

The Uncertainty Principle and Covalent Bonding

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Abstract: A conceptually correct model for covalent bonding, suitable for teaching at the undergraduate general chemistry level, is presented. The quantum mechanical basis for the stability of the covalent bond can be derived from a qualitative discussion of the uncertainty principle, which relates the electron's spatial confinement to its kinetic energy. The qualitative discussion is backed by quantitative data obtained from the analytical quantum mechanical solution of the H_2^+ molecule. In addition, the stability of molecules is used as a tangible background against which the inferences emerging from the philosophical debate between classical determinism and the Copenhagen interpretation can be tested.

The covalent bond is a central concept in chemical thinking, which students need to acquire early on in the chemistry curriculum. When it is first mentioned in most textbooks, it is vaguely introduced as a force that “holds” two atoms together. Later on, a more detailed discussion about the nature of the forces involved in this “holding” are discussed. Typically, the H_2^+ molecule serves as a prototype for this discussion, and the electrostatic interactions between the two protons and the electron are analyzed. Through the years, several chemistry education papers have argued against this oversimplified model of covalent bonding as presented in general chemistry textbooks [1–6]. Nevertheless, a look at a selection of recent textbooks [7–11] reveals that not much has changed in this regard. All these textbooks still use a purely classical electrostatic explanation for the stability of the covalent bond, despite the fact that the state of electrons in chemical systems can only be described in the context of quantum theory and its postulates. The probable reason for the persistence of classical explanations is that all the newly proposed models require familiarity with the mathematical nitty-gritty of quantum mechanics—even the most simplified models [1, 2] still require a formal solution of the particle-in-a-box model. Such skills are out of the scope of most general chemistry textbooks, which only present the basic ideas of quantum mechanics, without any mathematical rigor.

There is a need, therefore, for a model of covalent bonding that is based on quantum mechanical concepts, on the one hand, but that avoids a rigorous quantum mechanical treatment, on the other. To be suitable for inclusion in general chemistry textbooks, such a model should fulfill the following requirements [12]:

1. It should be conceptually correct, that is, consistent with the basic postulates of quantum mechanics.
2. It should be mathematically simple—requiring skills only in algebra and the simplest operations of calculus.

3. It should give a clear and succinct answer to the question, “Why is the H_2^+ molecule stable?”

One of the key concepts of quantum mechanics, which emphasizes the fundamental conflict with classical mechanics, is the *uncertainty principle*. This concept is introduced in all modern general chemistry textbooks as a cornerstone of quantum theory. Consequently, this concept can serve as a common ground on which a widely accessible quantum mechanical description of covalent bonding can be constructed. It will be shown that in addition to classical electrostatics, familiarity with the uncertainty principle and its implications is a necessary and sufficient condition for conceptual understanding of the covalent bond.

In the first part of this paper we introduce the uncertainty principle in historical perspective, and discuss an important implication of this principle—the association of kinetic energy with spatial confinement. The historical discussion might seem too philosophical and maybe even irrelevant at first, but the main point of this paper is that an in-depth understanding of the uncertainty principle is essential for a coherent description of covalent bonding. This would become apparent in the second part, where we use the association of kinetic energy with spatial confinement to explain the repulsive force in the H_2^+ molecular system and derive a minimal bonding model for this molecule that is conceptually consistent with a rigorous quantum mechanical solution.

The Uncertainty Principle

General chemistry textbooks (for example, [7–11]) express the content of Heisenberg's uncertainty principle as the observer's inability to simultaneously measure the position and momentum of a particle with arbitrary accuracy. This idea is easy to get across, considering the significant obtrusive effect of observation at the atomic scale; however, such a simplistic explanation addresses position and momentum as well-defined attributes of the object, and only precludes our ability as observers to *measure* both simultaneously. It does not preclude the possibility that a particle *possesses* definite values for its position and momentum that fully determine its motion when it is not subjected to a measuring experiment. But nature is more

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complex than this, and much evidence speaks to the contrary of this simplistic, classical view of the uncertainty principle.

The second part of the paper discusses the currently accepted quantum mechanical explanation for the stability of the covalent bond. This explanation presumes that an electron shared between two nuclei intrinsically possess unsharply defined values for its position and momentum, regardless of observation. This presumption contradicts classical determinism, and calls for a more complex interpretation of atomic properties, known as the "Copenhagen interpretation," mainly associated with Werner Heisenberg and Niels Bohr. A careful reading of their original papers provides important insights into the most fundamental difference between classical and quantum mechanics.

Heisenberg's View. The uncertainty principle was introduced by Heisenberg in 1927 in an article entitled "The physical content of quantum kinematics and mechanics"[13]. In his article, Heisenberg advocates an operational definition of atomic scale physical quantities such as "position" and "momentum":

When one wants to be clear about what is to be understood by the words "position of the object", for example the electron...then one must specify definite experiments with whose help one plans to measure the "position of the electron"; otherwise these words have no meaning.

That is, a concept has a physical *meaning* only if it can be measured in an experiment. These experiments don't have to be practically feasible, but they must be physically possible in principle. For example, in order to measure the position of an electron, one can illuminate the electron and observe it under a microscope. A microscope is only able to resolve features that are larger than the wavelength used for illumination—the diffraction associated with the wave property of light will blur any smaller details; therefore, the shorter the wavelength of the illuminating light, the higher the resolving power of the microscope. Heisenberg considered a hypothetical microscope illuminated by γ -rays, whose ultra-short wavelength offers maximal resolution, and therefore the best determination of the electron's position; however, an important feature of short wavelength light is the Compton effect, in which light scattered from an electron changes the electron's momentum [13]:

At the instant of time when position is determined—therefore, at the moment when the photon is scattered by the electron, the electron undergoes a discontinuous change in momentum. This change is the greater the smaller the wavelength of the light employed, that is, the more exact the determination of the position. At the instant at which the position of the electron is known, its momentum therefore can be known up to magnitudes which correspond to that discontinuous change; thus, the more precisely the position is determined, the less precisely the momentum is known, and conversely.

