COMMENTS ON EXOTIC CHEMISTRY MODELS AND DEEP DIRAC STATES FOR COLD FUSION

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Abstract

Several models are examined in which it is claimed that cold fusion is the result either of tight binding of the electrons in H isotope atoms or molecules, or of an electron-H isotope resonance which allows a higher probability of Coulomb barrier penetration. In the case of models in which the electron is tightly bound to the H isotope atom, we show that states below the most deeply bound (–16.39 eV) are impossible in principle. We also present evidence against the possibility of the existence of electron-H isotope resonances. Finally, a lower bound is found for the binding energy of H isotope molecules which is above that calculated in the tightly bound electron-H isotope models.

1. Tightly Bound Hydrogen and Deuterium

A number of models assume the existence of an exotic chemical system whose occurrence either precedes nuclear synthesis or makes it quite unnecessary. The similarity of these postulated models is in their tight binding of electrons in atoms and/or molecules. In one of the simplest, the authors[1] claim that in addition to the normal energy levels for the H atom, a more tightly bound sub-ground state of –27.17 eV is possible. For them, the excess Cold Fusion (CF) power, with no nuclear products, is simply the extra 13.68 eV/atom obtained as H isotopes go into the sub-ground state. If their tight H abounds in the universe, one may ask why this spectral line has not been seen long ago.

Mayer and Reitz[2] claim that resonances of ep, ed, and et are created which, if they survive long enough, allow a high probability of Coulomb barrier penetration and subsequent nuclear reaction. Their resonance model is based on that of Spence and Vary[3], who used single photon exchange in the Coulomb gauge. Recently, McNeil[4] reformulated the ep problem in a qualitative yet gauge-invariant way and finds no evidence for a resonance in the ep system in the energy range of interest. Therefore, it is possible that the results of Spence and Vary[3] and hence Mayer and Reitz[2] are spurious.

2. Deep Dirac States

Recently, Maly and Va'vra[5] carried out a calculation for the hydrogen atom based upon irregular solutions of the relativistic Dirac equation and obtained an extremely tightly bound electron orbit. They get a binding energy of ~ 500 keV, and a radius of ~ 5×10^{-13} cm, a nuclear dimension. For them, CF is primarily chemical. The excess energy is 500 keV/atom as these tightly bound atoms are formed. They suggest that this chemical ash of tightly bound H or D atoms may account for the missing mass (dark matter) of the universe. Their electron orbit radius of ~ 5 fm is 50 times smaller than muonic orbits of 250 fm. If such tight D atoms existed, they should produce fusion upon collision at a much higher rate than in muon-catalyzed fusion. Moreover, there are some serious errors in their analysis. At the nuclear surface, $r = r_n \neq 0$, both regular and irregular solutions are allowed simultaneously for $r \geq r_n$. Therefore, a general solution is a linear combination of them for $r \geq r_n$. When the boundary conditions are imposed at $r = r_n$, it can be shown that the irregular component becomes nearly negligible compared to the regular component[6]. The results of Maly and Va'vra[5] are incorrect, since they assumed erroneously that the irregular solution is a general solution independent of the regular solution, as shown below in detail.

The radial part of the relativistic Schrödinger equation is[7]

$$\frac{1}{\rho^2}\frac{d}{d\rho}(\rho^2\frac{d\psi}{d\rho}) + \left[\frac{\lambda}{\rho} - \frac{1}{4} - \frac{\ell(\ell+1)-\gamma^2}{\rho^2}\right]\psi \;=\; 0 \qquad (1)$$

for a point Coulomb potential $e\phi(r) = -Ze^2/r$, where

$$\rho = \alpha r, \gamma = \frac{Ze^2}{\hbar c}, \alpha^2 = \frac{4(m^2c^4 - E^2)}{\hbar^2 c^2}, \lambda = \frac{2E\gamma}{\hbar c\alpha}. \qquad (2)$$

and E and m are the total energy and mass of the electron, respectively. Because of the centrifugal barrier, we need consider solutions of this equation for $\ell = 0$ only because the energies corresponding to $\ell > 0$ must be higher than the lowest $\ell = 0$ energy. As $\rho \to 0$, the wavefunction ψ has the behavior

$$\psi \;\sim\; \rho^{s_\pm}, \qquad (3)$$

where

$$s_\pm \;=\; -\frac{1}{2} \pm \sqrt{\frac{1}{4} - \gamma^2}. \qquad (4)$$

Because the wavefunction has the boundary condition $\psi(\rho \to \infty) = 0$, from eq. (2),

$$E \;=\; mc^2(1 + \frac{\gamma^2}{\lambda^2})^{-1/2}, \qquad (5)$$

and $\lambda_\pm = n' + s_\pm + 1$, where n' is a positive integer. Furthermore, because $\gamma = \frac{Ze^2}{\hbar c} \approx \frac{Z}{137} \ll 1$,

