Atomic and Molecular Stability

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Klaus Ruedenberg once wrote that there are no ground states in classical mechanics. In other words, quantum principles are required to understand the stability of atoms and molecules, and the nature of the chemical bond. Quantum mechanics is not mathematically more difficult than classical physics, the real challenge it offers is of a conceptual nature. That's because it says that understanding the stability of matter requires that it possess both particle and wave properties. The conceptual challenge is that particle and wave are contradictory concepts.

http://www.users.csbsju.edu/~frioux/q-intro/WaveParticleDualityDeBroglie.pdf

Investing matter with wave behavior subjects it to interference effects and leads immediately to a redefinition of kinetic energy. In quantum mechanics the concept kinetic energy should be replaced with confinement energy, because the former implies classical motion. According to quantum mechanical principles a confined particle, a **quon**, because of its wave-like character is described by a wave function which is a weighted superposition of all possible positions. Quons do not execute trajectories in the classical sense. They are not here and later there; they are here and there simultaneously. As Werner Heisenberg said, "There is no space-time inside the atom." In other words there is also no space-time for confined **quons**.

"A **quon** is any entity (electron, proton, neutron, atom, molecule, C60 etc.), no matter how immense, that exhibits both wave and particle aspects in the peculiar quantum manner." Nick Herbert, *Quantum Reality*, page 64. The following tutorial outlines the origin of de Broglie's wave hypothesis for matter and how it transforms classical kinetic energy into quantum mechanical confinement energy.

http://www.users.csbsju.edu/~frioux/q-intro/WaveParticleDualityShort.pdf

The stabilities of hydrogen and helium, the most abundant elements in the universe, are now explained using rudimentary quantum principles.

http://www.users.csbsju.edu/~frioux/stability/AtomicStability.pdf

Scientists work almost exclusively in coordinate space when they do quantum calculations. There are two other options, momentum space and phase space, as the following tutorial shows. Calculations on the hydrogen atom are provided for all three computational venues in the following link.

http://www.users.csbsju.edu/~frioux/wigner/Wigner1DHatom-rev.pdf

The phase space calculations require the Wigner distribution function. The following link provides further information about the Wigner distribution and how it repackages quantum weirdness.

http://www.users.csbsju.edu/~frioux/wigner/wigner.pdf

Sometimes practitioners of quantum mechanics misinterpret energy contributions when studying the details of atomic behavior. This can happen when classical concepts are allowed to intrude on the quantum realm where they are not valid.

http://www.users.csbsju.edu/~frioux/stability/EngelCritique.pdf

Further evidence that confinement energy is not kinetic energy is seen in the following analysis of the effect of lepton mass in the hydrogen atom. In what follows the electron is replaced by the muon and the tauon in the hydrogen atom. Positronium, in which the proton is replaced by the positron, is also examined. These analyses also provide a graphical illustration of the uncertainty principle.

http://www.users.csbsju.edu/~frioux/stability/VariMassHatom.pdf

Many in the chemical education community teach chemical bonding as simply an electrostatic phenomenon. I and many others have argued against this incorrect, simplistic view on many occasions. In an effort to get a better understanding let's look at an overview of the nature of the chemical bond written by Frank E. Harris many years ago.

http://www.users.csbsju.edu/~frioux/h2bond/ChemBondQM.pdf

We go deeper with the following treatment of the covalent bond in the hydrogen molecule ion using the virial theorem (John C. Slater) and *ab initio* quantum mechanics (Klaus Ruedenberg). In my opinion, Slater and Ruedenberg are the true pioneers in understanding the covalent chemical bond. Many books have been written about the chemical bond, but few are as insightful as the papers published by Slater and Ruedenberg.

http://www.users.csbsju.edu/~frioux/h2-virial/H2p-Morse-MOT.pdf

The following link provides graphical displays of the electron density in the hydrogen molecule ion.

