Increasing Exclusion: The Pauli Exclusion Principle and Energy Conservation for Bound Fermions are Mutually Exclusive

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ABSTRACT

A review of standard quantum mechanics, including the Pauli Exclusion Principle, as it is applied to atomic species shows that the standard theory is not consistent with energy conservation. Particular focus is given to helium in which it is shown that energy conservation is only possible if the ‘ground state’ has electrons at two distinct energies. If the two electrons in the ground state, per current theory, are at the same energy as the ionization energy, it is demonstrated that according to the standard theory approximately 30 eV are lost during ionization, or alternatively, about 30 eV of energy are created during ionization/electron attachment. The same issue of energy loss during ‘relaxation’ of energy levels following ionization is shown to exist for all atomic species, thus demonstrating that the Pauli Exclusion Principle and energy conservation are not consistent for any atomic species. In contrast, a new model of quantum mechanics, Classical Quantum Mechanics (CQM), invented by R. Mills, is shown, following some modification, to be consistent with energy conservation for bound electron systems. This new model is based on the validity of Maxwell’s Equations and Newton’s Laws at all scales. Detailed, and remarkably simple, computations for determining the ‘ground state’ energy levels in one and two electron systems using CQM are presented. Excellent agreement with data is found.

INTRODUCTION

This article is intended to support two hypotheses. First, that standard quantum mechanics is inconsistent with known ionization energies. The ionization energies of the simplest multi-electron system, helium, are used to illustrate the point. In particular, we will endeavor to show that standard quantum fails because the proposed ‘relaxation’ of electron energy levels in atoms following ionization is inconsistent with the conservation of energy. This failing appears to be an inevitable consequence of assuming the Pauli Exclusion Principle (PEP) as generally understood. (The PEP as generally understood: No two electrons can have the same quantum numbers, and hence an orbital is ‘full’ when two electrons, identical other than having different spin directions, are in that orbital.) Second, we will show that the description of two electron systems based on a new paradigm of quantum mechanics, Classical Quantum Mechanics (CQM), developed by Randall Mills (1), but with a simple modification introduced herein, is consistent with energy conservation. Hence, it is concluded that modified CQM is a superior theory for the range of bound electrons. Extension to free electrons is left for future essays.

In order to provide support for the above dramatic hypotheses, we include sections normally not found in scientific articles. First, we find it expedient to include a description of the scientific process as it applies to physical sciences. Second, we find it absolutely necessary to offer a new means to classify standard quantum theory. Specifically, a novel classification scheme is presented to help ‘untangle’ the net of
quantum theories. It is argued there exist two distinct ‘standard’ quantum mechanics, the one ‘expository’ or ‘descriptive’ version employed by chemists and the quantitative version. Finally, there are the theories ‘between’ which are shown not to be true quantum in their very nature, indeed, they do not even employ Hamiltonians. These various versions of quantum are not compatible. Once we show that quantum is not even a coherent single theory, and that the inclusion of the PEP in any quantum model makes the model inconsistent with energy conservation, we argue it is scientifically rationale, in fact scientifically obligatory, to discuss alternatives to standard quantum theories. Only at this point in the presentation do we address the second hypothesis of the paper. To wit: It is shown that a new theory of quantum mechanics based solely on classical physics, particularly Maxwell’s equations and Newton’s Laws, and arguable one postulate regarding the strength of the interaction between two bound electrons, does give a totally satisfactory, algebraic, closed form, model of helium photo ionization with no variable parameters. Not only is it completely quantitatively consistent with all observations, but unlike standard quantum mechanics, the model is simple, self-consistent and consistent with energy conservation.

SCIENTIFIC PROCESS

In brief, physical science is a set of processes designed to produce an objective and predictive description of nature. Relevant to the present discussions are three types of scientific processes. One set of processes is designed to measure and record phenomenon in nature. In physics, observations considered scientifically objective share certain characteristics, including being repeatable and quantifiable. Also, through comparison/contrast with general observed patterns of nature, objective observations are categorized. For example, photo ionization of helium is one of the most studied processes in atomic physics. It has been repeated in countless labs and the quantities associated with the process have been verified repeatedly. Thus, the measured aspects of the process are ‘scientifically objective’, and it is clear the process is classified as one of a set of objectively observed processes, all similar in nature, known as photo ionization. The photo ionization of helium is a good example of a scientifically objective observation as it is clearly a highly repeatable process that has been precisely quantified, and belongs to a larger set of related processes, similarly repeatable and quantified.

A second process of physical science is finding ‘rules’, ‘descriptions’, and in physics in particular, quantitative THEORIES. These theories are valuable in that they can be used to predict behaviors quantitatively. A scientifically acceptable theory must be consistent with all objective scientific observations that are known for the proposed range of validity of the theory. Also, scientific theories should be self-consistent, and consistent with theories that are known to be consistent with all observables over the proposed range of validity. What is a ‘proposed range of validity’? The best example is the fact that, standard quantum theory is purportedly valid at all size scales, but classical physical theories including Maxwell’s Equations and Newton’s Laws are only believed to be valid for descriptions of physical processes at scales ‘greater than h-bar’ (Correspondence Principle).

Theories come and theories go. There is no heuristic for inventing theories. The best seem to come as epiphanies and involve simple ideas. The core equation in
Einstein’s special relativity revealed itself to him in a dream. In contrast there is a simple method for eliminating theories: scientific testing, the third category of scientific process relevant to this paper. A theory that fails scientific testing must be eliminated. Scientific testing is conceptually simple: A theory cannot be proved, but it can be disproved. Indeed, if a theory is shown to be inconsistent with just ONE objective scientific observation, either qualitatively or quantitatively, it is disproved. At a minimum, a theory shown inconsistent with a single objective scientific observation is no longer valid, or at least not valid over some range. Thus, for example, if quantum theory can be shown not to be consistent with any objective scientific observation, regarding valid scientific data for bound electrons, it is a rational, scientific, activity to seek new theories for bound electrons.

The above section/lecture should not be necessary. The fundamentals of the scientific process should be broadly understood. Unfortunately, the author believes many in the community are not aware that no theory is proven, hence questioning any theory is a scientifically sound activity, whereas arguing against even the consideration of alternative theories, as many distinguished scientists have in regard to quantum theory, is unscientific and irrational.

REVIEW OF STANDARD QUANTUM THEORY APPLIED TO BOUND FERMIONS

It is important in the context of the core of this paper to recognize that prior to the acceptance of the quantum model (QM) in its earliest form about 80 years ago, physicists believed that Newton’s Laws and Maxwell’s Equations applied at all size scales. However, no physicist succeeded in finding a means to explain the ‘quantum’ nature of stable energy levels in atoms, discovered via spectroscopy (e.g. Balmer series), using these laws. Hence, a new theory, herein called standard quantitative quantum mechanics (SQQM), was born that produced results quantitatively consistent with the quantum behavior of hydrogen. In time it was realized that this new theory, SQQM, was totally inconsistent with classical physics laws at size scales ‘less than h-bar’. For example, according to SQQM bound electrons, in single electron systems, are ‘point particles’ that jump randomly, obeying only a statistical description of their position- not forces, not conservation of momentum, etc., hence in violation of Newton’s Laws. Another clear example of the violation of Newton’s Laws: In those cases in which the point electron in a one electron system is far from the nucleus, allowed and expected according to the probability distribution used to describe the electron, it has nearly zero potential energy. At those positions in order to preserve the total binding energy, that is the sum of the potential and kinetic energy, the electron is presumed to have negative kinetic energy. This is clearly not consistent with Newtonian mechanics, even if it is argued these states only last a tiny fraction of a second.

The violations of Maxwell’s equations are equally clear. The random travels of the electron in the single electron system anticipated on the basis of the probabilistic model, result in instantaneous jumps into/out of the nucleus. In a classical sense this is accelerated motion, which by Maxwell’s equations should require the emission (jump toward nucleus) or absorption (jump away from nucleus) of energy. Yet according to SQQM these processes occur without the emission or adsorption of energy, hence SQQM is a clear violation of Maxwell’s equations.
To make SQQM match the older classical theories the community, under the guidance of Bohr, adopted the notion of the ‘Correspondence Principle’ more than 70 years ago. At some size scale, around h-bar, the two theories give identical predictions. Still, there are many who never were satisfied with this explanation. Einstein was very unhappy with the statistical description of the behavior of sub-atomic particles given in quantum theory, as succinctly put in his now famous comment, ‘God does not play dice with the universe.’

