete. It does not account for dark matter, for instance, while STQ defines *all possible elementary particles* in our 4-dimensional space-time. STQ accounts also for astrophysical observations, concerning dark matter and dark energy and even for the Big Bang, since hc/a is the highest possible energy. In this context of successive generalizations, it is also useful to reanalyze the concept of orbital motions that are determined by classical mechanics, but quantized.

In *chapter* 2*,* we consider the motion of two electrons in the ground state of

H_2 molecules and their dissociation process ($H_2 \to 2H$). *Chapter* 3 is devoted to the treatment of H_2^+. There is only one electron, but its orbit could not be determined, in spite of great effort. This problem will be solved. *Chapter* 4 presents conclusions and discusses the physical relevance of the concept of electron orbits.

2. The Electron Pair in H2 Molecules

2.1. Bohr's Model for the Ground State

Let us begin with recalling Bohr's treatment of hydrogen-like atoms. He assumed that the electron is moving on a circular orbit around a proton or a point-like ion of charge $+Ze$. It follows then from classical mechanics and the quantization rule that the orbital radius r and velocity v of the electron are related to one another so that

$$\frac{Ze^2}{r^2} = \frac{mv^2}{r} \quad \text{and} \quad 2\pi rmv = nh \quad \text{or} \quad rp = n\hbar$$

The Coulomb force is expressed in natural units ($4\pi\varepsilon_o = 1$) and the energy of this system is

$$E = V + T = \frac{-Ze^2}{r} + \frac{mv^2}{2} \quad \text{where} \quad \frac{mv^2}{2} = \frac{n^2}{2r^2}\frac{\hbar^2}{m} = \frac{Ze^2}{2r}$$

$$\text{Thus,} \quad r = \frac{n^2}{Z}a_o \quad \text{where} \quad a_o = \frac{\hbar^2}{me^2} = 52.918\ \text{pm}$$

$$E = \frac{-Z}{n^2}E_o \quad \text{where} \quad E_o = \frac{e^2}{2a_o} = 13.606\ \text{eV}$$

In honor of Niels Bohr and to facilitate comparisons with H atoms, we adopt the Bohr radius (a_o) and the ionization energy of hydrogen atoms ($E_o = 1\,\text{Ry}$) as natural units. So-called "atomic units" are defined by setting $\hbar = m = e = 1$, which yields $a_o = 1$, but $2E_o = 1$ Hartree. We note that

$$V = -2T \quad \text{and} \quad E = -T \tag{4}$$

What happens for H_2 molecules? Bohr assumed that the protons are bound to one another when both electrons are moving on the same circular orbit, situated in the median plane of the protons. The electrons are there always opposite, to minimize their mutual repulsion. This model is represented in **Figure 1(a)**. Dynamical equilibrium and the quantization rule for $n = 1$ require that every electron is attracted towards the symmetry axis by the Newtonian force

$$F = \frac{2r}{d^3} - \frac{1}{4r^2} = \frac{a_o}{r^3} \quad \text{where} \quad d^2 = r^2 + x^2 \quad \text{and} \quad d^3 = \frac{8r^4}{r + 4a_o}$$

Thus $d = d(r)$ and $x = x(r)$, but $r \ge (4/7)a_o$. The energy of the molecule is

$$E(r) = \frac{1}{x} + \frac{1}{r} - \frac{8}{d} + \frac{2a_o}{r^2} \tag{5}$$

This function displays a minimum when

$$r = r_o = 0.9532a_o \quad x = x_o = 0.550a_o \quad E_{\min} = -2.201E_o$$

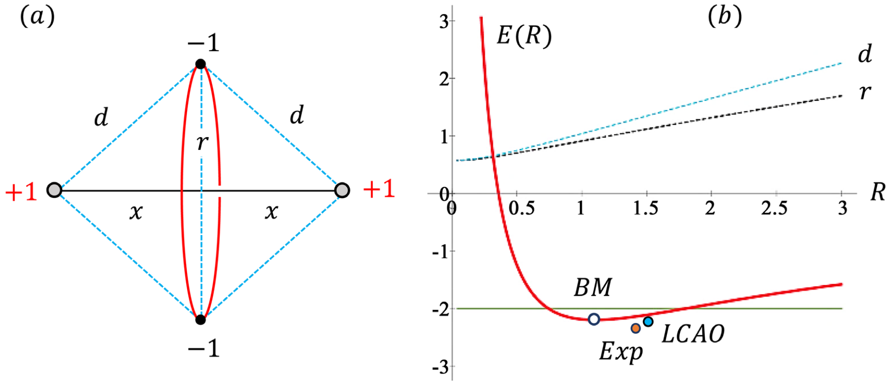

Figure 1. (a) The Bohr model (BM) for H_2 molecules in their ground state. (b) The resulting energy curve is $E(R)$ when R is the separation of the protons. The ground state would thus be situated at the white dot. Experimental measurements did yield the red dot and the first wave-mechanical calculation predicted the blue dot. The units are $E_o = 1$ and $a_o = 1$.

In parametric representation, we get the red curve of **Figure 1(b)** where $R = 2x$. The measured separation of the protons is $R = 1.40a_o$ and the measured dissociation energy for $H_2 \to 2H$ is $0.329E_o$. This energy is determined with respect to the energy level $-2E_o$ of two separated hydrogen atoms [14]. Today, the dissociation energy of hydrogen molecules is known with very high precision [15]. **Figure 1** implies that both electrons are always moving in the medium plane of the protons. The orbital radius r and the distance d would thus be constantly increasing until the molecule is completely decomposed ($H_2 \to 2H^+ + 2e^-$). When this state defines the energy level $E = 0$, the ground state energy $E \to -2.329E_o$.

The first wave-mechanical treatment of H_2 molecules was performed by Heitler and London and published in 1927. They belonged to Schrödinger's group and demonstrated the power of his equation [16]. It was sufficient, indeed, to consider the sum and difference of atomic wave functions, to get constructive or destructive interference in the median plane of the protons. *Linear Combination of Atomic Orbitals* (LCAO) could thus account for the bound state and the first excited state. According to this approximation, the ground state would be situated at $E = -2.23E_o$ and $R = 1.51a_o$. These results were reported by Pauling and Wilson [17], who did extensively use this method for other molecular structures.

Recent quantum-mechanical calculations for H_2 provide excellent agreement with observations [18]. The probability density is then maximal near the proton, but increased in the median plane. Bohr's model indicates that it is sufficient to assume that the electrons are only moving in the median plane to get a bound state. This approximation applies to average positions, of course, though they are assumed to be well-defined. Schrödinger attributed Bohr's concept of "stationary states" to the existence of stationary waves. Since they yield a static charge distribution, they restored agreement with Maxwell's theory, but led also to the idea that covalent bonds do merely result from electrostatic effects. Ruedenberg insisted therefore in 1962 on the fact that *motions* of both electrons are essential for these bonds [19]. He did that by computing the quantum-mechanical average values of the potential energy V and the kinetic energy T. It appeared that $\langle V\rangle = -2\langle T\rangle$ and thus that $\langle E\rangle = -\langle T\rangle$. This is a generalization of (4) and the *virial theorem*, which was established already by Clausius in 1870 for any isolated system that is composed of charged particles and has reached its equilibrium state. Bacskay and Nordholm [20] did also perform tedious computations of quantum-mechanical average values for other divalent molecules. However, it is easy to verify that SQM accounts already for the virial theorem. It is merely due to Coulomb forces and independent of more or less detailed quantum effects. The word "virial" stems even from the Latin word for force, which survived in the adjective "virile".

