

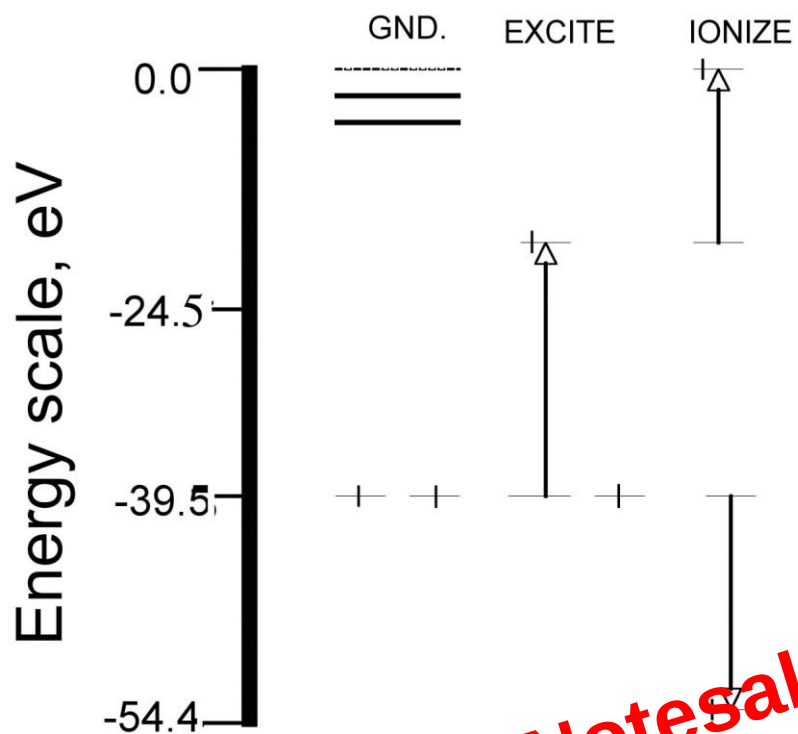
out of the atom. There are three versions for helium. In the 'NON INTERACTING' model the two electrons do not interact, and the 'unexcited' electron remains at its initial energy level until ionization. The key features are i) both electrons are initially at ~ -39.5 eV (agrees with total observed electron energy of -79 eV), ii) None of the energy levels of excited states are the same as in the 'Standard Model', iii) spacings between energy levels are the same as in Figure 1, iv) no energy level corresponds to -24.5 eV, v) there is a gap of about 15 eV between the highest excited state and the vacuum energy and vi) the jump to the vacuum level occurs when the 'unexcited' electron falls to its final energy of nearly -55 eV. In the 'INITIAL DROP' model, the electrons also do not interact, but the 'unexcited' electron falls to its final energy state under any and all excitation processes. Thus the first excitation process puts the energy of the non-ionizing electron 'drop', all the way to -54.4 eV, into the excited/ionized electron. After the first step the nonionizing electron remains at its 'ionized' He level though all subsequent excitation or ionization processes. In this model, the excited state energy levels of the 'excited/ionized' electron match those of the 'STANDARD MODEL' and there is no large energy gap between excited states and the vacuum.

In the 'STAGED DROP' model, it is assumed that there is electron-electron interaction energy. The total energy of each electron is -39.5 eV, but that energy is made up of negative energy of binding with the nucleus and some positive, repulsive, 'bond' energy coming from the interaction between the electrons. For example, there could be a (repulsive) total 'bond' energy of $+10$ eV, and each electron could be bonded to the nucleus with an energy of -44.5 eV. As the two electrons are identical, it is rational to assign half of the 'bond' energy to each electron. Thus, the net energy of each electron is -39.5 , as shown. (This assignment of half the bond energy to each electron is certainly consistent with standard quantum which always assumes the existence of a repulsive force that is positive energy between electrons, yet assigns specific energy levels to the electrons.) With each photon adsorption/excitation process there is a concomitant drop in the energy of the unexcited electron. Thus the 'unexcited' electron occupies an entire set of energy levels, one for each excited state. Other notable features of this model: All of the excited states are at lower energies than those given in the 'Standard Model', and all of the energy spacings between excited energy levels are larger than those of the standard DQM model.

All of the features of all of the energy level models present in Figure 2, EXCEPT THOSE OF THE STANDARD MODEL, are consistent with the PEP, and an energy balance. That is, the energy required for ionization in the standard model is -24.5 eV, exactly the observed input energy during the first ionization of helium. Thus, there is no accounting for the energy lost when the 'unionized' electron falls nearly 30 eV in energy following the first ionization. In contrast, the other models all account for the energy lost by the 'unionized' electron when it looses, in all the new models, about 15 eV. That energy, plus the input energy of 24.5 eV are required to boost an electron initially at 39.5 eV to the vacuum level. The 'Staged Drop' model is unique in that the positive repulsive interaction energy is given up in a series of steps, however, all energy is accounted for in this model.