The act of measuring one property introduces an *instantaneous discontinuous change* in another property of the electron. This means that it is impossible to measure simultaneously both the position and momentum of the electron with arbitrary accuracy. Taking into account that the position of the electron can be determined with an uncertainty Δx , which is on the order of the wavelength of the illuminating light (λ), and that the momentum change of the electron in the Compton effect

(Δp) is on the order of h/λ (where h is Planck's constant), Heisenberg estimated the limit of uncertainty in both measurements to be:

$$\Delta x \cdot \Delta p \sim h \quad (1)$$

This result can be generalized to any simultaneous measurement of position and momentum, because in every experiment the act of measurement has to involve an interaction between the investigated system and a probe. The relation between the probe's wavelength and its momentum is always $p = h/\lambda$, whether the probe is electromagnetic radiation (the Compton effect [14]) or a matter particle (as proposed by de Broglie and established experimentally by Davison and Germer [15]). A similar relation was worked out for the uncertainty in a simultaneous measurement of time and energy:

$$\Delta t \cdot \Delta E \sim h \quad (2)$$

It is important to note that in an idealized thought experiment, the estimated uncertainty is not a measure of some random experimental inaccuracy, but rather a fundamental limitation inherent in this kind of measurement. However, Heisenberg's thought experiment does not exclude the possibility of the electron *having* a definite position and momentum; it only excludes the possibility of *knowing* both of them with arbitrary accuracy. A naïve interpretation, based on classical causality, might be that the act of observing the electron's position causes it to change its momentum from one definite value to another. As a result, there is a de facto restriction on the information we can gather from this experiment, even though the system follows a deterministic path in principle. Such an interpretation implies that Heisenberg's aim was epistemological and that his argument intended to put a limitation on what we can *know* about atomic scale particles. This is the standard textbook interpretation of his work, as discussed earlier. But Heisenberg took the conclusions of his analysis one step further. His choice of the words "physical content" in the title of his article implies an ontological discussion of nature, concerning what we can *meaningfully say* about the intrinsic properties of such particles [16]. Following Heisenberg's operational definition, all concepts used in classical mechanics are also well defined in the realm of atomic processes, because each one is associated with a definite experiment in which its quantity can be measured, but each and every experiment that serves to provide such a definition for one quantity is subject to particular indeterminacies, obeying relation (1), which prohibits it from providing a simultaneous definition of the conjugate quantity. For Heisenberg, this implies that the uncertainty is not just a result of the specific act of observation. If the definition of "position" and "momentum" only has a meaning when it is associated with an experiment, and there is no conceivable experiment which can provide a simultaneous definition of both, then the electron simply does not possess a definite value for its position and momentum at the same time [13]:

But what is wrong in the sharp formulation of the law of causality, "When we know the present precisely, we can predict the future", is not the conclusion but the assumption. Even in principle we cannot know the present in all detail.... As the statistical character of quantum

theory is so closely linked to the inexactness of all perceptions, one might be led to the presumption that behind the perceived statistical world there still hides a 'real' world in which causality holds. But such speculations seem to us, to say it explicitly, fruitless and senseless. Physics ought to describe only the correlation of observations.

According to classical theory, the state of a particle is fully defined by its position and momentum. Based on the knowledge of its state at a given moment in time, all its future states can be calculated using classical mechanics. This deterministic view is referred to as "causality." Heisenberg rejects this classical notion in principle. His analysis defines a new perspective on what should be regarded as "state" and "explanation." An electron exists in a quantum mechanical state, one that cannot be fully defined using the classical terms of position and momentum. Because the state of the electron is only partially defined, and *in principle cannot be known in all detail*, it also cannot offer an explanation of physical phenomena based on a cause and effect mechanism. Nevertheless, such a state can provide an explanation by the *correlation of observations*. In our case, we will use the uncertainty principle to correlate kinetic energy and spatial confinement, a correlation by which the stability of the covalent bond can be explained.

Bohr's View. At the time Heisenberg worked out his uncertainty principle, Bohr was occupied by a closely related problem—that of "wave-particle duality." When trying to interpret the behavior of both light and matter on the atomic scale, it seemed that two different modes of communication were necessary to accommodate the full range of known phenomena. Some experiments, such as the diffraction patterns produced by a beam of light or of electrons reflected from the face of a crystal (X-ray diffraction and the Davison-Germer experiment), were described using the language of waves. Other experiments, such as the exchange of energy and momentum between a photon and an electron (the photoelectric and Compton effects), were discussed in terms of particles. All known atomic scale phenomena nicely fitted into either the wave or the particle models [17]; yet, these two ways of communication are mutually exclusive: whereas a particle is always localized, the very definition of the notions of wavelength and frequency requires an extension in space and in time. Bohr viewed the apparent contradiction as a limitation of language—no matter how abstract and subtle the concepts of modern physics may be, they are essentially an extension of our ordinary language and are therefore, limited by our classical perception of physical reality [18].

The two views...are rather to be considered as different attempts at an interpretation of experimental evidence in which the limitation of the classical concepts is expressed in complementary ways.

That is, the interpretation of observations associated with atomic scale phenomena requires new concepts; however, our language (and therefore our thought [19]) is limited to concepts which arise from our everyday experience with physical reality at the macroscopic scale. The use of the classical concepts of waves and particles to account for atomic scale phenomena is just an *attempt at an interpretation of experimental evidence* and should not be considered to imply a literal one-to-one correspondence to physical reality at the atomic level.

In what ways then do the two classical concepts correspond to experimental evidence, and what are their limitations? We shall exemplify this by considering the dual wave and particle nature of light. The concept of waves is rooted in our everyday experience with periodic disturbances traveling through a medium (e.g., water waves or sound waves). Disturbances from two different sources that act on the same medium can enhance (constructive interference) or diminish (destructive interference) their total effect, depending on the relative direction of the disturbances. This results in a pattern of alternating strong and weak disturbances (e.g., wave height or sound volume), which is called an "interference pattern." A similar pattern of alternating light and dark areas is formed when light can reach a point in space by two different paths. This experimental evidence is interpreted by analogy to the classical wave model as the interference of disturbances in an intangible medium we call the "electromagnetic field." While the electromagnetic field can be vividly imagined as an array of wiggling arrows or fluttering jello, it has no observable properties, and, therefore, no existence that is independent of the interaction of light and electrical charges [20]. Unlike sound or water waves, light requires no medium to travel through, and the physical reality of light cannot be attributed to a disturbance in a medium. Even though the classical wave model accurately captures the essence of light's observable interference patterns, this is but one property of light related phenomena, and it should not lead us to conclude that light is a wave in every classical sense.