2.2. Dissociation Process and Metastable Molecules

SQM has the advantage to describe what is essential during the dissociation of hydrogen molecules by means of a *modified Bohr model* (MBM). The two electrons are again assumed to move on circular orbits, but the orbital planes are separated, as shown in **Figure 2(a)**. The electrons are always moving as far as possible from one another. **Figure 2(b)** represents the limit of applicability of the BM. The value of r_1 is unknown, but $x_1 = x(r_1)$ as for the BM of **Figure 1**. The energy curve $E(R)$ is then bifurcating, since $E \to 0$ for the BM, while $E \to -2E_o$ for the MBM. **Figure 2(c)** shows that the MBM should allow for a *metastable state* when $x = x_2$, since two hydrogen atoms could polarize one another. The orbital plane is then separated from the median plane by the distance $z_2 < x_2$ and the orbital radius $\rho = \rho_2$.

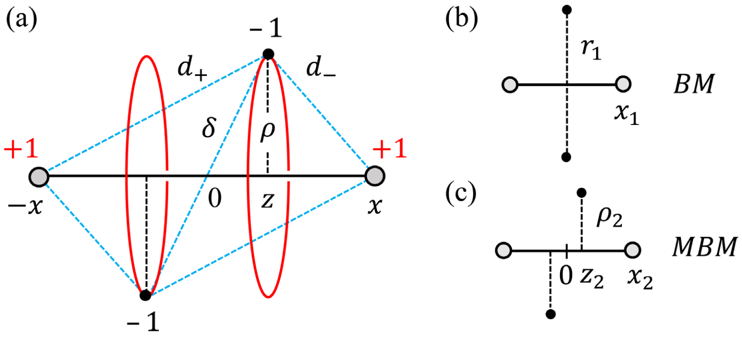

Figure 2. (a) The modified Bohr model (MBM) for H_2 molecules accounts for separated orbits of the electrons. (b) There is a limit of validity of the BM. (c) The dissociation process should allow for a metastable state for mutually polarizing hydrogen atoms.

Even the MBM of **Figure 2(a)** led to difficulties and it is useful to see the reasons. Svidzinsky and his collaborators treated this problem in 2005, by means of dimensional scaling [21]. The result was amazing, since the energy curve of **Figure 1(b)** was modified so that the minimum did coincide with the red dot. Such a precise agreement with experimental results without wave mechanics, could have been suspicious, but was published in several scientific journals. A didactical version appeared in Physics Today [22]. However, D-scaling was merely a hypothetical procedure, suggested by Witten to solve the riddle of elementary particles [23].

We mentioned already in the introduction that they can be distinguished from one another by means of empirically defined quantum numbers. Since this fact cannot be explained by conventional theories, it has been proposed that elementary particles could be strings, instead of points. These strings should even have peculiar structures, to allow for unobservable degrees of freedom. Another hypothesis was that space could have more than 3 dimensions. Momentum vectors do then have more components and the expression of kinetic energies is modified. However, when the number D of dimension is increasing, the limit $D \to \infty$ yields finite results. Witten recognized that "so far there has not been much tangible progress", but since it was possible to apply this formalism to hydrogen atoms [24], it seemed credible that it could also account for dissociating hydrogen molecules. However, the viral theorem cannot be satisfied when the kinetic energy T is modified, while the potential energy V is still defined by Coulomb forces. Moreover, the riddle of elementary particle physics can be solved by means of space-time quantization [7].

Yang and Hou did also examine the problem of dissociating hydrogen molecules [25]. Though their article was published in 2019, they ignored Svidzinsky's theory. They tried also to modify the BM, to get perfect agreement with experimental results, but they modified the potential energy V instead of the kinetic energy T. This would also contradict the virial theorem. Actually, they proposed that Coulomb interactions would be affected by screening effects. However, there are only 4 interacting particles for SQM.

Allmendinger considered the MBM in 2018, without modifying the expressions of V or T. This approach was realistic [26] and required that the energy is defined by

$$E_1(x, z, \rho) = \left(\frac{1}{x} + \frac{1}{\delta} - \frac{4}{d_+} - \frac{4}{d_-} + \frac{2a_o}{\rho^2} \right) E_o \tag{6}$$

The last term accounts for the kinetic energy of both electrons and the quantization rule for circular motions. It results also from **Figure 2(a)** that

$$\delta^2 = z^2 + \rho^2 \quad \text{and} \quad d_\pm^2 = (x \pm z)^2 + \rho^2$$

Since the electron orbits have to be radially and laterally stable,

$$\frac{\rho}{d_+^3} + \frac{\rho}{d_-^3} - \frac{2\rho}{(2\delta)^3} = \frac{a_o}{\rho^3} \quad \text{and} \quad \frac{x+z}{d_+^3} = \frac{2z}{(2\delta)^3} + \frac{x-z}{d_-^3} \tag{7}$$

Unfortunately, Allmendinger replaced the first condition (7) by the requirement that the forces applied on the protons should equilibrate one another. This is not necessary, since the energy (6) is calculated for various separations of positions of motionless protons. Computing the energy for several structures by Exel, Allmendiger found that the energy is minimal when

$$E_1(x,z,\rho)=E_1(0.705,0.488,0.892)=-2.127E_o$$

All distances are expressed in units a_o. Allmendiger did not consider the BM and was thus not aware that it yields a lower energy. To determine the metastable state, we have to account for both conditions (7) and require that the energy (6) yields a minimum for this state. Thus, $\partial E_1(x,z,\rho)/\partial x=0$. Solving these equations by Mathcad, we get

$$E_1(x_2,z_2,\rho_2)=E_1(0.817,0.706,0.9755)=-2.130E_o \tag{8}$$

These values define the metastable state of **Figure 2(c)**, but we would also like to know the value of x_1 in **Figure 2(b)**. SQM does even allow to describe the dissociation process, by introducing a new variable y to define the position of the proton for the MBM. The separation z between the orbital planes and the median plane of the protons is increasing so that $z\to x$ in an asymptotic way. The initial value of the orbital radius ρ is r_1 and its final value is $a_o=1$, but a metastable state would require that the total energy E is decreased by reducing the mutual repulsion of the electrons. These ideas are expressed by setting

$$x(y)=x_1+y \quad \text{where} \quad x_1=x(r_1) \tag{9}$$

$$z(y)=x(y)\left(1-\mathrm{e}^{-\alpha y}\right) \tag{10}$$

$$\rho(y)=1+(r_1-1+Ay)\left(1-\mathrm{e}^{-\alpha y}\right) \tag{11}$$

We get thus 4 adaptable parameters (α, r_1, A, y_2), where $y_2=x_2-x_1$. These parameters can be determined by solving the Equations (9)-(11) and (6) for the metastable state (8). These conditions yield

$$\alpha=42.468 \quad r_1=1.134 \quad A=12.545 \quad y_2=0.047$$

It follows that the branching point of the energy curves is situated at $x_1=x(r_1)=0.770$, well beyond $x_o=0.550$ for the ground state in **Figure 1(b)**. Svidzinsky's assumption led on the contrary to $x_1<x_o$ and did not account for a metastable state. The present results lead to **Figure 3(a)** for the functions $z(x)$ and $\rho(x)$. We see that dissociation occurs in an explosive way when $x=x_1$, since the orbital planes do then rapidly join the protons. The orbital radius ρ ceases to increase as for the BM and becomes rapidly equal to $a_o=1$ as in isolated hydrogen atoms, though the dissociation is not yet finished. The orbital radius ρ does not immediately decrease. There appears even a small initial increase. Since the mutual repulsion of the electrons is then decreased, it causes the existence of a metastable state, which is clearly indicated by the small potential well for the red curve in **Figure 3(b)**. The black curve shows that the BM remains valid in a large domain, since bifurcation of the energy curves occurs only when the separation $R=2x_1=1.54a_o$. **Figure 3(b)** accounts also for the fact that $E\to-2E_o$. This energy level is now replaced by $E=0$. It is approached in progressive way, since Coulomb forces have a quasi-infinite range. Their effects become only negligible when $R\approx 15$.