Given present information it is impossible to tell which, if any, is correct. It is abundantly clear that no current quantum model of the energy levels in helium agrees

'NON INTERACTING MODEL'



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electron from -24.7 to -54.4 is not accounted for. Hence, there is approximately 30 eV of energy 'lost to the universe' during the ionization process as it is described in the Standard Model.

THE REAL DEAL: SQQM

SQQM, is the actual quantitative quantum theory developed by Heisenberg, Schrödinger, Bohr, etc. As applied to atoms and ions SQQM does produce a model of photo ionization of helium that is consistent with energy conservation, but it must 'give up' all the physical content of DQM, in fact all physical meaning, in order to do so. Note: SQQM is a far more sophisticated mathematical 'theory' than DQM and hence different arguments must be brought to bear against it than those employed against DQM. Thus, the arguments given below, particularly those regarding the inherent inconsistency of the Pauli Exclusion Principle and Energy Conservation, as per the title of the manuscript, are distinct from those employed in the DQM section.

The core arguments against multi-electron SQQM are: i) the PEP is technically meaningless as applied to SQQM, ii) SQQM does not have physical meaning for multielectron systems, iii) SQQM is mathematically inconsistent because it switches back and forth between phase space and real space, iv) SQQM is self-inconsistent because for one electron the wave function is a probability map in real space whereas for multi-electron systems there is no real space map and no probability distribution (acceptable theories are consistent theories), and v) SQQM arbitrarily drops some elements of classical physics (Newton's laws, Maxwell's equations, magnetic force), keeps others (electrostatic potentials) and invents others (correlation energy).

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 (18):

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{Ze_1}{r_1} - \frac{Ze_2}{r_2} + \frac{e_1 e_2}{|r_1 - r_2|} \quad (6)$$

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

The reader can show that the wave function multiplied by its complex conjugate actually becomes the sum of four terms, each having four of the original one electron/hydrogen type wave functions. Two of these terms integrate to zero because the wave functions are orthonormal in both 3D phase spaces. Two of these terms integrate to one, because over both phase spaces the integrated values of the wave function and its complex conjugate are one, hence the product of the two integrations is one. It is notable that the number of dimensions required for integration/normalization increases with the number of electrons. For two electrons, two 3 dimensional phase spaces are required, for three electrons the total number of dimensions is nine, etc.

It might be reasonable to argue that the 'phase space' approach is acceptable if it were employed consistently. It is not. Indeed, the last term in the multi-electron Hamiltonian (Eq. 6) requires computing the energy of electrostatic interaction between two electrons in real space. (This in itself is odd. Given that Newton's Laws and Maxwell's equations are dismissed 'at the level of h-bar' why not electrostatic interactions? And why is there no term in the Hamiltonian for energetic interactions between the magnetic moments of electrons?) Apparently, and not for sake of consistency, it is believed that electrons cannot interact in 'phase space', they can only interact in real space!

Historically there has been a great deal of confusion on this very point. For example, we show below how two giants of quantum mechanics suggested means to understand and compute this interaction that are fundamentally flawed.

Examine the electron-electron interaction term in the two electron Hamiltonian (eq. 6), where r ($r=r_1-r_2$) is the distance between the electrons, in *real* space. Clearly, at any point in space where the two electrons are at the same position ($r=0$) there is a singularity at which point the repulsive energy term in the Hamiltonian goes to infinity:

$$E = \int \frac{1}{r} |\psi|^2 dr \quad (8)$$

where E in this case is the repulsive energy. Early in the development of SQQM, methods to evaluate this integral containing the very apparent singularity were offered. These explanations continue to be cited, and the results accepted. However, as we show below, they are clearly not correct. For example, Eyring *et al.* (20) suggested the following equality could be used, and would lead to a finite value of the repulsive energy

$$\frac{1}{r} = \sum_{n=0}^{\infty} \frac{(-1)^n (2n+1) r^{2n}}{2^{n+1} n!} \quad (9)$$

where r_{ij} is the "distance between the two particles" and " $r_>$ " be the greater of r_i and r_j and $r_<$ be the lesser". Developed using a 'proof' that appears questionable, Eyring's proposed substitution leads to the above expression, one in which the equal sign is clearly wrong. Indeed, consider that $r_<$ is at the origin, and $r_>$ is any point but the origin. In this case, every term in the sum contains a zero co-efficient ($r_</r_>$), thus each term is zero, and

$$E_{\text{ion}} = \Delta E_{\text{tot}} = (Z-1)e^2 / 4\pi\epsilon_0 r + \frac{1}{2} \frac{\hbar^2}{m_e r^2} \sqrt{s(s+1)} - \frac{1}{2} \frac{\hbar^2}{m_e r^2} \quad (35)$$

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. 30) is substituted in Equation 35 it can be shown:

$$- \frac{1}{2} \Delta E_{\text{Pot}} = \Delta E_{\text{Kin}} + \Delta E_{\text{Mag}} \quad (36)$$

It is interesting to reflect on the qualitative 'mechanics' of this equation. In inverse square force fields, standard orbital mechanics in gravitation fields for example, the magnitude of the potential energy equals twice 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. 35. In any event, Eq. 36 can be rewritten:

$$E_{\text{ion}} = \frac{1}{2} \Delta E_{\text{Pot}} = (Z-1)e^2 / 8\pi\epsilon_0 r \quad (37)$$

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. 37, and an equally simple solution for the radius, Eq. 30, 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.