A similar analysis can be applied to the particle nature of light. When speaking of particles, our everyday experience leads us to visualize small pieces of matter, which are both countable (discrete, noncontinuous) and localized (each one has a definite position in space and time). The interaction of light and matter shows a countable behavior, in that momentum and energy are transferred in discrete amounts (quanta), as observed in the photoelectric and Compton effects; however, no definite position in space and time can be attributed to the countable particles of light (photons), without denying them of their wavelike attributes discussed in the previous paragraph. Consequently, the physical reality of light cannot be attributed to point-like particles, and only the countable property of particles is valid during interaction with other particles.

It turns out that the applicability of the classical concepts becomes dependent on the experimental context. The wave model offers a valid description of the continuous propagation of light and matter in space and time; the particle model works well for the noncontinuous exchange of a quantum of momentum or energy during the interaction of light and matter. Each one of the two representations always applies to the measurement of specific variables: the wave model is associated with the space-time coordinates of the atomic system, whereas the particle model relates to the momentum-energy coordinates. While each model is viable in respect to its own domain of validity, it is subject to essential limitations in respect to the other model's domain of validity, and so neither offers a complete description of nature at the microscopic scale. In order to fully describe reality the two ways of communicating experience should be viewed as *complementary*, rather than contradictory.

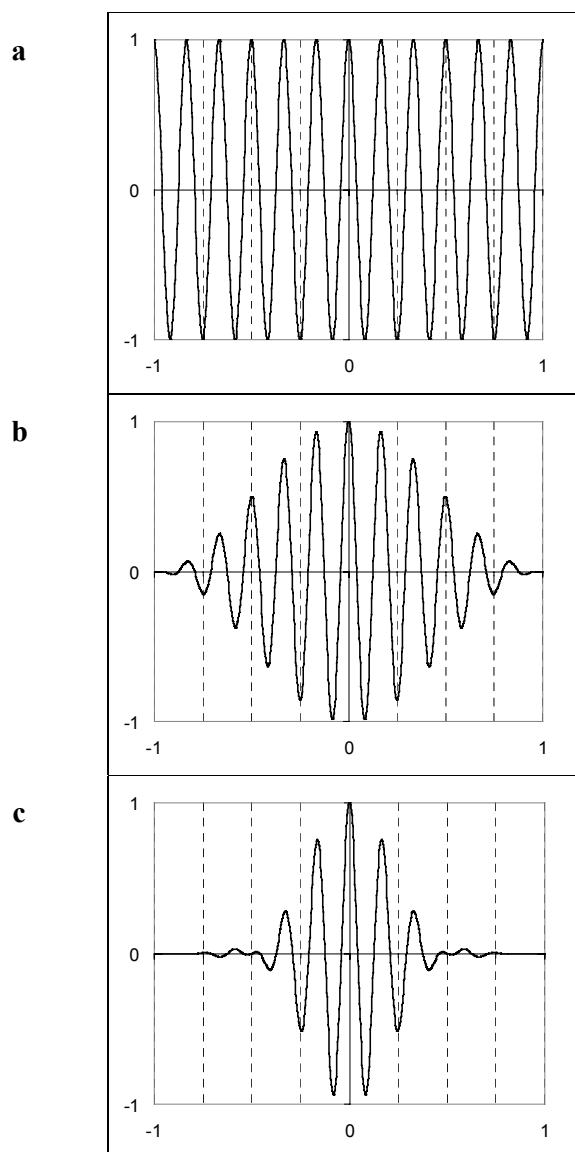


Figure 1. Building a wave-packet: $\Psi(x) = \sum_k g(1/\lambda) \cdot \cos(\frac{2\pi}{\lambda}x)$ where $g(1/\lambda)$ values are given in Table 1.

Table 1. $g(1/\lambda)$ values used in Figure 1.

$1/\lambda$	4.5	5	5.5	6	6.5	7	7.5
Fig.							
1a	0	0	0	1	0	0	0
1b	0	0	0.25	0.5	0.25	0	0
1c	0.034	0.125	0.216	0.25	0.216	0.125	0.034

The complementarity of the two models is best illustrated by an experiment with feeble light interference [21]. When light from a single source can reach the surface of a photographic plate by following two different paths, the resulting image shows an interference pattern. This phenomenon, which is associated with the spatial distribution (space–time coordinates) of the light, is readily explained by the wave model. Using the same setup, the light intensity is diminished until the interference pattern is lost and the plate only shows individual dots of light over a dark background. The interaction of light with the photographic substance, which is

associated with energy exchange (momentum–energy coordinates) between light and matter, exhibits a countable particle-like behavior; however, when the exposure time (rather than intensity) is increased, the individual dots accumulate back into an interference pattern. A similar behavior is observed in low intensity electron beams [22]. This shows that the particle behavior does not replace the wave behavior at low intensities, but rather coexists with it, each governing different aspects (or coordinates) of the total behavior. The wave and particle nature of light and matter are not two different modes of existence, but two faces of the same underlying physical reality, each exposed under different types of observation.

Although the two models govern different coordinates of observation, they are not independent. The Compton and photoelectric effects show that the fundamental parameters of the two models are correlated. This correlation is summarized in the “quantum postulate” [23], which relates the discrete amount of momentum (p) or energy (E) that is exchanged during the interaction of two particles, to the wavelength (λ) and frequency (ν) of the associated wave:

$$p\lambda = E/\nu = h \quad (3)$$

It follows from the quantum postulate that particles that exhibit a higher momentum and energy when interacting with other particles will also exhibit a shorter wavelength ($\lambda = h/p$) and higher frequency ($\nu = E/h$) in their space–time distribution and interference. For example, if we change the wavelength of the light source in the feeble-light interference experiment, the change will affect not only the spatial appearance of the recorded interference pattern, but also the feasibility of the photographic process itself. A longer wavelength (which has a lower frequency) will produce a larger separation between the dark areas in the interference pattern, but will also have a lower energy of interaction. Using standard black-and-white photographic film, going from blue light to green light will produce a pattern with larger separations, but red light will produce no pattern at all, because standard B&W photographic substance is not sensitive to the low energy red photons [24].