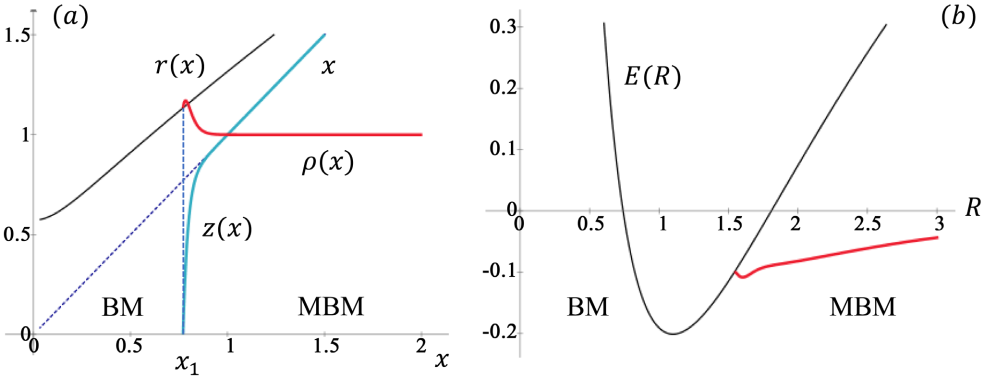

Figure 3. (a) The displacement z of the orbital planes with respect to the median plane does rapidly increase for the MBM. Even the radius ρ of circular obits is very soon the same as in isolated hydrogen atoms, but there is a small peak for the metastable state. (b) The red energy curve for the MBM of H_2 confirms its existence for mutually polarizing hydrogen atoms.

At present, it is possible to solve Schrödinger's equation for hydrogen molecules, by accounting even for correlated motions, as well as relativistic and quantum-electrodynamic effects [27]. This yields an energy curve that agrees with precise measurements of the dissociation energy and even with the infrared spectrum for vibrating hydrogen molecules [28]. Schrödinger's equation could also be solved for excited states of H_2 molecules [29]. However, it is astonishing that wave mechanics yields an energy curve that becomes suddenly flat, as if the dissociation $H_2 \to 2H$ were immediately complete. There is not even the slightest sign of a metastable sate. It might thus be useful to launch a more specific search in this regard.

3. The Tricky Problem of Hydrogen Molecular Ions

3.1. The BM and MBM for the Electron in H_2^+

Niels Bohr considered already the apparently simple case where only one electron is attracted by two protons. He adopted of course the model of **Figure 4(a)**, but found that H_2^+ would then be unstable [1, part III, p. 867]. It was not yet known that hydrogen molecular ions are slightly stable. The search of an explanation led to enormous difficulties. We begin therefore with Bohr's model. Dynamical stability requires that the force

$$F = \frac{2re^2}{d^3} = \frac{mv^2}{r} \quad \text{where} \quad d^2 = x^2 + r^2$$

The values of r and x are also determined by the quantization rule $rmv = n\hbar$. Thus,

$$d^3 = \frac{2r^4}{n^2 a_o}$$

For the ground state $n = 1$, the energy of a hydrogen molecular ion is

$$E_i = \left(\frac{1}{x} - \frac{4}{d} + \frac{a_o}{r^2}\right) E_o = E_i(r) \tag{12}$$

Since $x = x(r)$, parametric representation yields the red curve of **Figure 4(b)**, where $R = 2x$ is the separations of the protons. The ground state would thus be situated at the white dot, where $R = 1.731a_o$ and $E_i = -0.878E_o > -E_o$. According to the BM, hydrogen molecular ions would therefore be unstable. It should be noted that x has to be real, but that concerns only small values of R. The LCAO approximation did yield the blue dot, while experimental results are represented by the red dot.

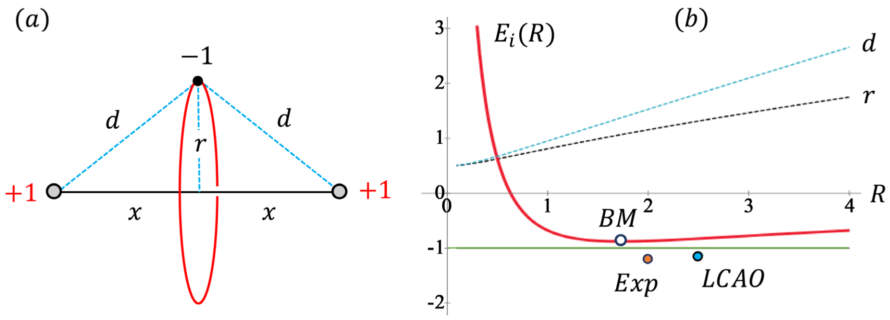

Figure 4. (a) The BM for H_2^+ assumes that the single electron is orbiting in the median plane of the protons. (b) The resulting ground state (white dot) is higher than experimental results (red dot) and the first wave-mechanical prediction (blue dot).

Since H_2^+ molecular ions are at least slightly stable, the initial BM has to modified. This can be done by adopting the model of **Figure 5(a)**. The modified energy is then

$$E_m(x,z,r) = \left(\frac{1}{x} - \frac{2}{d_+} - \frac{2}{d_-} + \frac{a_o}{r^2}\right)E_o \tag{13}$$

Radial and lateral stability of the electron orbit requires that

$$\frac{1}{d_+^3} + \frac{1}{d_-^3} = \frac{a_o}{r^4} \quad \text{and} \quad \frac{x+z}{d_+^3} = \frac{x-z}{d_-^3}$$

Bifurcation of the energy curves occurs when $E_m(x_1, 0, r_1) = E_i(r_1)$, while the lowest possible energy for the MBM is reached when $\partial E_m(x,z,\rho)/\partial x = 0$. The solution of these equations is

$$x_1 = 0.583 \quad r_1 = 0.871 \quad x_2 = 46.668 \quad z_2 = x_2 \quad \text{and} \quad \rho_2 = 1$$

Since $x_1 < 0.866$, bifurcation of the energy curves occurs now before reaching the white dot in **Figure 4(b)**. However, the dissociation process is again described by of (9)-(11). Thus,

$$\alpha = 99.413 \quad A = -1.624 \quad \text{and} \quad y_2 = x_2 - x_1 \approx 46$$

The resulting effects are represented in **Figure 5(b)**. Dissociation occurs when $R = R_1 = 2x_1 = 1.166a_o$. This process is explosive, since the displacement z of the orbital plane with respect to the median plane of the protons is suddenly increased. The electron does even immediately join the chosen proton ($z \to x$). The orbital radius ρ becomes immediately equal to a_o as in an isolated hydrogen atoms. Nevertheless, this electron is still attracted by the other proton. Their separation d_+ is increasing and the energy $E_m \to -E_o$ in a progressive way. Since the value of x_2 is enormous, polarization effects are negligible. Nevertheless, there does exist a metastable state, since the (black) energy curve E_i for the BM is replaced by the red curve when $R \geq R_1$.