The above issues are well rehearsed even in basic quantum theory courses. However, the problems with SQQM are far deeper for multi-electron systems, e.g. helium, than they are for single electron systems. In particular: There is no physical meaning in quantum theory for the ‘description’ of electrons found in multi-electron SQQM. The wave function (multiplied by its complex conjugate) for a single electron can be interpreted as a probability: the probability that a point charge exists at a particular location in space. For multi-electron systems there is absolutely no physical meaning that can be attached to the wave function. For example, if the multi-electron wave function (multiplied by its complex conjugate) is interpreted as a ‘probability’ the question is: Probability of what? In fact, in most numerical work the wave function is treated as an actual charge distribution, in contradiction to the theory. This is discussed in more detail later.

Another issue is the notion that anything regarding SQQM is proven. Indeed, is the, above described, division of physics at a size scale of h-bar proven? No. A theory shown to be consistent with all known phenomenon is still not proved, just shown to be ‘likely’. After all, science is empirical, hence not susceptible to absolute proof. Although proving a theory is difficult, disproving one is simple. Indeed, all that is required to disprove or at least limit the applicable range of a theory is to show that the theory fails to accurately describe a single ‘objective scientific observation’. Indeed, this is the rationale given for restricting the domain of applicability of Newton’s Laws and Maxwell’s Equations to scales ‘greater than h-bar’.

It is still possible that Newton’s Laws or Maxwell’s equations do apply to mater on all scales. It has not been proven that they do not, all we know is that earlier efforts failed! Thus, the argument at the core of this manuscript, that a single epiphany regarding the correct geometrical description of elementary particles ‘allows’ correct (i.e. matches objective scientific observations) values to be obtained using classical laws of physics on all scales, cannot be summarily rejected as ‘unscientific’. If such a claim is made, it must be tested. In our case we provide a first test of the CQM physical description of bound electrons. We show that the new ‘physical’ model of the bound electron provides quantitative consistent with all presently known objective scientific phenomena. Will the physics community recognize the primacy of the scientific process and not be guided by the weight of tradition? Will they even consider questioning SQQM?

Another difficulty in a critique of quantum mechanics is the difficulty of ‘pinning down’ the actual theory. There is actually a ‘parallel’ quantum theory, herein called ‘Descriptive Quantum Mechanics’ (DQM), that is often erroneously conflated with SQQM. In fact, DQM is the theory generally taught to scientists and engineers. In the DQM theory, electrons are quasi-independent particles that independently occupy (hydrogen like) ‘orbitals’ and have energies/spins and other properties associated with the orbital they occupy. They can move between orbitals without significantly disturbing
electrons in other orbitals. Each electron in a multi-electron system has a particular energy, associated with the quantum level it occupies. The total energy of the electron system, say helium, is the sum of the energies of the individual electrons. The total spin of the system is the sum of the ‘spins’ of the individual electrons. Thus, for example, helium in the ground state has two identical electrons at approximately -25 eV each.

DQM also can explain phenomenon such as XPS data from multi-electron atoms in which it is clear that there are a multitude of ionization energies. That is, it is recognized that both ‘interior electrons’ and the highest energy electrons occupy stable orbitals with precise energy levels. Since its description of an atom indicates that electrons occupy specific energy levels, it is consistent with the supposition that atoms at lower energies (inner orbitals) can be ‘knocked-out’ of the atom (ionized) with a bolt of the correct energy. A cascade of radiation (either photons or electrons) with precise energies will follow as the outer orbital electrons in their independent orbits ‘fall in energy’ to fill the lower energy ‘holes’ created by the ionization of inner orbital electrons.

Is DQM a valid physics theory? As shown below, DQM cannot even produce an energy balance consistent with photoionization of helium, thus clearly DQM cannot be considered a valid scientific model. Is SQQM a valid physics theory? The answer is also no! It is true that in contrast to DQM, SQQM can produce a valid energy balance for the photo ionization of helium, but it will be shown it is completely inconsistent with other clearly measured phenomenon such as precise ionization energies for ‘inner’ electrons. This failure cannot be dismissed as minor as it leads to absurd conclusions, such as the notion that ‘ionization’ followed by electron capture could actually generate energy, a kind of quantum perpetual motion (details below). Moreover, the quantitative analysis offered by SQQM requires abandoning our intuition, Newtonian mechanics, Maxwell’s Equations, and, in fact, any physical picture of bound electrons.

Deposing DQM- Postulate: If quantum theory cannot explain photo-ionization of helium, then it is not a valid scientific model for any bound electrons. Below it is shown that the DQM model cannot explain either photo-ionization of helium or related phenomenon, for example electron attachment to He+.

The DQM model of the photo ionization process for atoms is that a photon with sufficient energy is absorbed by a bound (atomic) electron and hence ‘frees’ the electron. For example, in the case of hydrogen it is well established that a photon with a minimum energy of 13.6 eV is required to ‘free’ an electron, that is bring it to a state in which it no longer feels any force from its original nucleus. The fact that SQQM predicts a binding energy exactly equal to the measured ionization energy is one of the great triumphs of SQQM.

A second aspect of the model of relevance is the postulate that for all two electron atoms in their ground state, the two electrons are identical in all respects, except for their spin direction/spin quantum number. In particular, the two electrons have identical energy. For helium the energy of both electrons in the DQM model is approximately -24.7 eV, because, that is the energy required for ionization. In the DQM model the magnitude of the ionization energy and the magnitude of the energy of the electron that is being ionized are equal, just as it is the case for one electron systems. That is, the value -24.7 eV does not come necessarily from a direct quantitative theory (and DQM as defined here is not quantitative), but rather from objective scientific observation of the ionization process.
A third aspect of DQM of relevance is that after/during ionization the remaining electron in He+ ‘falls’ to a lower energy state. The measured value of ionization for the electron in He+ is -54.4 eV, a value in close agreement with the ionization calculated using Shrodinger’s equation for the ground state of a one electron atom with a two proton nucleus. Thus, the electron that remains after He is ionized ‘falls’, according to this theory, from approximately -24.7 to -54.4 eV.

The fourth and final aspect of DQM of relevance to is the inclusion in the theory of the Newtonian law of energy conservation. There is no ‘scale’ at which this general principle does not apply.

The reader, armed with the four ‘aspects’ of DQM discussed above can demonstrate to himself the fact that DQM cannot provide a satisfactory explanation for the simple process of photionization of helium. Thus, one concludes that the nice physical picture of the atom at the heart of DQM is not valid, and hence DQM is not a scientific theory. Specifically, the reader can show that DQM is not valid simply by consideration of the following questions. Remarkably, there is no need for math any more complex than basic algebra to disprove DQM.

1. During/after ionization the electron that is not ionized falls in energy from -24.7 to -54.4 eV. Where do the nearly 30 eV lost by the remaining bound electron in this process go? Since chemical reactions are basically the movement of electrons between states, this conundrum can be readily written in the symbolism of chemical reactions:

\[
\text{He (}-49.4 \text{ eV}) + \text{hv (+24.7 eV)} \rightarrow \text{He}^+(-54.4 \text{ eV}) + e^-(0 \text{ eV}); \quad \Delta H_{rxn}= -29.7 \text{ eV} \quad (1)
\]

Where the energy of the species, assuming the Pauli Exclusion Principle is correct, are provided.

2. During electron attachment to He+ to recreate atomic helium, where does the energy come from to raise the electron energy from -54.4 to -24.7 eV? In fact, it is an objective scientific observation that during electron attachment to helium almost 24.7 eV of energy is released as a photon. The release of energy during the process of electron attachment to He+ is in fact required to maintain ‘microscopic reversibility’.

\[
\text{He}^+(-54.4 \text{ eV}) + e^-(0 \text{ eV}) \rightarrow \text{He (}-49.4 \text{ eV}) + \text{hv (+24.7 eV)}; \quad \Delta H_{rxn}= +29.7 \text{ eV} \quad (2)
\]

3. Why is electron attachment spontaneous if the total energy of two bound electrons in atomic helium is lower than that of ionized helium? The total energy of the electrons in atomic helium (2*-24.7) is -49.4 eV. In contrast, for ionized helium, the total energy of the free electron (0 eV) and the one bound electron is -54.4 eV. Clearly ionized helium is in a lower energy state than helium. Accordingly, helium should spontaneously ionize.

\[
\text{He (}-49.4 \text{ eV}) \rightarrow \text{He}^+(-54.4 \text{ eV}) + e^-(0 \text{ eV}); \quad \Delta H_{rxn}= -5 \text{ eV} \quad (3)
\]

The failure of DQM to be consistent with energy conservation is not subject to additional study. Energy and energy change are state properties. All that is needed to evaluate consistency with energy conservation are the initial and final energy values. Study of how the process occurs cannot impact the net energy change, any more than a study of the path a balloon travels from the top of the Sandia Mts. in New Mexico (10,
600 ft) to my front yard (5200 ft.) in Rio Rancho, NM changes the fact that the balloon lost 5400’ of altitude in the process.