The inseparability of the intrinsic properties of the wave and particle models has led Bohr to the same conclusion as Heisenberg, based on completely different reasoning. His arguments require basic knowledge of wave analysis, so if you are not familiar with the ideas of wave packets and spectral decomposition, this would be a good time to read the appendix. The quantum postulate associates the momentum and energy of a particle with a wavelength and a frequency of an idealized wave. An idealized wave has no boundaries—it has an infinite extent in space and time, therefore losing the classical sense of “where” and “when” (space–time co-ordination). This excludes any observation of the particle, because in any observation process the observed particle is spatially and temporally confined by the measuring apparatus. Because the spatial distribution is governed by the wave model, the confinement should be represented by a wave with a finite extent. This excludes the possibility of associating a unique wavelength and frequency to the particle. Yet, a confined wave can be described as the superposition of many wave components, a “wave packet,” which interfere constructively within the confinement region and destructively outside of it (Figure 1), but then, the state of the particle is associated

with more than one unique wavelength and frequency and, therefore, with more than one unique momentum or energy value. The act of observation excludes the ability to uniquely define the momentum and energy of a particle, preventing a deterministic description of the interactions in the system (causality). In Bohr's words [18]:

The very nature of the quantum theory thus forces us to regard the space-time co-ordination and the claim of causality, the union of which characterizes the classical theories, as complementary but exclusive features of the description, symbolizing the idealization of observation and definition respectively.

Bohr's analysis drops the footing under Heisenberg's arguments, in which he considers a measurement process involving a photon with a definite momentum, thus denying any wavelike properties of light [25]; however, Bohr was able to re-establish the uncertainty relations by taking into account wave-particle duality. He regarded the two idealized pictures, that of a completely localized particle (idealization of observation: $\Delta x \rightarrow 0$, $\Delta t \rightarrow 0$), and that of an infinitely unbounded wave (idealization of definition: $\Delta p \rightarrow 0$, $\Delta E \rightarrow 0$), as extreme cases of a continuum in which both uncertainties have finite values [18]:

...The idea of a coincidence of well-defined events in a space-time point being replaced by that of unsharply defined individuals within finite space time regions.

In all practical cases, the state of a particle should be represented by a nonidealized wave packet with a finite uncertainty of observation and definition. The spread of the wave packet in space and time determines the uncertainties Δx and Δt . The composition of the wave packet in terms of wavelengths and frequencies determines the uncertainties $\Delta(1/\lambda)$ and $\Delta\nu$. The relation between the wavelength and frequency composition of a wave packet and its spread in space and time is given by (see appendix):

$$\Delta x \cdot \Delta(1/\lambda) \sim 1 \quad (4)$$

$$\Delta t \cdot \Delta\nu \sim 1 \quad (5)$$

Combining eqs 4 and 5 with eq 3 gives back eqs 1 and 2. By assuming that the quantum postulate holds for every component of the wave packet, and not just for an idealized wave, the uncertainty relations directly emerge from the mathematical properties of wave-packet spectral decomposition. Thus, while Heisenberg's results still hold under Bohr's complementarity theory, his thought experiment is shown to be flawed: it is impossible to measure both position and momentum (or time and energy) simultaneously with arbitrary precision, not because the measurement process interferes with the state of the particle, but because the state of the particle cannot have in principle a sharp value of both properties. Such pairs of properties that cannot be measured simultaneously are called "complementary properties."

The philosophical implication of the uncertainty relations is that the physical reality of a particle should always be associated with a partly localized wave packet and never with a definite point in space and time. The practical implication is that the extent of this localization has a direct effect on the momentum and energy associated with the particle. These two

implications will serve as the basis for our simplified quantum mechanical model of covalent bonding.

The Kinetic Energy of Confinement. An essential corollary of the uncertainty relations is that the confinement of a quantum particle is associated with an increase in its kinetic energy. Before we elaborate on this, we must first explicitly define the terms "kinetic energy" and "confinement" in their quantum mechanical sense.

In classical mechanics, the energy content of a particle can be separated into two contributions:

1. Potential energy: energy which is associated with the interaction of the particle with other particles.
2. Kinetic energy: energy which is associated with the space-time coordination of the particle, regardless of any other particles.

In quantum mechanics, potential energy essentially keeps the same meaning as in classical mechanics. Kinetic energy, on the other hand, acquires an additional meaning. While in classical mechanics "space-time coordination" addresses the state of motion of a point particle, in quantum mechanics it also takes into account the spread in momentum associated with the wavelike character of the particle. To illustrate the difference, let us consider an electron emitted by the cathode in a CRT at one point in time and hitting the screen at a later time. The time between the application of voltage on the accelerating anode and the appearance of the sparkle on the phosphorescence screen can be measured. The higher the voltage on the anode, the less time it takes an electron to reach the screen. This phenomenon can be easily explained using classical mechanics, by describing the electron as a point particle moving from the anode towards the screen with a constant velocity v . The velocity is determined by the accelerating voltage of the anode—a higher voltage will result in a faster moving electron. The momentum of the electron is defined as $p = mv$, and its kinetic energy is $E_k = mv^2/2 = p^2/2m$. In quantum mechanics, the wave-like character of the electron determines its space-time coordination, so the motion of the electron cannot be described by a trajectory of a fully localized point particle. On the other hand, the electron in this case cannot be described by an idealized wave with a definite wavelength, because an idealized wave extends simultaneously throughout all space, while the electron is known to be around the cathode at one point in time and around the screen at a later time. The solution is to describe the electron as a wave packet: a partly localized combination of many wave components with different wavelengths λ_i , each associated with a different momentum value $p_i = h/\lambda_i$. This partly localized wave packet propagates through the CRT with an overall velocity of $v = \langle p_i \rangle / m$, where the angle brackets denote an average. The classical relation between momentum and kinetic energy holds for every wave component; therefore, the overall kinetic energy of the wave packet is $E_k = \langle p_i^2 / 2m \rangle = \langle p_i^2 \rangle / 2m$. This value looks almost similar to the kinetic energy of a classical particle with a momentum $p = \langle p_i \rangle$, which is $E_k = \langle p_i \rangle^2 / 2m$; however, because $\langle p_i^2 \rangle$ (the average of the square) is always greater than $\langle p_i \rangle^2$ (the square of the average) [26], the average kinetic energy of a wave packet is always greater than the classically calculated value for a particle with momentum $\langle p_i \rangle$. So, while part of the kinetic energy of the wave packet is analogous to the classical "energy of motion," there is another part, which has no classical analog, that is associated with the

spread of momentum values of different wave components inherent in a partly localized wave.