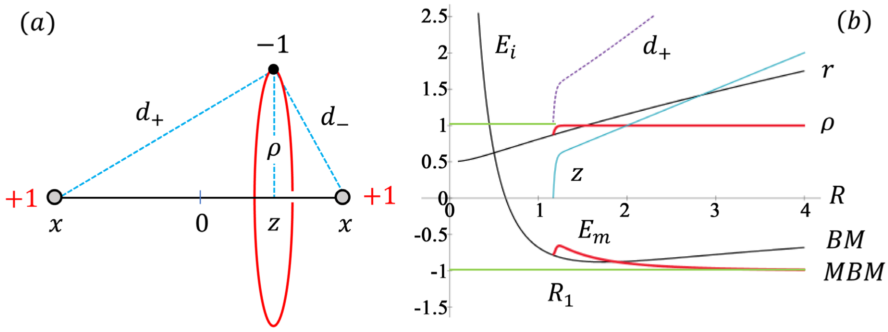

Figure 5. (a) The MBM for a dissociating H_2^+ molecule. (b) This model leads to a bifurcation of the energy curves and a metastable state when the separation of the protons $R = 2x = R_1$.

The sudden increase of the orbital radius ρ does only reduce the attraction of the electron by the departing proton. Hydrogen molecular ion would thus be slightly stable, but for a peculiar reason. We ignore if the resulting metastable state can be observed or not.

3.2. Wave-Mechanical Studies and Intensive Search of the Electron Orbits

A general introduction that insists on basic concepts, also for hydrogen molecules and molecular ions, was provided by Beiser [30]. Schrödinger's equation was solved in 2006 for H_2^+ with remarkable precision [31]. In 2021, the energy curves were computed for the ground state and several excited states with an accuracy of 40 digits [32]. The BM of **Figure 4(a)** was already abandoned very soon, to search for another orbit. This adventure was initiated by Sommerfeld, since he considered elliptical orbits for the single electron in hydrogen atoms. His excellent results suggested that the single electron, attracted by two protons in H_2^+ could be moving around both protons. It would then be sufficient to consider a particular sagittal plane. The ground state seemed to require a lemniscate. It is an 8-like orbit, but is not defined by some nice mathematical formula.

It results from Coulomb forces, when the electron is turning around both protons, but the electron can also keep them together by passing through the center. Since all sagittal planes are equally probable, this would generate two closed conical shells that touch one another. They would generalize Bohr's concept of spherical shells for hydrogen atoms. Sommerfeld advised thus his brilliant student *Wolfgang Pauli* to examine this problem for his PHD thesis. He accepted and used elliptical coordinates [33]. When the electron is separated from the protons by the distances r_1 and r_2 and when R is the separation of these protons, they are defined by

$$\xi = \frac{r_1 + r_2}{R} \quad \text{and} \quad \eta = \frac{r_1 - r_2}{R}$$

Any possible position of the electron is thus determined by the intersections of confocal ellipses and confocal hyperbola. However, Pauli used the first quantization rule (2) as Sommerfeld had done for elliptical orbits in hydrogen atoms. This approach led only to a classification of possible motions in 1922. The actual shape and size of the electron orbit for the ground state could not be determined. Karl Niessen came to the same conclusion [34]. These results did contribute to abandoning "old quantum mechanics", but the essential reason was the development of wave mechanics. Heitler and London did solve Schrodinger's equation by means of the LCAO approximation [10]. That is even simpler for one electron than for two electrons and presented in most textbooks on quantum mechanics. Since this procedure requires to calculate some integrals, it is useful to know how that can be done [35].

Burrau [36] did even solve Schrödinger's equation for stationary states of H_2^+ without any approximation. He did also use elliptical coordinates, since Schrödinger's equation yields then two separable equations. Computations were not easy with available tools, but Burrau concluded that the ground state would be situated at $E = -1.20E_o$ and $R = 2.0a_o$. Grivet presented in 2002 a method for simplifying the numerical calculations [37]. It appeared then that the differential equation for ξ led everywhere to well-behaved solutions, but the other differential equation did only yield precise results for low and high values of η. The computed curves did even meet with an unphysical discontinuity for an intermediate value of η. Grivet proposed an interpolation procedure to overcome this difficulty. Actually, he discovered a much more profound problem.

Strand and Reinhardt [38] presented in 1979 a very thorough and detailed study of this issue. They thought that the *semiclassical* approximation of wave mechanics is more realistic than the assumption of sharply defined positions in old quantum mechanics. The WKB approximation of wave mechanics leads, indeed, to Newtonian laws of motion for any trajectory of an electron. Since the average position is then defined by a wave packet, it accounts for Heisenberg's uncertainty relations. However, a wave packet can penetrate into the walls of a potential well. The separation of the turning points for the most probable position of the electron is then greater than when the electron is merely reflected by these walls. Strand and Reinhardt adopted therefore the quantization rule

$$\oint p_i \mathrm{d}q_i = \left(n_i + \alpha_i\right) h \tag{14}$$

It is a generalization of the first relation (2). For parabolic potential wells, $\alpha_i = 1/2$. Rotation around the symmetry axis requires an angular variable φ, but $\alpha_i = 0$ for this degree of freedom. Even these precautions did merely yield a classification of possible orbital motions. The expected 8-like orbit could be partially determined, but there appeared a "gap" in the region where the separation of the protons $R \approx 2a_o$. This is precisely the region where the ground state is situated, according to experimental results. That was a disappointing result and the cause of this failure was not explained.

About a dozen other authors tried thus to circumvent the enigmatic obstacle, but we mention only the enduring effort of Knudson. In 2006, he published a review for chemists [39], where he mentioned that "the motivation for such studies is the insight into the quantum behavior offered by the classical viewpoint". However, new computations could only confirm the existence of a "gap" in the critical region. It was even quite large ($0.83a_o < R < 2.30a_o$) for H_2^+. Knudson suggested that this defect might be due to the "inability to account for electron tunneling". He reanalyzed this problem [40] by modifying (14) to get two quantum numbers (n_i and m_j). This increased the flexibility of the semiclassical approximation, but the "gap" was still there, even for HeH^{2+} and for LiH^{3+}. Knudson returned to this nagging problem in 2022, as emeritus [41]. More computations were presented, but the gap did stubbornly resist. Knudson recognized then that this "disagreement… is not just quantitative, but qualitative in nature". He concluded even that "old quantum mechanics does not work… for the ground state near its known equilibrium position". However, he added that the concept of electron orbits is not totally useless. Orbital motions are more intuitive than probability distributions.

It is also noteworthy that the problem of dynamically stable closed orbits was already raised by Euler in 1760 for gravitational forces in classical mechanics. This apparently simple problem was treated by eminent scientists, to no avail. Wild [42] has shown that the differential equations of motion can be solved by means of personal computers. It is sufficient to proceed step by step for given initial conditions, but this applies to open orbits. It is even well-known that continued motions will become chaotic. Stability requires closed orbits. They were computed by Arensdorf for satellites turning around the Earth and the Moon [43]. They were not quantized and could have different sizes and display several lobes of variable shape.

3.3. Rehabilitation of Simple Quantum Mechanics

The LCAO approximation of wave mechanics did solve Schrödinger's equation for stationary states, but implied that the electron can be close to both protons with equal probabilities. The resulting probability distribution was static. However, Feynman proved that it can oscillate [44]. This requires to solve the time-dependent Schrödinger equation, which is possible and indicates that the electron is not simultaneously, but *alternatively* close to these protons. Feynmann called this a "flip-flop model". It did innovate quantum-chemistry, but provides also a powerful justification of orbital motions. However, Pauli and Niessen, Strand and Reinhardt, as well as Knudson and other authors had not succeeded to determine the orbit when the electron does successively move around the protons.