Most physicists conflate SQQM and DQM and attempt to save DQM because they perceive a threat to SQQM in the failure of DQM. In other words, they feel that the failure of DQM is a failure of the entire quantum hypothesis, because they don’t recognize the basic duality of standard quantum theory. As we shall see, they are wrong. However, it is interesting and revealing to discuss the many arguments posited to save DQM. These arguments, actually proposed ‘modifications’ to DQM, are considered below.

Two categories of modification are most common: First, are the ‘missed release’ models. These modifications always involve a release of energy never previously observed during photo ionization. Clearly, this is not part of any standard model. Second are the ‘stored’ energy models. Modifications of this type involve energy ‘storage’ in the He+ ion following ionization in the form of increased mass or in ‘fields’. Each category of answer is examined below.

It can quickly be shown, again with simple arguments, that all ‘missed release’ models lead to absurd conclusions. The patent office will not issue patents for perpetual motion machines, yet the missed release model of helium photo ionization can be shown to be equivalent to perpetual motion. Consider the following thought experiment. Helium gas is placed in a chamber with perfect mirrors. A pulse of 24.7 eV light from a laser is added. This energy will ionize the helium. In consequence, in these models, there is an increase in the effective nuclear charge to a full +2 on the remaining electron. At this point, almost 30 eV are released, presumably in the form of a photon. This is the ‘missed release’ of energy, ‘missed’ as it has never been observed. Next, as per valid scientific observation (and the principle of microscopic reversibility) the free electrons re-attach to He+ ions to reform atomic helium. This process is known to release the same amount of energy as required for ionization, nearly 25 eV of energy! Clearly, this model again violates the energy balance. The system starts and ends in the identical form: helium. No fuel is burned, yet a net of almost 30 eV of ‘free’ energy is generated for each photon of 25 eV put into the system. Solution to the energy crisis? Think again.

The proposed missed emission process can be written as two steps. First, helium is ionized and emits a photon:

\[
\text{He} + h\nu (+25 \text{ eV}) \rightarrow \text{He}^+ + e^- + h\nu (+30 \text{ eV}); \Delta H = +5 \text{ eV}
\]  

(4)

And then the helium ion recaptures an electron:

\[
\text{He}^+ + e^- \rightarrow \text{He} + h\nu (+25 \text{ eV}); \Delta H = +25 \text{ eV}
\]  

(5)

Another of the ‘missed emission’ modifications of SQM is that the ionized electron and the remaining He+ absorb the energy in ‘re-coil’. However, as in the co-ordinate system of the original atom momentum must be conserved, the electron, being almost 8000 times lighter than the ion, will have virtually all of the released energy. Is it possible the physics community never noticed 30 eV electrons produced during photo ionization? In any event, the Perpetual Motion argument applies to this model as well.
The ‘stored energy’ models all suffer from a lack of precision and quantification. Where is the energy stored? In the form of mass? Which particle in the ion gains mass during photo ionization? Is this even possible given that the rest mass of fundamental particles is immutable? The conversion of mass to energy involved entire particles, not parts thereof. How is the mass reconverted to energy during electron attachment? If the energy is stored in ‘fields’ the question is: What fields? Such a model must be quantified to be given any credence.

Explaining and Questioning SQQM- SQQM, as applied to atoms and ions, does produce a model of photoionization of helium that is consistent with energy conservation, but it must ‘give up’ all the physical content of DQM in order to do so. In SQQM applied to multi-electron systems, there are no ‘individual electrons’. Indeed, there is no such quantity as ‘the energy of an electron’ or the ‘spin of an electron’ or the ‘angular momentum of an electron’, or even the ‘probability distribution of an electron’. In SQQM one develops a single ‘wave function’, from a single Hamiltonian, not a number of Hamiltonians, that ‘number’ being set equal to the number of electrons. That would be the number required to obtain wave functions for each ‘particular’ electron. The Hamiltonian is intended to express all the energies arising from forces. Surprisingly, it never includes a magnetic interaction between electrons. For two electron systems, the Hamiltonian is written in non-operator form (2):

\[
H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|r_1 - r_2|}
\]  

(6)

Where \( p \) is the momentum, \( Z \) the nuclear charge and \( m \) is the reduced mass. The generalization to many electron systems is clear. One adds an additional kinetic and nuclear electrostatic term for each electron, and the number of two electron repulsive terms is one less than the number of electrons. This leads to the generation of a complex wavefunction that is most compactly expressed in the form of a Slater determinant (2), which automatically yields the anti-symmetric (independent of the labels on the electrons) form appropriate for Fermions (fractional spin particles). In particular for a two electron system the wave function is most easily expressed as a product-sum of ‘single particle’ wave functions and has this general form:

\[
\Phi = \frac{1}{\sqrt{2}}[\phi_1(A)\phi_2(B) \pm \phi_1(B)\phi_2(A)]
\]  

(7)

Where the subscripts represent the different ‘single particle’ wave functions (\( \phi \)), and the letters in parentheses are the electron identifiers. The above is actually multiplied by a ‘spin function’, and the nature of the spin function determines the identity of the +/- . A minus sign is correct if the spins are parallel and positive if they are anti-parallel, to insure total antisymmetry of the wavefunction. Note that mathematically all electrons are ‘indistinguishable’. That is, if the electrons are interchanged , the wave function is not changed. The mathematical indistinguishable nature of the electrons is presumed to reflect the ‘real’ world. In other words, the bound electrons of an atom are sort of ‘one big electron’, hence describable by one big Hamiltonian.

And exactly what is the ‘meaning’ of the wave function of this ‘one big electron’? It is not a ‘probability distribution’, because it is for the system of electrons. It is not
intended to be a descriptor of a single electron. NO INFORMATION ABOUT ANY SINGLE ELECTRON IN THE MULTI-ELECTRON ATOM IS PRESENT IN THIS WAVE FUNCTION. To insist that the wave function for a multi-electron system is a probability distribution, immediately raises the unanswerable question: *Probability of What?* It is not at all like the single electron system for which one could answer, ‘the probability that the infinitely small electron occupies particular co-ordinates’. One cannot say for two electron systems that the product of its wave function and its complex conjugate represent the probability that two electrons occupy particular co-ordinates. Nor can one say that the single energy value that can be calculated from the multi-electron wave function is that of a single electron. It is the sum of the energy of all the electrons. Thus, we conclude, as stated earlier, there is absolutely no physical meaning to a multi-electron wave function derived from proper employment of a multi-electron SQQM Hamiltonian. This leads to an additional puzzle regarding the Pauli Exclusion Principle that can be expressed in terms of a three electron atom: If electrons are indistinguishable AND only two can occupy a particular orbital (with opposite and paired spins), which two? In other words, as applied to SQQM the PEP as generally understood is not meaningful. In SQQM there are no independent identifiable electrons, thus it doesn’t make sense to present an argument regarding how many independent electrons occupy an orbital.

What is the value, therefore, of the multi-electron wave function when correctly determined according to the true theory? Answer: It can be used to compute ‘expectation values’ for the entire electron collection. That is, it can produce an expectation value for energy and radius and in a manner of speaking, spin. But these values are for the ‘system as a whole’. There is absolutely no means to separate electrons and speak of the energy of this or that electron. After all, there is only one Hamiltonian and it produces one wave function, that yields one energy.