Confinement, in the classical sense, means that a particle's motion is limited to a specific region in space, because its potential energy is lower in this region (a potential well), and its kinetic energy is insufficient for it to break loose. In quantum mechanics, a particle can be spread around a potential well without moving at all. It is the extent of the particle's wave packet that is limited, not its motion—the wave packet has appreciable values over a length of Δx and quickly vanishes outside of this region.

A confined wave packet can be stationary, which means its space-time distribution stays constant over time; still, even in such a stationary state, it follows from Bohr's interpretation that the associated momentum of a confined wave packet has an uncertainty of $\Delta p = h/\Delta x$. This uncertainty is independent of any measurement process in the sense that it reflects an inherent spread in the particle's momentum and not a spectator's inability to measure it. So, even if there is no net movement of the wave packet, which means the momentum values of all wave components average to zero, individual wave components have nonzero momentum associated with them, ranging in the order of $-\Delta p/2$ to $+\Delta p/2$. The kinetic energy associated with the particle should reflect this spread, because kinetic energy is a positive quantity and would not average out to zero [27]. A rough approximation of the kinetic energy associated with a confined particle of mass m is, therefore,

$$E_k = \langle p^2 \rangle / 2m \sim (\Delta p/2)^2 / 2m \sim h^2 / 8m\Delta x^2 \quad (6)$$

where the quantum relation between overall kinetic energy and the momentum of individual wave components was used in the first step, a rough estimate of $\langle p^2 \rangle$ in terms of the uncertainty Δp was used in the second step, and eq 1 was used to transform Δp to Δx in the last step. The kinetic energy is therefore inversely proportional to the square of the length of the confinement—the smaller the spread in position, the larger the uncertainty in momentum, and the larger the overall energy. We will address this manifestation of kinetic energy in quantum mechanics as “kinetic energy of confinement.”

The kinetic energy of confinement has no classical analog because it is not associated with motion. The nonzero value is due to the spread of momentum values associated with the wave components that constitute a confined wave packet. Thus, the kinetic energy is inherent in the unsharply defined state of the particle and should not be interpreted as indicative of particle motion in the classical sense. An example of such a classical miss-interpretation of the kinetic energy of electrons confined in an atom can be found in [28]: “When the fan is stationery you can identify the number of blades, but as it is turned full blast is it possible to identify each blade? No, it is blurred. Therefore it is the same with electrons, hence the name electron cloud. You cannot identify each and every electron since they are moving at a high speed.” Such interpretations are inconsistent with the Copenhagen interpretation of quantum mechanics because they attribute to the electron a point-like particle property at each instant of its motion in space and time. This contradicts the idea that space-time coordination is always associated with a wave model. The electron “cloud” should be interpreted as a stationary wave

packet in which the position and the momentum of the electron are not sharply defined.

A Model for Covalent Bonding in H_2^+

A scientific model is a conceptual representation of structure in a physical system [29]. The physical system has measurable properties, which exhibit certain regularities. The scientific model represents a subset of these properties and regularities. As such, a scientific model is not judged for being “true,” but rather for being “valid,” that is how well it fits the phenomena at hand and how it relates to other models and theories in the domain of interest. Many times it is advisable to use a simplified model, even if we know it is incomplete or inaccurate, in order to emphasize specific features of the physical system. This promotes qualitative insight and quantitative appreciation at the expense of numerical exactness.

For molecular systems, there are two features that are worth emphasizing at the general chemistry level: their size and force of cohesion. We think of molecules as a collection of atoms, held together by “covalent bonds.” These bonds have a characteristic length, which defines the size of the molecular world—on the scale of angstroms. They also have a characteristic strength, which defines the energy scale of chemical transformations—on the scale of hundreds of kJ/mol. A valid model for covalent bonding should be able to reflect these scales, and relate them to the theory of quantum mechanics.

In this part of the paper we consider the hydrogen molecule ion as a prototype of covalent bonding. We present three possible models to describe the covalent bond in this molecule: an analytic quantum mechanical solution, a crude approximation based on the uncertainty principle, and a classical model. We will show that only the first two are valid models, while the classical one fails on both accounts—it cannot produce quantitative appreciation of molecular scales, and it is inconsistent with the quantum mechanical description of atomic scale systems.

Analytic Solution. Systems composed of more than two bodies, such as the H_2^+ molecule, do not lend themselves to exact analytic solution; however, if we take into account the large difference between the masses of the nuclei and the mass of the electron, we can separate the three-body problem into a single-body problem (the electron distribution under the influence of two stationary nuclei) and a two-body problem (the nuclei moving under the influence of an average electron-charge distribution). This separation of time scales is called the Born–Oppenheimer approximation.

According to the Born–Oppenheimer approximation, we can calculate the energy of the molecular system assuming the nuclei are fixed. This means we take into account the electrostatic attraction between the electron and the nuclei (V_{en}), the electrostatic repulsion between the nuclei (V_{nn}), and the kinetic energy of the electron (T_e), but ignore the kinetic energy of the nuclei. For each internuclear separation, there will be a specific electron distribution that will yield the lowest molecular energy (the ground state). Thus, we can carry out a calculation process in which we decrease the internuclear separation in steps, and at each step calculate the lowest possible energy of the electron distribution. A word of warning is in place: this process is a stationary mathematical process and does not model the dynamic physical process of two atoms