There are several reasons. The use of elliptical coordinates suggested that separated differential equations do allow for different quantization rules. This led to imposing the first relation (2), even when the electron is attracted by two protons. The second relation (2) requires only one quantum number and is justified by de Broglie's interpretation of Bohr's quantization rule. It applied to circular orbits, but can be generalized for any closed orbit. The momentum vector $\boldsymbol{p}$ is everywhere tangential to this orbit and applies also to a progressively varying wavelength $\lambda = h/p$. It is thus sufficient that

$$\oint p\mathrm{d}s = nh \quad \text{where} \quad (p\mathrm{d}s)^2 = (\dot{x}\mathrm{d}x)^2 + (\dot{y}\mathrm{d}y)^2$$

This applies to Cartesian coordinates and the chosen unit of the electron mass ($m = 1$). Since $\mathrm{d}x = \dot{x}\mathrm{d}t$ and $\mathrm{d}y = \dot{y}\mathrm{d}t$, the quantization condition is

$$\int_0^{T_0} V_o^2 \mathrm{d}t = nh \quad \text{where} \quad V_o^2 = V_x^2 + V_y^2 \tag{15}$$

V_o is the speed of the electron and T_o is the period for motions on the closed orbit. We might object that Newton's laws of motion are not compatible with Heisenberg's uncertainty relations. That is not true, since the electron can move on a well-defined orbit, though we ignore where it is situated at some particular instant. In other words, we have to abandon the idea that Newton's laws of motion can *only* be solved by providing initial conditions. That is not necessary, even for a vibrating string, since it is possible to consider the general solution with adaptable parameters. Their values are then determined by boundary conditions and not by initial conditions.

It was also believed that the semiclassical approximation of wave mechanics has to be used with the quantization rule (14). That leads to complications, which are not necessary to account for Heisenberg's uncertainty relations. According to classical mechanics, a harmonic oscillator can be at rest at its equilibrium position. That is excluded in wave mechanics, by means of a zero-point energy and α_i in (14). However, for orbital motions it is automatically excluded that an electron could be somewhere at rest. Condition (15) is sufficient.

In 2008, it was claimed [45] that old quantum mechanics was abandoned for "wrong reasons". That is true, but not because of the proposed linear oscillations of the electron along the interproton axis. They are mathematically possible, but the turning points would be situated beyond the protons and thus require that the electron can pass through these protons. That is impossible. The electron has to turn around them, but that requires specific developments.

3.4. Computed Orbits of the Electron in H_2^+

To determine the orbit of a single electron, moving around two protons in an arbitrarily chosen sagittal plane, we can use Cartesian coordinates (x, y). The motionless protons are situated at ($\pm c, 0$) and attract the electron by Coulomb forces. The resulting potential energy of the electron is

$$V(x,y) = -\frac{1}{d} - \frac{1}{D} \quad \text{where} \quad d^2 = (c-x)^2 + y^2 \quad \text{and} \quad D^2 = (c+x)^2 + y^2$$

Near the center, we get thus

$$V(x,0) = -\frac{1}{c-x} - \frac{1}{c+x} \approx -\frac{2}{c^2} - \frac{2x^2}{c^4} \quad \text{and} \quad V(0,y) \approx -\frac{2}{c^2} + \frac{2y^2}{c^4}$$

At the center (0, 0), the potential is $-2/c^2$, but it is parabolically decreasing along the *x*-axis and parabolically increasing along the *y*-axis. The center is thus a saddle point. Oscillations on the *y*-axis are excluded, since they would be unstable. The coordinates *x*(*t*) and *y*(*t*) have thus to describe orbital motions. Newton's laws of motion yield two coupled equations:

$$F_x = \frac{c-x}{d^3} - \frac{c+x}{D^3} = \ddot{x} \quad \text{and} \quad F_y = \frac{-y}{d^3} + \frac{-y}{D^3} = \ddot{y} \tag{16}$$

Since the functions *x*(*t*) and *y*(*t*) are periodic, they can be expressed by Fourier series. Closed orbits are thus *Lissajous curves*. Such an orbit can pass through the center, but near the center

$$F_x = \frac{4x}{c^3} = \ddot{x} \quad \text{and} \quad F_y = \frac{-2y}{c^3} = \ddot{y} \tag{17}$$

The first equation does not allow for a single sine function and it would be arbitrary to assume that this is possible for *y*(*t*). The simplest general solution of (16) is thus

$$x(t) = a\left[\sin(\theta) - k\sin(3\theta)\right] \quad \text{and} \quad y(t) = b\left[\sin(2\theta) - K\sin(4\theta)\right] \tag{18}$$

It is not necessary to assume that this motion results from initial condition, as for a projectile that would be thrown or shot from the center or some other point with a precisely computed velocity to get a closed orbit. According to (18), the electron is passing thought the origin when $\theta = 0$, but we can set $\theta = \omega t + \phi$, where ϕ has any constant value. The period would always be $T_o = 1/2\omega$. We consider thus motions that are characterized by adaptable parameters. Since (18) has to be compatible with (17), it is necessary that

$$k = \frac{4+\mu}{3(4+3\mu)} \quad \text{and} \quad K = \frac{1-2\mu}{2(1-8\mu)} \quad \text{where} \quad \mu = \omega^2 c^3 \tag{19}$$

The parameter μ is a constant of motion, which indicates that smaller separations of the protons require higher angular frequencies. The value of k is always quite small and positive, while the value of K can diverge and change sign. The general solution (18) implies that *x*(*t*) will reach its maximal value $x_o = a(1+k)$ when $\theta = \pi/2$. Since (16) has to be satisfied at this turning point,

$$\frac{1}{(x_o - c)^2} + \frac{1}{(x_o + c)^2} = \omega^2 a[1 + 9k] \tag{20}$$

The turning points for *y*(*t*) are reached when $V_y = 0$ and thus already when $\theta = \tau$ and

$$\cos(2\tau) - 2K\cos(4\tau) = 0 \tag{21}$$

The values of the coordinates x and y are then

$$X = a\left[\sin(\tau) - k\sin(3\tau)\right] \quad \text{and} \quad Y = b\left[\sin(2\tau) - K\sin(4\tau)\right]$$

The distances d and D are there defined by

$$d^2 = (c - X)^2 + Y^2 \quad \text{and} \quad D^2 = (c + X)^2 + Y^2$$

The equations of motion (16) require therefore that

$$\frac{c - X}{d^3} - \frac{c + X}{D^3} = -a\omega^2 \left[\sin(\tau) - 9k \sin(3\tau) \right] \tag{22}$$

$$\frac{Y}{d^3} + \frac{Y}{D^3} = 4b\omega^2 \left[\sin(2\tau) - 4K \sin(4\tau) \right] \tag{23}$$

The actual orbit has also to be compatible with the quantization condition (15). It requires merely integration of squares and products of sine or cosine functions over one period. It is thus sufficient to consider average values. They yield the relation

$$\omega^2 \left[a^2 \left(1 + 9k^2\right) + 4b^2 \left(1 + 4K^2\right) \right] = n\hbar \tag{24}$$

Using units where $E_o = a_o = m = 1$, it follows that $\hbar^2 = e^2 = 2$. Since k and K are function of μ, there remain only 5 parameters (a, b, c, μ, τ). Their values are determined by Equations (20)-(24). It follows that

$$a = 1.026 \quad b = 0.031 \quad c = 0.622 \quad \mu = 0.133 \quad \tau = 0.407 \quad \text{for} \quad n = 1$$

$$a = 1.728 \quad b = 0.88 \quad c = 1.413 \quad \mu = 1.044 \quad \tau = 0.857 \quad \text{for} \quad n = 2$$

The resulting orbits are represented in Figure 6. It is thus possible to determine electron orbits that are dynamically stable and quantized, but we get only a simple 8-like orbit for the exited state.