The total energy for all the electrons, computed using full scale SQQM, can have predictive value. In the case of helium, this methodology correctly yields a total electron energy equal to the sum of the two measured ionization energies, approximately 79 eV. Can this be interpreted to mean that each electron has an energy of -39.5 eV? No. To repeat: there is no information about individual electrons that can be extracted from an application of SQQM theory to a multi-electron system. So, is this result really consistent with the known ionization energies? Yes, but a second calculation must be performed. The ionization energy is defined to be the difference between the system at the beginning of ionization and at the end of ionization, that is between a system of N electrons and one with N-1 electrons (more below). Hence, it is always necessary to make two calculations, one for a system of N electrons and one for a system of N-1 electrons. In the case of helium the calculation for an N-1 system is really simple as it is for a one electron system and this can be computed using Shrodinger’s equation and is approximately -54 eV. So, the approximate ionization energy is computed to be:

$$E_{\text{ion}} = -54 \text{ eV} - (-79 \text{eV}) = -25 \text{ eV} \quad (8)$$

in agreement with experiment.

The fact that the SQQM model successfully predicts ionization energies does not make it a scientifically acceptable theory. Can it produce the multiple ionization energies
measured with XPS etc? Not directly, as the only energy value it provides is for the total system of electrons and since it is organized to indicate the electrons in an atom are indistinguishable. No energy for individual electrons can be extracted from this formalism by its very structure.

Other problematic issues regarding SQQM not pursued here: Why is it that for helium all excited states are computed assuming the ‘unexcited’ electron stays unperturbed in its original energy level of -24.7 eV? Isn’t the ‘screening’ reduced when one electron is excited? According to SQQM, once the screening of an electron is modified so is its stable energy level. Another quantitative change that is never considered: following ‘excitation’ there must be seen in a change in the ‘correlation’ energy between the two electrons behavior for excited helium. Why isn’t the impact of that on the energy of the ‘unexcited’ electron considered? What is the basis for computing a ‘correlation energy’ from integration of a term with units of force, if such a force has ever been measured? In contrast, why is there no term in the Hamiltonian of SQQM or any of its derivatives for magnetic interaction energy, a force/energy easily measured? At exactly what stage/level of the excitation process does the ‘unexcited’ electron fall to the energy it has in ionized helium, -54.4 eV and ‘emit’ nearly 30 eV of energy?

Descriptive/Quantitative Quantum Models (D/Q)- As DQM has no quantitative content (e.g. can’t close an energy balance) and as SQQM cannot even begin to explain many well known physical phenomenon (e.g. multiple ionization energies in multi-electron systems) there is a natural tendency to invent models that are a bit of both.

Simple or naïve models are not satisfactory. For example, a first effort to ‘combine’ these two theories might be to ‘assume’ that distinct electrons occupy the ‘single particle’ wave functions that are combined to create the fully antisymmetric wave function required by SQQM (e.g. Equation 7) and that the overall wave function is just a means to express this mathematically. This can easily be shown to be wrong. If this were true, one could find the energy for each of these states, add the energies and get the same energy as for the fully anti-symmetric multi-electron wave function. It is clear that this is not true just by examining the expressions derived from the multiplications of the wave function(s) and their complex conjugates. There is no overlap in the expressions for the terms in the energy expression from the assumption that the electrons are in independent ‘single particle’ orbitals, and those for the true result for the full multi-electron wave function. In the ‘naïve’ one electron ‘interpretation’:

\[ E_{\text{tot}} = \sum_i \langle \phi_i(A)|H_i|\phi_i(A)\rangle \]  \hspace{1cm} (9)

where the Hamiltonians in the above expression are some type of ‘effective’ Hamiltonians, and the sum is over the total number of electrons in the system. In the theoretically correct case (SQQM), using the two electron example for simplicity, the total energy is computed from this expression:

\[ E_{\text{Tot}} = \frac{1}{2} \langle [\phi_1(A)\phi_2(B) + \phi_1(B)\phi_2(A)] | H | [\phi_1(A)\phi_2(B) + \phi_1(B)\phi_2(A)] \rangle \]  \hspace{1cm} (10)
There is no overlap of any of the terms in Eq. 9 and Eq. 10. Moreover, simply using single particle wave functions derived from perturbation theory it is easy to show that for helium Eq. 9 yields about 70% of the measured total energy whereas Eq. 10 yields better than 95% (4). The low energy computed on the basis of the assumption of independent electrons is one demonstration of the quantitative fallacy of this approach.

Note, single particle wave functions, derived from perturbation theory, lead to notions like ‘effective nuclear charge’, and ‘look’ like ‘hydrogen orbitals’, but from nuclei with reduced ‘effective nuclear charge’. However, other ‘basis’ functions can be used that are not hydrogen like orbitals. In fact, the ‘best’ basis set of orbitals by definition is the set that produces the lowest total system energy, not the set composed of hydrogen-like orbitals (3). This leads to other questions: If the orbitals don’t even resemble hydrogen like orbitals, on what basis does one still speak of “orbital angular momentum”? And in the absence of clear values for orbital angular momentum, on what basis do selection rules exist? In general, selection rules for transitions are rationalized on the basis that only transitions that conserve angular momentum are permitted.

The naïve approach outlined above does not work, but it does indicate some necessary elements of any ‘theory’ that produces both the ‘descriptive’ elements of DQM and the quantitative elements of SQQM. One element is the requirement that there be a set of Operator equations, one for each ‘independent’ electron in the multi-electron system. Solving a set of these equations leads to ‘eigenfunctions’ and ‘eigenvalues’ the former are then associated with orbitals and the latter with orbital energy levels. In fact, a significant fraction of all the effort of quantum theorists is focused on defining Hamiltonian-like operators, that is something like the $H_i$ of Eq. 9, as well as the best single electron wave functions (basis set) to use in these operator based quantitative quantum theories.

These methods do improve the performance for predicting energy that match observed ionization energies in some cases, although as illustrated below for the illustrative example selected for this essay, two electron system ionization energies, the computed energy values leave the conundrum of the unclosed energy balance unresolved. However, these methods are not to be confused with SQQM. They do not create a single wave function with total symmetry as required by the theory. Instead, employing a variety of assumptions, they treat a multi-electron system as composed of individual electrons with distinct energies. Moreover; the equations solved are not Hamiltonian equations. There are sets of operator equations, but these are not Hamiltonians. Moreover, there is one operator equation for each electron, not a single operator equation for all the electrons. This leads to a set of ‘orbitals’ each with a distinct energy, and in the final analysis the ‘orbitals’ generated are presumed (by adoption of PEP) to be doubly occupied by spin paired electrons and the eigenvalues are presumed to be the energies of these electrons. That is, the ‘single electron’ Hamiltonian methodologies are a means to create a middle, ‘quantitative’, ground between DQM and SQQM. To do this they must be neither.

There are many fundamental problems with attempting to make a theory that is somewhat in the middle of SQQM and DQM. For example, interaction energies are determined in these ‘one electron’ methods employing an inconsistent set of physical interpretations. For example, in the Hartree-Fock method (3) the operator equations (not Hamiltonians!) include two types of integrals that both represent the energetics of
interactions between ‘distinct electrons’: Colobmic repulsion integrals that require the electrons to be independent entities with charge distributions that are ‘decreed’ to be fully described by ‘single particle wave function x single particle wave function’*, and a second type of repulsive integral for which the underlying basis is ‘correlated motion’ of point particles (3). (Note, reference 3 contains a detailed example of the use of the Hartree Fock method to obtain the 'orbitals' and 'energy levels' of helium. This includes details of the two operator equations, with all the complexity of coupling between the equations fully revealed, that must be solved to obtain eigenfunctions and eigenvalues for the ground state of helium.)

There are clearly at least three major inconsistencies with SQQM inherent in this approach: i) The electrons are treated as independent (against the basic assumption of SQQM) particles, ii) these independent particles repel each other both as charge distributions and as point particles, and iii) in order to compute the magnitude of both types of repulsive interactions the wave functions, which in SQQM theory are probability distributions, are treated as charge distributions. Moreover, these ‘charge distributions’ have no ‘self-interaction’ energy, and magnetic interaction energy is not considered.

Final notes: i) Each Quasi-Hamiltonian operator involves integrations that depend on precise expressions for all the other one electron wave functions. Thus, computations are complex as they must be done interatively until the final wave function set employed in computing the Hamiltonians is nearly identical to the ‘estimated’ set of the previous iteration. ii) Full wave functions developed from the set of individual wave functions are not written in a symmetric form, despite the requirements of SQQM (3).