http://www.users.csbsju.edu/~frioux/h2pvirial/H2P-MOs.pdf

The following calculation shows that the lepton mass effect in molecules is the same as it is atoms. This mass effect provides a challenge for those who think atomic and molecular stability can be explained solely in terms of electrostatic potential energy effects. The mass effect is important because quantum mechanical kinetic energy (confinement energy) is inversely proportional to mass, but classical kinetic energy is directly proportional to mass.

http://www.users.csbsju.edu/~frioux/h2-virial/H2p-LCAO-MO-Mass.pdf

Some might feel uncomfortable relying on a one-electron molecule to gain an understanding of the chemical bond. After all don't chemical bonds consist of electron pairs? So we move to the hydrogen molecule for a quantum analysis of the more traditional two-electron bond. The only new contribution to the total energy is electron-electron potential energy, and the significance of confinement energy in understanding molecular stability survives.

http://www.users.csbsju.edu/~frioux/h2-virial/h2-bond-virial.pdf

I apologize for the considerable overlap in the following, but it does provide some additional interpretive graphics. It also contains references to the publications of Slater and Ruedenberg.

http://www.users.csbsju.edu/~frioux/h2-virial/H2-virial.pdf

I close with a rather mystical description of the chemical bond by Charles A. Coulson, the author of *Valence*, an influential monograph on the chemical bond published in 1952.

> Sometimes it seems to me that a bond between two atoms has become so real, so tangible, so friendly, that I can almost see it. Then I awake with a little shock, for a chemical bond is not a real thing. It does not exist. No one has ever seen one. No one ever will. It is a figment of our own imagination.... Here is a strange situation. The tangible, the real, the solid, is explained by the intangible, the unreal, the purely mental.

Addendum
The Bohr Model of Atomic and Molecular Stability

The purpose of this study was to outline the success of quantum mechanics in explaining the stability and structure of matter. But quantum mechanics didn't emerge out of a vacuum; it had a precursor – the Bohr model. So I thought it appropriate to take a brief look at that precursor and present its explanation of atomic and molecular stability.

> My starting point (for the development of the Bohr model) was not at all the idea that an atom is a small-scale planetary system and as such governed by the laws of astronomy. I never took things as literally as that. **My starting point was rather the stability of matter, a pure miracle when considered from the standpoint of classical physics.** Niels Bohr

All matter consists of elements that are made up of electrons, protons and neutrons. Given that the electron and the proton have opposite charges and therefore are attracted to one another provides the problem that classical physics has in explaining the stability of matter. What keeps these oppositely charged building blocks apart? There is no more fundamental question in science and Bohr was the first to attempt an explanation of atomic stability by creating, by fiat, the necessary rudimentary quantum mechanical concepts.

We begin with the Bohr model for the simplest element, the hydrogen atom. In the following tutorial the Bohr model is enriched with de Broglie's hypothesis of wave properties for the electron. This allows the reinterpretation of some of the apparently arbitrary features of Bohr's initial atomic model.

http://www.users.csbsju.edu/~frioux/stability/deBroglieBohr.pdf

The Bohr model gives correct results for any one-electron atomic atom or ion. The following tutorial shows that it is also accurate when applied to the rather esoteric and short-lived hydrogen atom analog positronium, in which the proton is replaced the positron, the electron's antiparticle.

http://www.users.csbsju.edu/~frioux/stability/BohrPositronium.pdf

After reviewing the Bohr model for the hydrogen atom, the following tutorial outlines Bohr's model for the hydrogen molecule. It shows that it yields plausible values for bond energy and bond length.

http://www.users.csbsju.edu/~frioux/stability/H-H2-BohrModel.pdf

The examples presented in this addendum are based on classical pictures of the hydrogen atom, positronium, and the hydrogen molecule that have been moved in the quantum direction with de Broglie's hypothesis of wave-particle duality for matter. Bohr and de Broglie are the early quantum theorists who cut a path for those who created modern quantum theory.