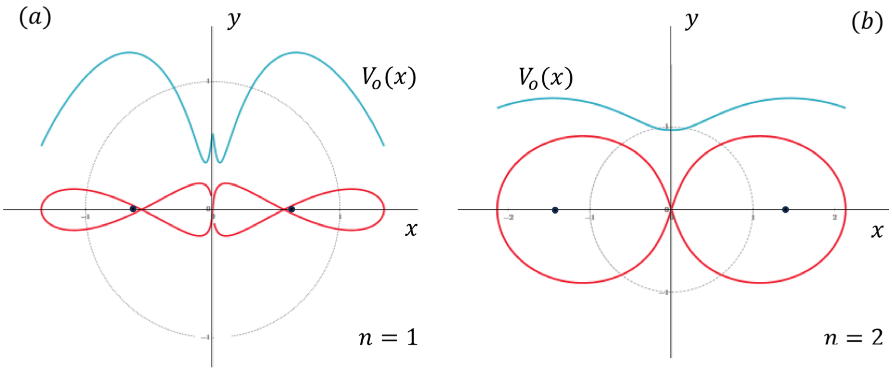

Figure 6. (a) The electron orbit for the ground state (in red) and its speed (in blue). (b) The electron orbit and the speed for the first exited state of hydrogen molecular ions.

Figure 6(a) SQM determines the orbit of the electron for the ground state of hydrogen molecular ions. This orbit (red line) defines all possible positions of the moving electron and not where it is situated at a particular instant. (b) The first excited state allows for an 8-like orbit and the separation of the protons (represented by black dots) is greater. The scales are indicated by light gray circles of radius a_o. The speed of the electron (blue curves) varies more for the ground state than for the excited state.

The ground state requires thus a double 8-like orbit and that the electron does pass very close to the protons. It is then strongly accelerated but slows down when it approaches the potential barrier between the adjacent wells. The predicted separation $R = 2c$ of the protons is then only $1.24a_o$ for the ground state and thus notably smaller than the measured value. The BM or SQM is much less useful for a single electron than for electron pairs. Nevertheless, it is possible to determine the orbit. The total energy E is then

$$E = \frac{1}{2c} - \frac{1}{d} - \frac{1}{D} + \frac{1}{2}V_o^2 = E(a, b, c, \mu, \theta)$$

It is not a constant of motion, but when all positions are equally probable on the computed orbits, the average value $\langle E \rangle = -2.53E_o$ for the ground state. This value is determined with respect to the energy level $E = 0$ for complete dissociation, but is much lower than the experimentally measured value in **Figure 4(b)**. Because of **Figure 1(b)**, it is obvious that SQM yields a better approximation for an *electron pair* in the median plane than for a single electron that is alternatively turning around both protons. For the excited state, the separation of the protons would be $2.8a_o$ and the average energy $\langle E \rangle = 0.06E_o$. The angular frequencies are respectively $\omega = 0.743$ and $\omega = 0.220$ for the ground state and the excited state. The essential result is, of course, that the electron orbit in H_2^+ could not be determined during more than 100 years, but is possible by means of conceptual clarifications.

We considered also motions that are symmetric with respect to the median plane, instead of being antisymmetric with respect to the center. They would be described by the functions

$$x(t) = a\sin(\theta) \quad \text{and} \quad y(t) = b\left[\cos(\theta) - \sigma\cos(3\theta)\right]$$

The electron does then pass through the median plane when $y = b(1-\sigma)$. This could happen at the center when $\sigma = 1$, but also without touching the interproton axis or by crossing it. We established the required equations, but found no acceptable solution for this kind of quantized motions. That is not required anymore. It is more useful to spare some time for basic considerations.

4. Conclusions and the Meaning of Electron Orbits

A discovery of phenomena that cannot be explained by already existing theories, requires the construction of a new one. It may not be easy to discover the needed concepts. Fortunately, it was possible to progress by successive approximations. This applies also to "old quantum mechanics", which should not be depreciated, but reconsidered in a broader context. It appeared also in the course of this research that there were hampering misunderstandings.

It is even necessary to become aware of the fact that, in general, we are too easily distracted or blinded by *preconceptions*. This did not only happen when it was believed that the Earth is the center of our Universe. At present, we know that the development of the theory of relativity and quantum mechanics revealed the existence of two universal constants (c and h). They impose restrictions on some types of measurements. Nevertheless, we continue to believe that it should be possible to measure always smaller and smaller space-time intervals, without ever reaching a finite limit. This assumption allowed us to use differential equation, but they do not prove the existence of a "space-time continuum". Today, it is more plausible that there does exist a *quantum of length* (a) that is also a universal constant, though its value is not yet known and could be extremely small.

Variations of wave functions and fields in space and time can then only be described by means of finite-difference equations. Their physical meaning results from generalizing the definition of local values of the components of the momentum vector $\boldsymbol{p}$ and the value of the instantaneous energy E of any particle. This theory of space-time quantization (STQ) is logically consistent and explains mysterious facts [7]. They are at least partly known and appear already as being of fundamental importance, in particular for understanding the nature of dark matter.

There are other examples of preconceptions. We recall what happened for "water memory" [46]. Careful experimental investigations had proven that when some types of biologically active molecules are dissolved in pure water and repeatedly diluted, the resulting water does still display the same effects. That was declared to be impossible, since all active molecules have been eliminated and since we "know" that thermal agitation of water molecules in the liquid state prevents any structuring. It would even have to be specific for different types of diluted molecules. Homeopathy had already revealed the efficiency of this procedure, but the underlying mechanism was not understood. Instead of trying to discover what is really happening, it was merely declared that all observed facts are illusions. The medical doctor who proved the reality of water memory was even treated by the editor of a famous scientific journal and a professional magician in a radically unscientific way.

Actually, water molecules are known to be electric dipoles. They can thus constitute crystals, like magnetic dipoles in ferromagnetic materials. However, electric dipoles can only be ordered inside very small spheres. We proved that in a theoretical way and drew then logical conclusions. The nano-sized ice crystals are stronger electrical dipoles and are thus spontaneously aligned. The constitution of these filaments is initiated by dipolar parts of the initially dissolved biologically active molecules. These parts oscillate at very low frequency, depending on the type of molecules. They produce standing waves on detached chains when they have reached the appropriate length. All chains have thus the same length, but a part of them is broken by vigorous succussions after every dilution. However, all broken parts grow again until they reach the same length as the unbroken chains. This results from their collectively generated electric field. The number of tuned chains is thus progressively increased and they produce the same electric signal as the initially dissolved molecules. This secret could have been discovered long ago, but that was prevented by preconceptions and arrogance.

The case of virus destruction by resonance and missed treatment of cancer by

EM waves [47], the explanation of the ball-lightning phenomenon [48] or cold fusion and biotransmutations [49] are other examples, demonstrating the negative power of prejudices. Skepticism is necessary, of course, but also in regard to our own convictions. That is not always easy, but possible. Even the treatment of "simple quantum mechanics" is instructive, since it required some very important conceptual clarifications. Though SQM is merely an approximation of wave mechanics, it is logically consistent and combines classical mechanics with Heisenberg's uncertainty relations in an interesting way. This approach could even be useful to tackle complicated problems by focusing attention on essential features. In solid-state physics, for instance, it is customary to adopt the "independent electron model". It assumes that every electron is only subjected to the average force, exerted by all other electrons in a lattice of ion cores. Are correlated motions and the formation of electron pairs really impossible?