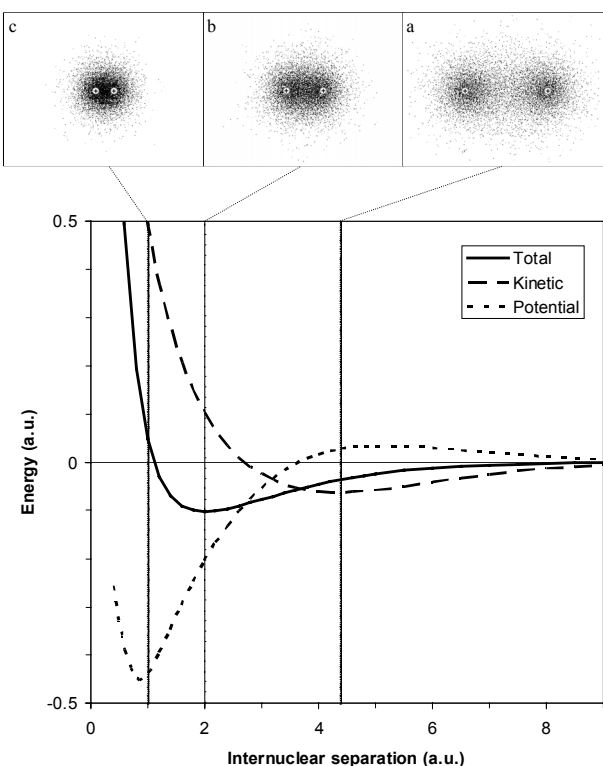


Figure 2. Analytic solution of the H_2^+ molecular system. The energy axis is relative to a separated proton and a hydrogen atom (-0.5 au relative to complete separation of all three particles, with a contribution of -1.0 au from potential energy and $+0.5$ au from kinetic energy). The spatial distribution of the single electron is represented by randomly plotting 10,000 points whose positions are distributed according to the square of the electronic wave function, thus forming an “electron cloud.”

approaching one another. In the physical process, the overall energy is conserved, and therefore a bond will never form unless a third body is present to take away the excess kinetic energy of the nuclei. In the mathematical process, the stationary molecular energy will vary with each internuclear separation because the electron is subjected to a different electrostatic field. The curve displaying the change of the molecular energy as a function of internuclear separation can be later used as an effective potential curve on which the dynamics of the nuclei will be calculated. The minimum in this curve represents the most stable configuration of the nuclei in the molecule, which is the bond length.

This mathematical process was carried out by Bates et. al. [30], who calculated the molecular energy and electron wave functions of H_2^+ for a large set of internuclear separations. Their results for the molecular energy are shown as the graph of total energy in Figure 2, along with illustrations of electron distribution at internuclear separation of 1.0 au, 2.0 au, and 4.4 au [31]. The molecular energy can be broken down into its potential energy and kinetic energy components, using the virial theorem [32]. The energy components are also shown in Figure 2.

At large internuclear separations (9.0 au), the energy of the system is similar to that of a hydrogen atom. This means that the electron distribution around each nucleus is mostly affected by the attraction to a single nucleus. When the two nuclei are positioned closer, the electron distribution that minimizes the overall energy is such that more of the electron density is in

between the two nuclei. This can be seen in Figure 2a as a slight asymmetry of the electron cloud around each nucleus at 4.4 au, which is slanted towards the middle. Going down from 9.0 a.u. to 4.4 a.u., the decrease in energy is due to two factors: the simultaneous attraction of the electron to both nuclei reduces the potential energy ($V_{\text{en}} = -0.200$ au), and the less tight confinement of the electron, which partly occupies the internuclear space, reduces the kinetic energy ($T_{\text{e}} = -0.064$ au). The apparent increase in potential energy is due to the nucleus–nucleus repulsive energy term ($V_{\text{nn}} = 1/R = 0.227$ au).

The trend of decrease in the electron–nuclei potential energy with decreasing internuclear separation continues at smaller separations. At 2.0 au, the simultaneous attraction of the electron to both nuclei reduces the potential energy ($V_{\text{en}} = -0.705$ au) more than the internuclear repulsion increases it ($V_{\text{nn}} = 0.500$ au). This is because a larger part of the electron density lies between the nuclei, as can be seen in Figure 2b; however, the same reason causes the trend for the kinetic energy to reverse. At separations smaller than 4.4 au, a decrease in internuclear separation results in a tighter confinement of the electron, because the electron is concentrated between the nuclei. The contracted distribution of the electron corresponds to a higher kinetic energy ($T_{\text{e}} = 0.103$ au at 2.0 au separation). The same trends are still observed when the internuclear separation is reduced to 1.0 au. As seen in Figure 2c, at this separation the electron density is also concentrated between the nuclei. The decrease in internuclear separation results in a big decrease in electron–nuclei potential energy ($V_{\text{en}} = -1.437$ au), still outweighing the increase due to internuclear repulsion ($V_{\text{nn}} = 1.000$ au). On the other hand, the tighter confinement increases the kinetic energy ($T_{\text{e}} = 0.485$ au).

At separations below 0.8 au the electron–nuclei potential energy continues to decrease with decreasing internuclear separations, but no longer outweighs the increase in potential energy due to internuclear repulsion, and the potential energy increases with decreasing separation.

Overall, in the range 0.8 au to 4.4 au, the potential energy increases with increasing separation, while the kinetic energy increases with decreasing separation. The two opposing trends result in a minimum in the overall static molecular energy at 1.997 au. Because the static molecular energy curve serves as an effective potential for the motion of the nuclei, the slope of the curve can be interpreted as the force acting on the nuclei. The positive slope of the potential energy curve can be interpreted as an attractive electrostatic force, in which the attraction of the electron to the two nuclei outweighs the electrostatic repulsion of the nuclei. The negative slope of the electronic kinetic energy curve can be interpreted as a repulsive quantum mechanical force, which has no classical analog. It is solely the result of the kinetic energy of confinement, which is a unique property of microscopic particles. This property is explained by the complementary wave-particle description, and quantified in the uncertainty principle. The attractive force is stronger at large intermolecular separations, and the repulsive force dominates at small separations. The bond length of the molecule is the distance in which these two forces are balanced. The value of 1.997 au ($= 1.057$ Å) is in excellent agreement with the experimental ground-state bond length of H_2^+ , which is 1.053 Å, and the molecular energy at the bond length is exactly the same as the experimental value of -269.4 kJ/mol [33]. We see

that the analytic solution provides numerical exactness in its results for the geometry and energy of the H_2^+ molecule.