D/Q type computational methodologies are so often presented as ‘quantum theory’ that it is easy to get confused and begin to ‘buy’ the notion that they are fundamental theory. In fact, they are often labeled as ab initio to suggest that they are based on the most fundamental rules of quantum theory. Yet, they are based on ‘multiple operators’ (not Hamiltonians), rather than a single Hamiltonian and generate multiple ‘orbitals’ each with a distinct energy. All of these features of the D/Q models are contrary to the real SQQM theory. These D/Q methods, which come in innumerable variations, are employed because there is no choice. Indeed, given the fact that the very structure of SQQM precludes the possibility of obtaining multiple ionization energies, and DQM is simply not quantitative, only these ‘computational methodologies’ can provide any numerical information that ‘sort of’ resembles observation.

Koopman’s theorem, is the basis for ‘teasing out’ individual orbital energies from ab initio calculations, including Hartree-Fock. This theory requires the construction of a wave functions from a set of N ‘single electron wave functions’ (e.g. from Hartree-Fock) from which any single single electron wave function has been removed. The energy of the new, N-1, wave function can then be calculated and the energy so calculated is the ‘energy level’ of the removed electron, or:

\[ E_{N} - E_{N-1} = E_{\text{removed orbital}} \]  

Moreover, Koopman’s theory requires that the total energy be the sum of all the orbital energies! This clearly does not apply to our standard example, helium! In the helium case Equation 11 becomes:
If this is correct, then the two electrons in helium, which according to SQQM must be identical, cannot be identical, because if they were the total energy of helium would be close to -50 eV, which is clearly NOT the value (-79 eV) calculated with SQQM or measured experimentally. Clearly, employing this method returns us to the list of conundrums, including the perpetual motion conundrum, discussed in the section on DQM, above.

To be specific the Koopman theory is not consistent with energy conservation for all two electron systems. As an example; in the case of the helium atom an excellent result would be for the Hartree Fock single electron energy level of both electrons to be approximately equal to the measured ionization energy. Thus, if an ‘excellent’ result would be achieved if the Hartree Fock method, or any other D/S computation method, predicted a first ionization energy precisely equal to that measured experimentally. However, if this is the energy computed, then as noted repeatedly in this essay, there is an energy balance problem. Precisely the same objections raised repeatedly, including the ‘perpetual motion’ objection, again indicate that the method provides energy levels not consistent with a closed energy balance, and yields a total energy value for the two electron system totally inconsistent with the total energy obtained using any ‘total’ wave function computation. In fact it is generally understood that ab initio approaches do not yield outer electron energies consistent with measured ionization energies (3). Thus, the performance of any pseudo one-electron method is assessed generally by comparing computed energy level spacings with measured energy level spacing. In contrast, ionization energies are usually only computed using the ‘double calculation’ method described above (3).

Are the failures of the Koopman theory to achieve energy self-consistency for helium unique or the rule? It is the rule, as shown below, demonstrating once again that SQQM really says nothing about individual electrons in multi-electron systems.

It can be shown that an absurd ‘free energy’, as per the section on DQM, is always produced when the Koopman hypothesis is employed to ‘tease out’ the energies of individual orbitals, no matter what ab initio technique is employed to derive the full wave equation of the multi-electron system. This is inevitable because it is an experimental fact for atoms that the second ionization energies are always higher than first ionization energies. Thus, the sum of the total energy after ionization is never simply the original N atom energy minus the energy of the ionized/missing electron. It is always far lower than that! The system ‘relaxes’, or at least does so theoretically, to a lower energy. As our first example, we consider alkali metals as presumably the outer shell of these atoms, like helium, is occupied by two ‘s-electrons’.

For all of the alkali metals the second ionization energy is nearly twice the first. Moreover, according to the Koopman model, the highest energy, easiest to ionize, electrons are both in identical ‘s-orbitals’ prior to ionization. Assume one of these electrons is ionized. Measurement of the second ionization energy clearly shows that the s-electron that was not ionized ‘fell’ in energy by almost 100%! This leads to the same set of questions we encountered in the DQM section. Where does the energy ‘go’ when the s-electron that is not ionized falls to a lower state? Can’t we capture that energy and
thereby solve the energy crisis? From whence comes the energy to bring that electron ‘back’ to its atomic state during electron capture? After all, if a precise amount of energy is required to ionize an atom, then exactly the same amount should be released when the atom recaptures the ionized electron and returns to its original configuration. If more energy is released, then there is a net energy increase in the universe, if less energy is released, then for the universe as a whole energy is being destroyed! In fact, microscopic reversibility is observed. Happily, in the real world energy is not lost or gained during ionization or electron capture.

Finally, it is clear according to the Koopman model that the net energy of an electron and an alkali metal ion is lower than that of the atomic alkali metal. Hence, this model leads to the absurd conclusion that alkali metal atoms should spontaneously ionize. In fact, a brief look at ionization energies shows that for ALL atomic species each ionization energy is larger than the preceeding one. There are never two ionization energies in a row for any atom that are the same. Where does the energy go each time the electrons ‘relax’ following ionization? Where do ‘relaxed electrons’ find the energy to regain their old energy status during subsequent electron re-attachment, a process known to release energy.

Alternative Models- Are there methods other than SQQM that yield solutions closer to the truth? Indeed, ‘methods’ such as the SCF Xa and DFT approach that abandon the ‘wave function’ mathematics, treats electrons as individual charge distributions (i.e. they have no ‘particle like’ properties at all), compute interaction energy on the basis that electrons are charge distributions with ‘extra repulsion’ due to ‘correlation’, etc. generally yield results closer to reality than SQQM. But, it is not tenable to claim that these are simply modifications of SQQM. These computational approaches are in fact distinct theories. They are not presented as such, probably for ‘political correctness’. However, as distinct theories they are not proper subjects of this essay.

Summary: SQQM is a very limited model, capable only of computing total properties for multi-electron systems such as total energy, average radius, etc. The mathematics of SQQM essentially treats a multi-electron system as ONE BIG ELECTRON. Absurd conclusions are inevitable when the method is misrepresented as a means to provide information about individual electrons in the multi-electron system. In other words, SQQM/ab initio models are acceptable for finding the total energy of a system, and the change in the total energy of a system once the electron in the highest energy orbital is removed. However, once ‘energy levels’ for individual electrons are assigned, and these are ‘matched’ to measured phenomenon, specifically ionization energy, the energy balance for the system cannot be closed. This was specifically discussed as it applies to two electron systems and for all the alkali metals.

Finding ‘better’ ab initio models or better basis sets may improve ‘total energy calculations’, but no amount of manipulation can change the fact that for multi-electron systems individual electron properties, such as energy levels that match experimental values, cannot be ‘teased’ out of SQQM. In particular, it is clear that energy level values ‘teased out’ of SQQM are fundamentally inconsistent with the proposition that there is post-ionization energy level relaxation. There is a fundamental misunderstanding about SQQM. The truth is the SQQM model cannot be employed or ‘manipulated’ to provide data regarding energy states, etc. for individual electrons in a multi-electron system.
Unfortunately, this fact is generally missed, possibly due to the blizzard of mathematical sophistry that ‘is’ standard quantum mechanics.

This inability to yield individual electron energies is not a minor issue. It means the theory is inconsistent with some of the clearest facts in physics such as well-defined, multiple ionization energies for atoms.

NEW MODEL

Where do we go from here? Since it was demonstrated that both DQM and SQQM are completely inconsistent with the most common observations, we clearly need a new theory. The new theory should: 1) Be consistent with all classical laws of physics at all scales, 2) Lead to quantitative computations that close all energy balances, 3) Be quantitatively consistent with the observation that in all multi-electron systems (e.g. atoms) distinguishable electrons are found in distinct, sharply defined, energy levels, 4) Provide a clear value of the angular momentum of each electron in the multi-electron system. Specifically, we need a paradigm shift. One is offered below. That is, we attempt to explain via one example how the Classical Quantum Mechanics (CQM) theory developed by R. Mills overcomes all of the inherent difficulties of SQQM and DQM. Specifically, via one example, bound two electron systems, we show how CQM closes the energy balance and provides first and second ionization energies in agreement with measurement. This work also leads to the conclusion that in order to close energy balances the Pauli Exclusion Principle must be amended.