Even the concept of *electron orbits* merits attention. Werner Heisenberg reported a discussion that he had in this regard with Albert Einstein [50]. Immediately after a meeting in Berlin, where he had presented matrix mechanics, Einstein invited him to his home for a private discussion. He appreciated Heisenberg's ingenuity, but was more than astonished that electron orbits should not be real, since the path of electrons is visible in cloud chambers. Heisenberg answered that the trajectory of electrons cannot be observed inside atoms and that physical theories should only be concerned with what is observable. Spectroscopic data provides at least a substitute (Ersatz) for the customary concept of trajectories. Einstein said, "You do not seriously believe that a physical theory can only accept what is observable." Heisenberg was surprised and answered: "I thought that just you adopted this idea for the foundation of your theory of relativity."

Einstein admitted that this interpretation is possible, but his purpose had been to describe reality. He was even profoundly convinced that "from the standpoint of principles, it is not correct to build a theory only on observables". In other words, he considered that reality is vaster than what can be observed from a particular point of view. Heisenberg insisted that our knowledge about the behavior of electrons in atoms does only result from transitions between quantized states. Einstein said, "You are only talking about what we know about Nature… and not about what Nature really does." Is reality more fundamental than our limited knowledge of it? This question is not a trivial one.

Less than one year later, Schrödinger presented his wave mechanics. The basic concept was there a function that varies in a continuous way in space and time. It has a real and an imaginary part, but the square of the absolute value of this wave functions defines a density that obeys a conservation law. Max Born realized that wave functions are only tools for making *probabilistic* predictions. It took some time to understand why this conservation law is not valid in relativistic quantum mechanics. At sufficiently high energies, electrons can be created or annihilated, but the essential point was that the outcome of precise position measurements is not always predictable. That was new.

Schrödinger did not like matrix mechanics, since he thought that wave functions provide a more realistic description of the behavior of electrons at atomic scales. He was thus invited to Copenhagen, where Bohr insisted that only "quantum jumps" are relevant. Heisenberg was present during these discussions, which reminded him of Einstein's objection. It was thus necessary to find out if it is really possible to observe the trajectory of an electron by other means than spectroscopic ones. This question led him to establish his famous uncertainty relations. They limit *simultaneous* knowledge of the position and velocity of a particle, because of the finite value of the quantum of action h. It stressed the importance of observables and the need of a radically new perception of reality and possible knowledge. That was a tremendous paradigm shift.

Since Einstein was not convinced, Heisenberg concluded that it is "infinitely difficult to abandon ideas that were hitherto adequate for scientific thinking and research". That is true, but we have to add that Einstein did keenly grasp what was radically new: the outcome of some types of measurements would be random and that contradicted past experience: *Gott würfelt nicht*! Quantum physics became the first physical theory that concerns *knowledge*. It should be noted that this knowledge is not merely limited, but richer. Wave functions have a real and an imaginary part at every point in space. That is much more than amplitude and phase. It appeared even that non-relativistic quantum mechanics accounts for the spin of point-like particles. This observable was unknown in classical mechanics and has an ensemble of possible values. Space-time quantization considers an irreducible "quantum of length" and abandons thus the concept of continuous functions, but that is precisely why there are more observables, characterizing elementary particles. Some of them had been experimentally discovered, but remained unexplained.

What is now the status of electron orbits? First of all, we have to recognize that this concept is similar to the concept of "light rays". They remain useful tools, though we know that there are light waves that can interfere. They are even EM waves and there are photons. The concept of quantized electron orbits remains valid as an approximation, but closed orbits are quantized. Feynman did even derive quantum mechanics from the idea that a particle can move from a point A to another point B by an infinity of conceivable paths [51]. Nature can be viewed and described in various ways. There is not only one possibility. Theories are thus adaptable. It is even remarkable that our understanding of the complexities of reality can be discovered and understood in a progressive way. There are already signs that reality is more complex than we think at present, because of unconventional technologies that are observable, but these facts are not easily accepted.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

References

[1] Planck, M. (1906) Vorlesungen über die Theorie der Wärmestrahlung. Legare Street Press.

[2] Bohr, N. (1911) Studier over Metallernes Elektrontheori. Ph.D. Thesis, University of Copenhague.

[3] Drude, P. (1900) Zur Elektronentheorie der Metalle. *Annalen der Physik*, **306**, 566-613. https://doi.org/10.1002/andp.19003060312

[4] Wilson, W. (1915) LXXXIII. The Quantum-Theory of Radiation and Line Spectra. *The London*, *Edinburgh*, *and Dublin Philosophical Magazine and Journal of Science*, **29**, 795-802. https://doi.org/10.1080/14786440608635362

[5] Sommerfeld, A. (1915) Zur Theorie der Balmerschen Serie, Münchener Akad. https://www.zobodat.at/pdf/Sitz-Ber-Akad-Muenchen-math-Kl_1915_0425-0458.pdf

[6] Ishiwara, J. (1915) Die universelle Bedeutung des Wirkungsquantums. *Physical Society of Japan*, **8**, 106-116. https://www.jstage.jst.go.jp/article/ptmps1907/8/4/8_4_106/_pdf

[7] Einstein, A. (1917) Zum Quantensatz von Sommerfeld und Epstein. *Deutsche Physikalische Gesellschaft*. *Verhandlungen*, **19**, 82-92.

[8] The Nobel Prize in Physics. https://www.nobelprize.org/prizes/physics/1929/broglie/biographical/

[9] Schrödinger, E. (1926) Quantisierung als Eigenwertproblem. *Annalen der Physik*, **384**, 489-527. https://doi.org/10.1002/andp.19263840602

[10] Born, M. (1926) Quantenmechanik der Stoßvorgänge. *Zeitschrift für Physik*, **38**, 803-827. https://doi.org/10.1007/bf01397184

[11] Heisenberg, W. (1925) Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen. *Zeitschrift für Physik*, **33**, 879-893. https://doi.org/10.1007/bf01328377

[12] Heisenberg, W. (1927) Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik. *Zeitschrift für Physik*, **43**, 172-198. https://doi.org/10.1007/bf01397280

[13] Meessen, A. (2021) Elementary Particles Result from Space-Time Quantization. *Journal of Modern Physics*, **12**, 1573-1605. https://doi.org/10.4236/jmp.2021.1211094

[14] Liu, J., Salumbides, E.J., Hollenstein, U., Koelemeij, J.C.J., Eikema, K.S.E., Ubachs, W., *et al.* (2009) Determination of the Ionization and Dissociation Energies of the Hydrogen Molecule. *The Journal of Chemical Physics*, **130**, Article ID: 174306. https://doi.org/10.1063/1.3120443

[15] Sprecher, D., Jungen, C., Ubachs, W. and Merkt, F. (2011) Towards Measuring the Ionisation and Dissociation Energies of Molecular Hydrogen with Sub-MHZ Accuracy. *Faraday Discussions*, **150**, 51-70. https://doi.org/10.1039/c0fd00035c

[16] Heitler, W. and London, F. (1927) Wechselwirkung neutraler Atome und homöopolare Bindung nach der Quantenmechanik. *Zeitschrift für Physik*, **44**, 455-472. https://doi.org/10.1007/bf01397394

[17] Pauling, L. and Wilson, E.B. (1935) Introduction to Quantum Mechanics with Applications to Chemistry. McGraw-Hill.