Simplified Electrostatic-Uncertainty Model. While the analytic solution is numerically exact, it cannot be used to teach the concept of a covalent bond at the high school or freshman level. The mathematics of the analytic solution is even beyond the scope of an advanced course in quantum mechanics. Simplified quantum mechanical models have been proposed [1–6], but all require a level of understanding of quantum mechanics that is beyond the scope of a general chemistry course. It is possible to construct a mathematically simple model of covalent bonding, which is still valid, if we relinquish numerical exactness in favor of quantitative appreciation. The emphasis of only a few key features promotes qualitative insight into the nature of the covalent bond.

In the analytic model, the electron distribution is concentrated between the two nuclei, which are separated by a distance R . In our simplified model, we assume it is totally confined to the internuclear region. This is related to the Lewis model of covalent bonding, in which bonding electrons are counted as “shared” between the two nuclei. In such an arrangement, the simultaneous electrostatic attraction of the electron and the two nuclei always outweighs the internuclear repulsion (as is the case in the range of 0.8 au to 4.4 au in the analytic solution). An increase in R will result in an increase in potential energy. On the other hand, the confinement of the electron is associated with its kinetic energy, which increases when R decreases. This explains the repulsive force, which is quantum mechanical in nature, in much the same way it is explained by the analytic solution—a localization of the electron is associated with increase in kinetic energy, as follows from the uncertainty relations.

In order to calculate the point of balance between the two forces, we need an estimate of the energy associated with each one. We can estimate the electron–nuclei potential energy by calculating the attraction of both nuclei to a point particle placed halfway between the nuclei: $V_{en} = 2[-k_e e^2/(R/2)] = -4k_e e^2/R$. The nuclei–nuclei potential energy is $V_{nn} = k_e e^2/R$. The kinetic energy is estimated by using eq 6 and substituting R for Δx . The total molecular energy as a function of R is therefore:

$$E(R) = V_{nn} + V_{en} + T_e = -3k_e e^2/R + h^2/8m_e R^2 \quad (7)$$

This function has a single minimum that can be found by differentiating E with respect to R and equating the derivative to zero:

$$dE/dR = 3k_e e^2/R^2 - h^2/4m_e R^3 = 0 \quad (8)$$

which gives a value for the equilibrium bond length of

$$R_{eq} = h^2/12m_e k_e e^2 \quad (9)$$

Substituting the values for Planck’s constant ($h = 6.63 \times 10^{-34} \text{ m}^2\cdot\text{kg/s}$), electron mass ($m_e = 9.11 \times 10^{-31} \text{ kg}$), electrostatic constant ($k_e = 8.99 \times 10^9 \text{ N}\cdot\text{m}^2/\text{C}^2$) and electron charge ($e = 1.60 \times 10^{-19} \text{ C}$) into eq 9, we get an estimate for the bond length of $R_{eq} = 1.7 \times 10^{-10} \text{ m} = 1.7 \text{ \AA}$. Substituting this value back into eq 7 will give the molecular energy value of -1200 kJ/mol at the bond length. Although these values are very different from the experimental values, they still give an

order of magnitude estimate for the properties of a covalent bond: bond length in the order of angstroms and bond energy in the order of hundreds of kJ/mol. We have therefore shown that the simplified electrostatic-uncertainty model also qualifies as a valid model for covalent bonding. It explains the source of both attractive and repulsive forces, in a way that is consistent with the basic postulates of quantum mechanics, and it provides a way of calculating the approximate geometry and energy of the H_2^+ molecule.

A Classical Model of Bonding. Most general chemistry textbooks (e.g. [7–11]) give a quantum mechanical description of the structure of a single atom. But when they move on to the description of molecules, they pursue a completely classical line of argumentation. We will show that a fully classical model is an oversimplification, which fails to explain the source of the repulsive force in the molecular system. Without a proper description of repulsive forces, there can be no appreciation of bond lengths and bond energies; therefore, such a model is ineffective for quantitative appreciation of the fundamental properties of covalent bonding.

The classical model converges with our proposed model in respect to the source of the attractive force between the nuclei, namely the mutual attraction of the nuclei to the electron. It differs in its interpretation of the repulsive force, which is claimed to arise from the mutual repulsion between the nuclei. All the textbooks mentioned above state that a covalent bond is formed when the nucleus–nucleus repulsive force offsets the nuclei–electron attractive force at the equilibrium distance. This claim sounds qualitatively plausible, but if we formulate it in quantitative terms it is easy to see it has no quantitative basis. Assuming the electron is halfway between the nuclei (if we put the electron closer to one of the nuclei, we will get an even lower (more negative) value for the total energy [6]), we get an expression for the total energy of the system:

$$E(R) = V_{nn} + V_{en} = k_e e^2/R - 4k_e e^2/R = -3k_e e^2/R \quad (10)$$

which amounts to rewriting eq 7 without the kinetic energy term; however, without this term, the total energy of the system always decreases with decreasing R , which means the nuclei will only feel an attractive force, and an equilibrium state can never be achieved. If this was the case, the beautiful architecture of molecules would collapse. A static array of charges can never be arranged in a stable equilibrium state [34].

Is it possible to add a kinetic energy term consistent with classical mechanics that will offset the decrease in potential energy in much the same way the tangential motion of the Earth keeps it in an orbit around the sun? The answer is no. An electron moving in a confined space has to accelerate in order to change its direction of motion; otherwise, it will escape its confinement. However, acceleration of a charged particle must be accompanied by the emission of electromagnetic radiation and the loss of energy. Unfortunately, this explanation is beyond the reach of most general chemistry audiences, who are usually not familiar with Maxwell’s equations. Still, even if the electromagnetic force did behave like gravitation (a common misconception) and accelerating electrons didn’t radiate energy, this system wouldn’t be stable. According to the Second Law of Thermodynamics, energy is more probable to dissipate between many particles rather than be concentrated in a single particle. An object moving in an orbit under the

influence of a centripetal force can lower its energy by reducing the radius of the orbit. The reason the earth doesn't fall into the sun is because it closely resembles an isolated system and cannot exchange energy with the environment. This is not true for atomic systems—the frequent collisions would quickly dissipate the excess kinetic energy.