The improvements of the CQM model over SQQM as applied to two electron systems are as follows: Maxwell’s equations and Newton’s Laws work on all scales. Each electron is an individual particle with its own energy, magnetic moment, angular moment and size. There is no wave equation. There is no uncertainty principle. There are no variable parameters (i.e. all constants employed below are from NIST). And the quantized energy levels have energies in complete agreement with ionization energies. However, unlike DQM, this is a quantitative theory. Unlike SQQM this is a quantitative theory that yields the energy levels, spin, orbital angular momentum, radii of individual electrons. And unlike SQQM the fundamental equations employed to compute energy levels are simple algebraic, Newtonian force balances. Also, there is no difficulty tracking angular momentum. It is explicit that each electron has a precise angular momentum. Finally, the CQM model suggests a truly revolutionary conclusion (a conclusion not supported by RM, the developer of CQM): The Pauli Exclusion Principle is wrong. A new exclusion principle is postulated, based on the notion that electrons are actually physical objects: No two electrons can occupy the same space at the same time. That is, even if the spins are ‘opposite’ no two electrons can be identical in all other respects.

CQM of Two Electron Systems: The CQM model, developed previously entirely by Dr. Randall Mills (1,5), includes the revolutionary hypothesis that bound electrons around single nuclei (atoms) are spherical symmetric bubbles of charge, with a very specific mass and very specific charge current pattern. These bubbles of zero thickness charge (‘orbitsphere’) are not solutions to a wave equation. (Note: The orbitspheres can
have orbital angular momentum, and in those cases two dimensional waves, solutions to
the two dimensional wave equation, are found on the two dimensional orbitsphere
surface. However, for helium and other two electron atoms in the ground state there is no
orbital angular momentum on either orbitsphere. Hence, for the systems discussed below
there is no need to ‘confuse the issue’ by any consideration of ‘waves’.) It is simply
postulated that these bubbles will have properties consistent with all the valid scientific
observations regarding bound electrons including the right quantized energy levels, the
correct magnetic moment (determined with Maxwell’s Laws) and the correct g-factor
/angular momentum determined using standard mechanics). Moreover it is postulated
that these bubbles of negative charge obey Maxwell’s equations and Newton’s Laws.
Most of the above has already been thoroughly demonstrated and vetted in the reviewed
literature (5). For example, it clearly is shown that these orbitspheres, with the postulated
current pattern, do have the correct angular momentum and magnetic moment. It is also
clearly shown that they will not radiate. Although sophisticated arguments are found
elsewhere to demonstrate that closed loops of charge in motion will not radiate, it is clear
enough from ordinary experience. Indeed, it is well known that currents in
superconductors, for example in magnets formed in loops, do not radiate.

Of particular importance in evaluating this model: There is no requirement in
physics for a bound electron to obey a wave equation. All that is required is that the
model be consistent with all objective scientific observations. For example, a model that
is consistent with energy conservation and involves no ‘wave’ is consistent with
observation and thus a valid model, whereas a model that waves but does not conserve
energy is not a valid model.

In this paper we do not have the ambition or need to repeat the arguments made for the
success of the orbitsphere in producing quantitative results in precise agreement with
objective scientific observations about angular momentum, magnetic moment, g-factor
e.tc. of bound electrons. The goal of this paper is simpler: To show that two electrons,
each assumed to be simply a spherical shell of charge of ‘zero’ thickness (an
‘orbitsphere’), that obeys Newton’s Laws and Maxwell’s equations, will provide a
solution to the above energy balance conundrum. The reader unfamiliar with the ‘proofs’
offered in earlier papers demonstrating that the properties of the orbitsphere are
consistent with objective scientific observation, is urged consider the arguments below
and to avoid the impulse to ‘fire from the hip’. These readers are urged to take the
following principled pledge of the honest skeptic: I will expend effort studying the CQM
model of the bound electron (i.e. orbitsphere), if and only if it can be shown the
orbitsphere model provides quantitative predictions for two electron atoms more
consistent with objective scientific observations, including energy conservation, than
SQQM. That is, if the reader emerges from a study of the arguments laid out below,
convinced that simple force balances applied to the CQM ‘orbitsphere’ produces
predictions of two electron systems completely consistent with all objective scientific
observations of two electron systems, then they should retire to detailed study of earlier
papers that purport to show that the ‘orbitsphere’ model of the electron has the properties
claimed, particularly: non-radiation, correct angular momentum, and correct magnetic
moment.
CQM Model of the Helium Atom: In this model the atom is built in two stages from its constituent parts. (As the structure of helium is a ‘state property’ the path of construction will not impact the outcome.) In the first step a single electron/orbitsphere is ‘added’ to a nucleus consisting of two protons, and one or two neutrons to create a He+ ion. In the second step, a second electron/orbitsphere is added to the ion created in the first step. A helium atom is the product of this second electron addition. For both steps, the arguments below only concern computation of stable final state properties, not the mechanism of the process.

Step 1: The following are postulated regarding the orbitsphere: It is a physical object shaped like a ‘soap bubble’ of zero thickness that symmetrically surrounds the nucleus, obeys Newton’s Laws and Maxwell’s Equations, has a constant angular momentum, $\hbar$. Clearly, it obeys standard orbital mechanics. Given these requirements, the following force balance equation pertains:

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\varepsilon_0 r^2}$$

(13)

Where $r$ is the unknown radius, $v$ is the velocity of all the mass on the orbitsphere surface, $e$ is the charge on an electron, $\varepsilon_0$ is the permittivity of free space and $Z$ is the number of protons in the nucleus. In essence this is a very simple statement of Newtonian mechanics: The centripetal force must equal the central force, and the central force is the standard form of the electrostatic interaction between opposite charges. Next, we replace ‘$v$’ by noting that the angular momentum of all electrons must be $\hbar$:

$$v = \frac{\hbar}{mr}$$

(14)

Substitution of Eq.14 into Eq. 13 yields:

$$r = \frac{4\pi\varepsilon_0 \hbar^2}{Ze^2 m_e}$$

(15)

In fact, $m_e$ should be replaced by reduced mass, $m_r$, where $m$ is the mass of the atom:

$$m_r = \frac{m_e m}{m_e + m}$$

(16)

even though this is a very small correction.

Given this definition of Bohr radius:

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{e^2 m_e}$$

(17)
A very simple formula for the radius of the first electron in any one electron system is obtained:

\[ r = \frac{a_0}{Z} \tag{18} \]

This is significant as the energy of any object bound by a central force with inverse square strength can be obtained from standard mechanics once the mass, radius and angular momentum are determined. In these central force systems the kinetic energy (always positive) is equal to one-half the magnitude of the potential energy (always negative). And the total binding energy will be the sum of kinetic and potential energies. Thus, the total binding energy \( E_B \) will equal, in magnitude (not sign), the total kinetic energy \( E_{\text{kin}} \):

\[ E_B = -E_{\text{kin}} = -\frac{1}{2} \frac{h^2}{2mr^2} = -\frac{1}{8 \pi e_0 a_0} \frac{e^2 Z^2}{r^2} \tag{19} \]

This simple equation can be solved to yield the one electron energy for all one electron atoms simply by changing one parameter, \( Z \) - the number of protons (Table I). (Note: it is a simple matter to determine independently the potential and kinetic energy of the orbitsphere, add them together, and obtain the same result.)

Several comments regarding the above development are of value. For example, terms not included in the energy balance include ‘self-interaction’. (No self interaction terms are included in SQQM either. Instead, the infinite self-interaction of point particles is swept away in a mathematical vortex known as ‘renormalization’.) Not including any self-interaction terms in the CQM model is fully justified by Maxwell’s Laws. First, as the orbitsphere is a perfect conductor, it has no field inside. Faraday’s Law: There is no field inside a closed conductor. Hence, there is no interaction between charge and an internal field. Is there a field inside the charge layer itself? It is clear that the field is discontinuous. Inside the orbitsphere there is no field, outside there is a well defined field, equivalent to that produced from a single charge at the center of the orbitsphere. Where is the discontinuity? It is on/in the charge layer itself. This is in fact a standard postulate of E&M. There is no field generated by the charge in the layer of the charge, hence there is no self-interaction term. Alternatively, symmetry indicates there can be no field in the plane of a sphere. If the charge distribution is symmetric, there can be no preferred direction. The net result is that at any single point, symmetry shows that the fields must cancel. All points on the orbit sphere are electrostatically equivalent, hence the fields cancel at all points.