[18] Pachucki, K. and Komasa, J. (2016) Schrödinger Equation Solved for the Hydrogen Molecule with Unprecedented Accuracy. *The Journal of Chemical Physics*, **144**, Article ID: 164306. https://doi.org/10.1063/1.4948309

[19] Ruedenberg, K. (1962) The Physical Nature of the Chemical Bond. *Reviews of Modern Physics*, **34**, 326-376. https://doi.org/10.1103/revmodphys.34.326

[20] Bacskay, G.B. and Nordholm, S. (2013) Covalent Bonding: The Fundamental Role of the Kinetic Energy. *The Journal of Physical Chemistry A*, **117**, 7946-7958. https://doi.org/10.1021/jp403284g

[21] Svidzinsky, A.A., Scully, M.O. and Herschbach, D.R. (2005) Simple and Surprisingly Accurate Approach to the Chemical Bond Obtained from Dimensional Scaling. *Physical Review Letters*, **95**, Article ID: 080401. https://doi.org/10.1103/physrevlett.95.080401

[22] Svidzinsky, A., Scully, M. and Herschbach, D. (2014) Bohr's Molecular Model, a Century Later. Physics Today, **67**, 33-39. https://doi.org/10.1063/pt.3.2243

[23] Witten, E. (1980) Quarks, Atoms, and the 1/N Expansion. *Physics Today*, **33**, 38-43. https://doi.org/10.1063/1.2914163

[24] Chen, G., Ding, Z., Lin, C., Herschbach, D. and Scully, M.O. (2010) Variational Justification of the Dimensional-Scaling Method in Chemical Physics: The H-Atom. *Journal of Mathematical Chemistry*, **48**, 791-811. https://doi.org/10.1007/s10910-010-9710-6

[25] Yang, Z. and Hou, J. (2019) Calculating the Ground State Energy of Hydrogen Molecules and Helium Hydride Ions Using Bohr's Quantum Theory. *European Journal of Physics*, **40**, Article ID: 065405. https://doi.org/10.1088/1361-6404/ab32ce

[26] Allmendinger, T. (2018) The Elucidation of the Ground State in the H-Atom-Model of Niels Bohr and Its Application on the Bond-Length Computation in the H_2-Molecule. *International Journal of Molecular and Theoretical Physics*, **2**, 1-10. https://doi.org/10.15226/2576-4934/2/1/00109

[27] Puchalski, M., Komasa, J. and Pachucki, K. (2017) Relativistic Corrections for the Ground Electronic State of Molecular Hydrogen. *Physical Review A*, **95**, Article ID: 052506. https://doi.org/10.1103/physreva.95.052506

[28] Roueff, E., Abgrall, H., Czachorowski, P., Pachucki, K., Puchalski, M. and Komasa, J. (2019) The Full Infrared Spectrum of Molecular Hydrogen. *Astronomy & Astrophysics*, **630**, A58. https://doi.org/10.1051/0004-6361/201936249

[29] Nakashima, H. and Nakatsuji, H. (2018) Solving the Schrödinger Equation of Hydrogen Molecule with the Free Complement-Local Schrödinger Equation Method: Potential Energy Curves of the Ground and Singly Excited Singlet and Triplet States, Σ, Π, Δ, and Φ. *The Journal of Chemical Physics*, **149**, Article ID: 244116. https://doi.org/10.1063/1.5060659

[30] Beiser, A, (1963) Concepts of Modern Physics. McGraw-Hill.

[31] Scott, T.C., Aubert-Frécon, M. and Grotendorst, J. (2006) New Approach for the Electron Energies of the Hydrogen Molecular Ion. *Chemical Physics*, **324**, 323-338.

[32] Fernandez, F.M. and Garcia, J. (2021) Highly Accurate Potential Energy Curves for the Hydrogen Molecular Ion. *ChemistrySelect*, **6**, 9527-9534.

[33] Pauli, W. (1922) Über das Modell des Wasserstoffmolekülions. *Annalen der Physik*, **373**, 177-240. https://doi.org/10.1002/andp.19223731102

[34] Niessen, K.F. (1923) Zur Quantentheorie des Wasserstoffmolekülions. *Annalen der Physik*, **375**, 129-134. https://doi.org/10.1002/andp.19233750205

[35] Fitzpatrick, R. (2010) H_2^+. https://farside.ph.utexas.edu/teaching/qm/Quantum/node100.html

[36] Burrau, Ø. (1927) Berechnung des Energiewertes des Wasserstoffmolekül-Ions H_2^+

im Normalzustand. *Det Kgl Danske Videnskabernes Selskab*, **7**, 2-18. https://gymarkiv.sdu.dk/MFM/kdvs/mfm%201-9/mfm-7-14.pdf

[37] Grivet, J. (2002) The Hydrogen Molecular Ion Revisited. *Journal of Chemical Education*, **79**, 127-132. https://doi.org/10.1021/ed079p127

[38] Strand, M.P. and Reinhardta, W.P. (1979) Semiclassical Quantization of the Low Lying Electronic States of H_2^+. *The Journal of Chemical Physics*, **70**, 3812-3827. https://doi.org/10.1063/1.437932

[39] Knudson, S.K. (2006) The Old Quantum Theory for H_2^+: Some Chemical Implications. *Journal of Chemical Education*, **83**, 464-472. https://doi.org/10.1021/ed083p464

[40] Buehler, E.J., Gooch, E.E., Dial, J.L. and Knudson, S.K. (2000) Semiclassical Energies of Low-Lying States of One-Electron Diatomics. *Chemical Physics*, **253**, 219-230. https://doi.org/10.1016/s0301-0104(00)00006-9

[41] Knudson, S.K. (2022) The Old Quantum Theory for One-Electron Diatomic Ions and Molecules.

[42] Wild, W.J. (1980) Euler's Three-Body Problem. *American Journal of Physics*, **48**, 297-301. https://doi.org/10.1119/1.12144

[43] Genova, A.L. and Aldrin, B. (2015) A Free-Return Earth-Moon Cycler Orbit for an Interplanetary Cruise Ship. https://ntrs.nasa.gov/api/citations/20150018049/downloads/20150018049.pdf

[44] Feynman, R.P. (1963) Other Two-State Systems. *The Feynman Lectures on Physics*, *Quantum Mechanics*, **III**.

[45] Bucher, M. (2008) Rise and Premature Fall of the Old Quantum Theory. https://arxiv.org/abs/0802.1366

[46] Meessen, A. (2018) Water Memory Due to Chains of Nano-Pearls. *Journal of Modern Physics*, **9**, 2657-2724. https://doi.org/10.4236/jmp.2018.914165

[47] Meessen, A. (2020) Virus Destruction by Resonance. *Journal of Modern Physics*, **11**, 2011-2052. https://www.scirp.org/pdf/jmp_2020122516060286.pdf

[48] Meessen, A. (2023) Explanation of Ball Lightning by Plasma Oscillations. *Journal of Modern Physics*, **14**, 1355-1381. https://doi.org/10.4236/jmp.2023.1411078

[49] Meessen, A., (2023) Explanation of Cold Fusion and Biotransmutations. *Journal of Modern Physics*, **14**, 1087-1116. https://www.scirp.org/pdf/jmp_2023062914321461.pdf

[50] Heisenberg, W, (1969) Der Teil und das Ganze. Piper.

[51] Feynman, R.P. (1948) Space-Time Approach to Non-Relativistic Quantum Mechanics. *Reviews of Modern Physics*, **20**, 367-387. https://doi.org/10.1103/revmodphys.20.367