160.06306 3236.459 3223.78 -0.003932961

170.05932 3670.0178 3658.521 -0.003142472

* Eqs 24 and 30, **Eq. 37, *****(Column 4-Column 3)/Column 4**

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. Indeed, in Mills's model a 'magnetic energy of pairing' is computed that dramatically improves the agreement with data (1, chapter 6), however, the origin of this correction is not clear to the present author. 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. That is, SQQM only computes the energy of both electrons together, and the values of energy computed with DQM and D/Q, always assume the PEP. In fact, there exists not a single D/Q computation for helium in which the only energy consistent with an energy balance, the PEP and the known ionization energies, that is -39.5 eV, is the ground state 'target' energy of the many computational manipulations. In contrast, in the modified CQM model, described above, the 'inner electron' energy is virtually the same as that given in Table 46. That is, if it is correct, the modified CQM model presented here *predicts* something truly unique: *it predicts that the PEP is wrong.*

Isn't there some experimental data that *proves* the Pauli Exclusion Principle? Note first that 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, according to any standard paradigm, or with the predictions of CQM, is reason for doubt. (The only paradigm consistent with PEP and an energy balance for helium is the one introduced at the end of the DQM section of this paper, e.g. both electrons are at -39.5 eV). 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. Hence, it is clear that any D/Q or DQM model that assumes the PEP must also assume 'boost'.

The reader is urged to avoid the confusion of further consideration of energy level 'relaxation' without direct emission. There is no 'proof' of it. We postulate relaxation is not a real effect, but only one required by DQM and D/Q M versions of standard quantum theory. There is no experimental support for this belief. **In fact** (not theoretical fiction) 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.

The addition of the 'boost' concept allows the PEP and an energy balance to be in harmony. However, if one adds the 'boost' hypothesis there are several new problems. First, it requires that the computed energy levels not match any experimentally measured value. For example, the PEP, with boost, requires energy level for each electron in the ground state of helium to be -39.5 eV, clearly very different from the first ionization energy of -24.5 eV or the second ionization energy of -54.4 eV. Second, major changes in the present theory would be required, such as entirely new computations of the energy state of the un-excited electron during excitation process. Not even a 'talking model' of the energy levels of the 'unexcited' electron currently exists. Indeed, the most basic issues, such as the impact of 'boost' on the energy of excited states relative to the vacuum have never been discussed (see Figure 2).

It is postulated herein that electron energy levels do not relax (not significantly) following ionization. A corollary is that there is no 'boost'. In fact, there is no experimental evidence of either relaxation or boost. Relaxation is only *believed* to occur because it is required by theory in some cases.

The energy balance failures of DQM are generally ignored, or are conflated with process steps, such as change in screening constant following ionization, which are irrelevant to computation of an energy balance (44). Indeed, as energy is a state property only the initial and final state values are required to determine the net amount of energy released and/or adsorbed during a state change. The nature of the particular process of change is not relevant to this computation. In fact, it has been shown the only means to have harmony between the PEP and an energy balance is to postulate that the energy levels of stable states in atoms do not match any measured experimental values.

The only 'category' of standard quantum modeling for which the PEP does not require the existence of energy levels that don't match ionization energies is SQQM. And that is because for this version of quantum the PEP is meaningless. Discussions regarding the application of PEP to SQQM are equivalent to arguing regarding the shape of red. Moreover, SQQM doesn't provide energy level information for individual electrons. It only provides the total electron system energy.

Although SQQM does not fail the two electron system energy balance test, it is shown that SQQM is not a particularly attractive theory. It is inconsistent with basic spectroscopy (e.g. multiple ionization energies for multi-electron atoms), Maxwell's equations, Newton's Laws, the existence of spin, requires renormalization of self-energy, and fails the self-consistency requirement of valid scientific theories. Moreover, if SQQM provided results in agreement with spectroscopy, the other classes of quantum theory would never have developed. It even requires a new force ('correlation energy'), a corresponding set of optimized variable parameters, and fails to account for obviously existing magnetic interactions between electrons. Multi-electron SQQM wave functions are also clearly not physical. There is no 3-D wave! At best there are waves in 3N (N is the number of electrons) phase space. Exactly where is 3N dimensional phase space?

In contrast, a slightly modified version of a new theory, CQM, developed by R. Mills is consistent with Maxwell's Equations, Newton's Laws and spectroscopy. It is a totally physical theory as it posits that electrons are real particles with very specific real shapes in real space. Magnetic moments arise from moving charge, as per the Maxwell equations. Forces from electrostatic and magnetic interactions are the only forces. There