There are small corrections that lead to even greater accuracy. For example, as the electron is a real object, it has real velocity and thus there should be relativistic corrections. As the number of protons increases, the radius decreases and the velocity increases in order to maintain \( \hbar \) of angular momentum. Thus, the relativistic correction is only significant for large \( Z \). This and other small corrections are discussed in detail elsewhere (1).
Table I: Force balance calculations of the ground state energy of Orbitspheres in one electron systems. Comparison with experimental values is excellent.

<table>
<thead>
<tr>
<th>Specie</th>
<th>Calculated Number of Bohr Radii (Eq. 11)</th>
<th>Calculated Kinetic Energy and Ionization Energy, eV (Eq. 13)</th>
<th>Experimental Ionization Energy, eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.00</td>
<td>13.61</td>
<td>13.59</td>
</tr>
<tr>
<td>He⁺</td>
<td>0.500</td>
<td>54.42</td>
<td>54.58</td>
</tr>
<tr>
<td>Li²⁺</td>
<td>0.333</td>
<td>122.45</td>
<td>122.45</td>
</tr>
<tr>
<td>Be³⁺</td>
<td>0.250</td>
<td>217.69</td>
<td>217.71</td>
</tr>
<tr>
<td>B⁴⁺</td>
<td>0.200</td>
<td>340.15</td>
<td>340.22</td>
</tr>
<tr>
<td>C⁵⁺</td>
<td>0.167</td>
<td>489.81</td>
<td>489.98</td>
</tr>
<tr>
<td>N⁶⁺</td>
<td>0.143</td>
<td>666.68</td>
<td>667.03</td>
</tr>
<tr>
<td>O⁷⁺</td>
<td>0.125</td>
<td>870.77</td>
<td>871.39</td>
</tr>
</tbody>
</table>

Finally, it is interesting to note that the CQM model is just as accurate as SQQM model for the one system to which SQQM can be applied without approximation or mathematical sophistry of any kind: the excited states of one electron systems, e.g. atomic hydrogen. Again, simply algebraic force balances are all that are required. This is discussed elsewhere (1) but will not be pursued here in depth, because it requires introduction of another concept: photons as trapped electromagnetic energy in resonant cavities (i.e. orbitspheres of precise size). In the CQM model, photons do not mysteriously disappear upon capture as they do in standard physics, their energy converted to a higher potential for an electron. Rather, in CQM photons never cease to exist, but they can be trapped in the resonator cavity that is the orbitsphere. In this essay the minimum number of CQM concepts required to produce a resolution to the issue of closing the energy balance are introduced. The reader interested in other topics such as the excited states of one electron atoms is urged to pursue the matter (1,5).

Step 2: In the second step, an atom is formed when a free electron is captured by the ion created in Step 1. As the free electron about to ‘attach’ approaches the ion it ‘feels a force’ from a net central field equivalent to that of a single proton. That is, as the single electron on the ion is spherically symmetric, it creates a field equivalent to that of a point electron at its center. (This ‘electron generated’ field is restricted to the region outside the orbitsphere. As noted earlier it creates no field inside itself.) Thus, the two proton fields and the one electron field sum to create a field, outside the single orbitsphere of the ion, equivalent to that of a single proton. In other words, the orbitsphere field cancels one proton field outside of itself. In addition, the free electron as it approaches the ion feels a force from the magnetic field generated by the moving currents of the orbitsphere already present on the ion.

A force balance is once again employed to determine the stable radius. (It is a given that the final stable geometry for both electrons will be that of an orbitsphere, as only in that configuration will a bound electron in a central field not radiate.) However, in this
case the force balance should have two terms, one for the net one proton central field and one from the magnetic interaction. The form of the electrostatic term in the force balance is standard, as per Eq. 1. However, a new postulate is required for the form of the magnetic interaction. To wit, it is postulated that the magnetic force between any two ‘nested’ orbitspheres, in which neither has orbital angular momentum, in any atom (of which two electron atoms are a subset), is described with this equation:

$$F_{\text{mag}} = \frac{\hbar^2}{r^3Z\mu_e} \sqrt{s(s+1)}$$

(20)

where \(r\) is the radius of the electron being acted on and \(s\), the spin quantum number, is 1/2. For the purposes of this essay, this expression for magnetic force between two electrons will be taken simply as a postulate. In the full development of CQM, available elsewhere, it is argued that this term is derived from the standard Lorentz force (1). It is a complex derivation. However, the expression given is acceptable as a postulate as it has a simple algebraic form, uses only the most standard constants (Plank’s constant, mass of an electron) and has no adjustable parameters. It is left to others to engage in a ‘postulate’ or ‘derived from Lorentz force’ debate. For those who must debate, please recall: Postulates are at the heart of all physics. They are permitted.

Clearly the outer electron feels two forces. It feels the magnetic force from the other electron and it feels a net electrostatic force equivalent to one proton. (As noted above the fields at the outer electron arising from the inner electron and one proton, both mathematically represented by point charges at the center of the atom, cancel.). In sum, this leads to the following force balance:

$$F_{\text{tot}} = \frac{mv^2}{r} = \frac{e^2}{4\pi\varepsilon_0r^2}(Z-1) + \frac{\hbar^2}{r^3Z\mu_e} \sqrt{s(s+1)}$$

(21)

This can be re-written, using Eq. 14, as:

$$\frac{\hbar^2}{m_r^3} = \frac{e^2}{4\pi\varepsilon_0r^2}(Z-1) + \frac{\hbar^2}{r^3Z\mu_e} \sqrt{s(s+1)}$$

(22)

Multiply through by \(r^3\), and \(r\) can be quickly obtained (Bohr radius defined by Eq. 17):

$$r = a_0\left[\frac{1}{(Z-1)} - \frac{\sqrt{s(s+1)}}{Z(Z-1)}\right]$$

(23)

This simple algebraic equation, derived from a straightforward two term force balance, will be shown to provide energies consistent with measurements of ionization energies, to better than two percent accuracy, for all measured two electron atoms. It also yields an absolute value to the size of the ground state for all two electron atoms, a dimension that can be used to predict scattering behavior.

Computing the energy of this second electron is not quite as simple as for the first, because in this case the central forces are not inverse square. The energy must be
calculated as the sum of the potential, kinetic, and magnetic energies. The energy balance for the system is:

\[ \Delta E_{\text{tot}} = \Delta E_{\text{pot}} + \Delta E_{\text{kinetic}} + \Delta E_{\text{magnetic}} \]  

(24)

where \( E_{\text{pot}} \) is the electric potential energy. Moreover, it is clear that the change in the magnetic energy is equal to the work done against the magnetic field in moving from \( r \) to infinity, and the change in the electric potential energy is equal to the work done against the electric field. Thus, the change in the magnetic energy is determined from an integration of Eq. 17:

\[ \Delta E_{\text{magnetic}} = \frac{1}{2} \frac{1}{Z} \frac{\hbar^2}{m_r} \sqrt{s(s+1)} \]  

(25)

Similarly, the change in the electric potential energy can be determined from integration of the electric force term:

\[ \Delta E_{\text{Pot}} = (Z-1)e^2 / 8\pi\varepsilon_0 r \]  

(26)

The change in the kinetic energy, of course, is from a positive value to zero. Hence:

\[ -\Delta E_{\text{kin}} = \frac{1}{2} \frac{\hbar^2}{m_r^2} \]  

(27)

Thus the total energy change of the outer electron during ionization, that is the energy input to bring the outer electron from the bound state to the free state is:

\[ E_{\text{ion}} = \Delta E_{\text{tot}} = (Z-1)e^2 / 4\pi\varepsilon_0 r + \frac{1}{2} \frac{1}{Z} \frac{\hbar^2}{m_r^2} \sqrt{s(s+1)} - \frac{1}{2} \frac{\hbar^2}{m_r^2} \]  

(28)

It should be noted that this equation explicitly shows that the kinetic energy, inherent in any physical object in a stable orbit, is ‘re-deployed’ such that it contributes to the ionization process. Once the simple formula for \( r \) (Eq. 23) is substituted in Equation 28 it can be shown:

\[ -\frac{1}{2} \Delta E_{\text{Pot}} = \Delta E_{\text{Kin}} + \Delta E_{\text{Mag}} \]  

(29)