Because both the static and dynamic classical models fail to consistently explain the stability of covalent bonds, quantum mechanics has to be taken into account when discussing the nature of the covalent bond. The simplified electrostatic-uncertainty model described in the previous section is the simplest way of introducing the quantum mechanical nature of the stabilizing forces without reverting to the complicated rigorous treatment of the system described in the analytic model. Students' acquaintance with the uncertainty principle is a necessary and sufficient condition for understanding the nature of the covalent bond.

Conclusions

Molecules, which constitute most of the observable matter surrounding us, are remarkably stable. The "glue" which keeps the intricate molecular architecture together is conceptualized as a covalent bond and is one of the most important ideas in modern chemistry. It is therefore crucial to find a simple explanation of the phenomena of covalent bonding that can be understood by beginning chemistry students. While the simplicity of the explanation can come at the expense of numerical exactness and scientific rigor, it should not contradict the basic premises of current scientific knowledge.

We have shown the deficiency of the current common textbook explanation for the H_2^+ system, which only addresses classical electrostatic arguments. The electrostatic system can only produce an attractive force, where a stable bond requires an equilibrium between an attractive and a repulsive force. We employed the uncertainty principle to formulate a static quantum kinetic-energy term, which finds its origin in the confinement of the electrons to the volume in between the nuclei. This kinetic energy term was shown to produce the necessary repulsive force. Our simple model gives an order of magnitude appreciation for the bond length and bond energy and is consistent with the more advanced analytical quantum mechanical treatment of the system. We argue that this simple model can be used at the freshman level to give students a better understanding of the underlying principles of covalent bonding. As for high school chemistry, the above discussion of the uncertainty principle might be an overkill. Nevertheless, we advise against using the purely classical model even at this level. We feel it is better to obscurely speak about a "mysterious" quantum mechanical repulsive force than it is to give the false pretense that classical mechanics can offer an adequate description of matter at the atomic scale.

The argument for the attractive force being associated with potential energy and the repulsive force being associated with kinetic energy is not limited to our test case, the H_2^+ molecule. The virial theorem [32] can be used to show that for any particle system at equilibrium (even solids), the derivative of the kinetic energy in relation to expansion is negative, and the derivative of the potential energy is positive. This means that a small expansion of the system will be accompanied by an increase of potential energy—the atoms are "pulled" by an electrostatic force. On the other hand, a small compression of the system will be accompanied by an increase of kinetic

energy—the atoms are "pushed" by a force whose origin is in the kinetic energy of confinement. Using the simplified model for the H_2^+ molecule can help get this idea across to students long before they have the mathematical tools needed to fully comprehend the arguments involved in the application of the virial theorem to molecular systems.

The applicability of the virial theorem to all molecular systems enables us to generalize our results and have an overall appreciation of molecular scale. The bond length represents the equilibrium point between two forces: the electrostatic force, $F_e \sim k_e e^2/R^2$, and the quantum mechanical "uncertainty" force, $F_u \sim h^2/m_e R^3$. A direct consequence of this balance is that the bond length of all covalent bonds is determined by a common length scale of $a_0 = h^2/(2\pi)^2 k_e e^2 m_e$ known as the Bohr radius. The size and shape of all observed molecular matter is determined by this scale. A miniature chemical world would exist if we could replace the mass of the electron, m_e , by a larger quantity. Such esoteric chemistry can be done by replacing electrons by muons with a mass of $207 m_e$ shrinking the covalent bond by that amount (This is also a short lived chemistry because the lifetime of muons is only ~ 2.2 microsecond). The consequence of the shorter bond length finds its use in catalyzing nuclear fusion reactions [35, 36]. Substituting all the electrons in an object with muons would have an effect similar to that of the potion Alice of Wonderland consumed which caused her to shrink.

Apart from the discussion of molecular scale, the simplified electrostatic-uncertainty model can be used to discuss the philosophical implications of the uncertainty principle. The common interpretation of Heisenberg's thought experiment, which attributes the uncertainty in the electron's momentum to the measurement process, can be easily challenged. Because we know molecules exist even if we don't probe them with photons, because we demonstrated that the stability of molecules depends on the existence of electronic kinetic energy, and because the average momentum of a bound electron has to be zero, we have to accept that the uncertainty in the electron's momentum exists even without measurement. This fuzzy definition of the state of the electron is an inherent property of its physical reality, as Bohr argued. The question of whether the electron has a definite momentum when we don't measure it is not just a philosophical question; it has an experimentally measurable consequence. The stability of molecular systems is the evidence for this unintuitive property of atomic scale particles.

In summary, the concept of covalent bonding and the concept of uncertainty are closely related. On the one hand, the uncertainty principle explains the stability of the covalent bond and facilitates appreciation of its energy and length scales. On the other hand, the stability of the covalent bond helps resolve the philosophical question about the physical reality of the uncertainty principle. Teaching these two concepts in unison, by using the simplified electrostatic-uncertainty model, will certainly enhance the conceptual understanding of both.

Appendix

According to the theory of spectral decomposition (Fourier analysis), every function can be expressed as the sum of harmonic waves. While each wave component has a constant amplitude throughout space (Figure 1a), the superposition of several wave components localizes the amplitude into a finite region (Figure 1b) [37]. This localized bundle of waves is

called a “wave packet.” The localization is achieved by constructive interference of the wave components within the region and destructive interference outside. As the maximum difference between the reciprocal wavelengths of the different wave components increases, the width of the wave packet decreases (Figure 1c).

If we define the uncertainty as the width of the wave packet at half its maximum value (FWHM—Full Width Half Maximum), we get the uncertainties $\Delta x \rightarrow \infty$, $\Delta x \sim 1$, and $\Delta x \sim 0.5$ for Figures 1a, 1b, and 1c, respectively. Using the same definition for the uncertainty in $1/\lambda$, we get $\Delta(1/\lambda) \rightarrow 0$, $\Delta(1/\lambda) = 1$, and $\Delta(1/\lambda) = 2$, respectively. In all cases, $\Delta x \cdot \Delta(1/\lambda) \sim 1$. Using similar arguments, it can be shown that this relation holds for the temporal width of a wave packet as well, giving $\Delta t \cdot \Delta \nu \sim 1$.

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- For example, the average of 8, 9, 10, 11 and 12 is 10, but the average of 8^2 , 9^2 , 10^2 , 11^2 and 12^2 is 102, which is greater than 10^2 .
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