It is interesting to reflect on the qualitative ‘mechanics’ of Eq. 29. In inverse square force fields, standard orbital mechanics in gravitation fields for example, the magnitude of the potential energy equals one half the magnitude of the kinetic energy. In the presence of an added central force (e.g. magnetic) the velocity required to maintain the object in stable orbit at any particular radius should be larger, hence the magnitude of the kinetic energy larger. Since the changes in kinetic and magnetic energy are opposite in ‘sign’ during ionization, this qualitative analysis is consistent with Eq. 26. In any event, Eq.28 can be re-written:
\[ E_{\text{ion}} = \frac{1}{2} \Delta E_{\text{Pot}} = (Z - 1)e^2 / 8\pi\varepsilon_0r \]  

(30)

Can two extremely simple one-dimensional formulas really quantitatively predict all the known ionization energies of two electron atoms? That is, can the simple formula for ionization energy with no adjustable parameters, derived from a simple algebraic energy balance, Eq. 30, and an equally simple solution for the radius, Eq. 23, derived from a one dimensional force balance also with no adjustable parameters, using only NIST values for physical constants really predict all of the known ionization energies for two electron atoms? The answer, as seen in Table II is a yes. Helium shows the worst agreement, yet is within two percent. As Z increases, the ions become smaller (literally!), and the relative error decreases to a small fraction of one percent.
Table II: Comparison of predicted and measured ionization energies in two electron systems.

<table>
<thead>
<tr>
<th>(Z)</th>
<th>Ionization Energy, (a_0^*)</th>
<th>Ionization Energy, CRC **</th>
<th>Relative Error***</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.5669</td>
<td>23.9965</td>
<td>24.587</td>
</tr>
<tr>
<td>3</td>
<td>0.35566</td>
<td>76.50902</td>
<td>75.64018</td>
</tr>
<tr>
<td>4</td>
<td>0.26116</td>
<td>156.289</td>
<td>153.897</td>
</tr>
<tr>
<td>5</td>
<td>0.2067</td>
<td>263.295</td>
<td>259.375</td>
</tr>
<tr>
<td>6</td>
<td>0.17113</td>
<td>397.519</td>
<td>392.087</td>
</tr>
<tr>
<td>7</td>
<td>0.14605</td>
<td>558.958</td>
<td>552.0718</td>
</tr>
<tr>
<td>8</td>
<td>0.12739</td>
<td>747.61</td>
<td>739.29</td>
</tr>
<tr>
<td>9</td>
<td>0.11297</td>
<td>963.474</td>
<td>953.112</td>
</tr>
<tr>
<td>10</td>
<td>0.10149</td>
<td>1206.552</td>
<td>1195.8286</td>
</tr>
<tr>
<td>11</td>
<td>0.09213</td>
<td>1476.84</td>
<td>1465.121</td>
</tr>
<tr>
<td>12</td>
<td>0.08435</td>
<td>1774.34</td>
<td>1761.8055</td>
</tr>
<tr>
<td>13</td>
<td>0.0778</td>
<td>2099.0537</td>
<td>2085.98</td>
</tr>
<tr>
<td>14</td>
<td>0.07216</td>
<td>2450.977</td>
<td>2437.63</td>
</tr>
<tr>
<td>15</td>
<td>0.0673</td>
<td>2830.1124</td>
<td>2816.91</td>
</tr>
<tr>
<td>16</td>
<td>0.06306</td>
<td>3236.459</td>
<td>3223.78</td>
</tr>
<tr>
<td>17</td>
<td>0.05932</td>
<td>3670.0178</td>
<td>3658.521</td>
</tr>
</tbody>
</table>

The values reported and those predicted will never be close enough to satisfy all physicists. Some small corrections are probably required. Several are under consideration. Still, the remarkable agreement between measured values and predicted values for such a simple formula cannot be dismissed with a wave of the hand and a reiteration of the cliché: ‘We can do better with our present methods that only requires many hours of supercomputer time.’ And the cliché ignores the fact that in the first part of this essay it was demonstrated that standard quantum theory is fundamentally wrong in that it presumes that the ionization energy is equal to the energy of BOTH/Either electron(s). That is, SQQM and DQM are absolutely and totally wrong about the energy of electrons in two electron systems. In contrast, in the modified CQM model, described above, the ‘inner electron’ energy is virtually the same as that given in Table I. Some perturbation (<1 eV) will occur, due to the removal of the magnetic ‘pull’ of the outer electron.

Isn’t there some experimental data that proves the Pauli Exclusion Principle? Quite the contrary. The existence of ‘relaxation’ in energy levels following ionization in all atomic systems disproves that theory. The only way to avoid the ‘perpetual motion’ arguments presented earlier in this essay is to insist that no two electrons have the same energy in atomic systems. Electrons energy levels don’t actually relax (not significantly, ca. <1 eV) following ionization of the highest energy electron. The energy level of all the lower energy electrons are at most slightly perturbed by the ionization event. They are already at the supposed ‘relaxed’ energy levels when in the atomic state!
the entire notion of a ‘proof’ is a misunderstanding in physics. As explained in the section on the scientific method it is possible to disprove a scientific theory. It is not possible to prove it. Also, demonstrating the falsehood of a theory only requires that one issue be unresolved. Thus, the failure of the Pauli Exclusion Principle to be consistent with energy conservation is more than sufficient evidence that the theory is not valid. Infinite evidence of ‘consistency’ with other types of data (e.g. spectroscopic) cannot overcome the failure of the model to be consistent with energy conservation.

The reader is urged to avoid the confusion of further consideration of energy level relaxation. Relaxation is not a real effect, but only one required by standard quantum theory. We also note that in fact (not theoretical fiction) and according to CQM the energy levels of the more tightly bound atomic electrons are only slightly perturbed by the ionization of the outermost/highest energy electron. And we note that contrary to standard quantum theory, this observation of fact, and its prediction by CQM theory, does provide consistency with energy conservation in the universe.

Other purported supports for the Pauli Exclusion Principle are equally simple to dispose. For example, all two electrons in a zero spin state are Bosons according to CQM theory. That is, as all electrons have h-bar angular momentum, and the two moments in ground state two electron systems are equal and opposite, they ‘cancel’. The objects have no net angular momentum. Thus, CQM two electron systems in the ground state are boson, as bosons have no angular momentum. If the magnetic moment of these bosons aligns with an applied field, as required for a species to produce an EPR effect, this means that there is a magnetic moment. If there is a net magnetic moment, and ‘g’ is not zero, then there must be angular momentum. Thus a contradiction in classical physics, the basis of the CQM theory, arises for any magnitude magnetic alignment with an applied field for a Boson. Hence, there is no magnetic alignment and no ESR/EPR signal for any two electron system in its ground state according to CQM theory. Hence, there is absolutely no basis for arguing that the absence of an EPR signal indicates that the two electrons are ‘identical’. Clearly, as is well known experimentally, in excited states of helium in which neither the angular nor the magnetic moments cancel, an EPR signal will be observed according to CQM theory.

SUMMARY

Numerous arguments are made in this essay regarding flaws in standard quantum theory as applied to atoms and ions, and an equal number are made in support of a new theory (although limited in this essay to the range of bound electrons), Classical Quantum Mechanics. The basic arguments against standard quantum could be classified as ‘The Emperor Has No Clothes’ arguments. It is overwhelmingly evident from experimental observation that the inclusion in standard quantum of the Pauli Exclusion Principle dooms the theory to failure on the basis of simple energy balance considerations. For example, it is demonstrated that if electron energy levels truly relaxed following ionization, the very process of ionization would generate energy, yes increase the energy in the universe without any concomitant mass loss. This is clearly not true. It is concluded that electron energy levels do not relax (not significantly) following ionization. In fact, there is no experimental evidence of such a process. It is only believed to occur because it is required by standard quantum. Energy balance failures are simply ignored.
Demonstrating the failure of the Pauli Exclusion Principle to be consistent with known ionization energies, a key plank of SQQM, deals a fatal blow to the entire theory of SQQM (at least as it applies to bound electrons). We show that this hole can be sealed by a slightly modified version of a new theory, CQM, developed by R. Mills after modification to include a more exclusive form of the exclusion principle. Specifically we show that the modified theory predicts very accurately the two distinct energies in two electron systems. That is, using simple one-dimensional, closed form, no variable parameter, Newtonian force balances, the two energies predicted by the theory nearly perfectly match the known first and second ionization energies of these systems.

REFERENCES