$$s_\pm \approx -\frac{1}{2} \pm (\frac{1}{2} - \gamma^2), \tag{6}$$

and the energy levels E_+ and E_- are

$$E_+ \approx mc^2(1 + \frac{\gamma^2}{(n' + 1 - \gamma^2)^2})^{-1/2} \tag{7}$$

$$E_- \approx mc^2(1 + \frac{\gamma^2}{(n' + \gamma^2)^2})^{-1/2}. \tag{8}$$

Note that eq. (8) gives a binding energy of $E_- - mc^2 \approx mc^2(\gamma\text{-}1) \approx -510$ keV, so that, if the solutions corresponding to s_- were acceptable, deeply bound electron states might exist. However, these solutions are incorrect. Furthermore, eq. (7) gives the correct observed binding energy of $E_+ - mc^2 = -13.6$ eV for $n' = 0$ and $Z = 1$.

The energy levels, eqs. (7) and (8), obtained from the relativistic Schrödinger equation, eq. (1), are similar to those of Maly and Va'vra[5] (their eq. (24)) for the Dirac equation[7]. The same shortcoming, detailed below, applies to their solution; however, it is less transparent than our example because the Dirac equation involves a set of coupled differential equations[7].

We can assume that the potential $e\phi(r)$ is given realistically by

$$e\phi(r) = \begin{cases} -\frac{Ze^2}{r_n}, & r < r_n \\ -\frac{Ze^2}{r}, & r \geq r_n \end{cases}. \tag{9}$$

The wavefunction $\chi(r) = r\psi(r)$ then, as $r_n \to 0$, has the following form:

$$\chi(r) = \begin{cases} AKr, & r < r_n \\ B\rho^{s_+ +1} + C\rho^{s_- +1}, & r \gtrsim r_n \end{cases}, \tag{10}$$

where $(\hbar c)^2K^2 = (E + Ze^2/r_n)^2 - m^2c^4$. Note that, in eq. (10), we have used the regular solution $\chi = A \sin Kr$ for the interior wavefunction. which is zero at the origin, as it must be for a finite potential, and the form of the exterior wavefunction comes from the analytic solution of eq. (1).

When we equate logarithmic derivatives

$$\frac{1}{\chi}\frac{d\chi}{dr}\bigg|_{r=r_n^-} = \frac{1}{\chi}\frac{d\chi}{dr}\bigg|_{r=r_n^+} \tag{11}$$

we obtain,

$$\frac{C}{B} = -\frac{s_+}{s_-}(\alpha r_n)^{s_+ - s_-} \approx -\frac{\gamma^2}{1-\gamma^2}(\alpha r_n)^{1-2\gamma^2}, \tag{12}$$

so that, for a physical wavefunction, as $r_n \to 0$, the solution corresponding to s_- does not contribute. However, because of the finite size of the nucleus, the wavefunction consists of a large component corresponding to s_+ and a small component corresponding to s_- with a binding energy which is thus very close to the original binding energy $E_+ - mc^2$. For instance, for the case of a proton, the proton radius $r_n \approx 1$ fm, $Z = 1$, and $E \approx E_+ = mc^2 -$ 13.6 eV; therefore $\alpha \approx 3.78 \times 10^{-5}$ fm^{-1}, and hence $C/B \approx -0.2 \times 10^{-8}$.

3. Tightly Bound H_2^+ and D_2^+ Molecules

The next set of models involve tight H isotope molecules of radius ~ 0.25 Å in which excess energy may result chemically, and/or from nuclear fusion as the tightly bound atoms more easily penetrate their common Coulomb barrier[8]. Actually, there seems to be no sound basis for assuming the existence of a superbound state of a D_2^+ ion. Some of the analysis is qualitative. The most critical region is barely at the boundary of applicability of the equations. An exact solution for the entire region under consideration will likely yield a potential with no local minimum. Thus the metastable state may not be present in a more rigorous analysis[9]. Hence, the superbound solution is at best unstable.

Gryzinsky[10] and Barut[11] present analyses to substantiate the existence of the metastable D_2^+ state based on three-body calculations for two d's and one electron. Gryzinsky treats the problem mainly classically, but invokes quantum mechanics to neglect radiation effects for his oscillating electron. Barut's analysis is based on the Bohr-Summerfeld quantization principle, and obtains a binding energy of 50 keV. Both authors, independently, conclude that a "superbound" $(D_2^+)^*$ molecular ion can exist in which an electron that is exactly half-way between the d's provides an attractive force and screens the d Coulomb repulsion. Vigier[12] presents an analysis almost identical to that of Barut[11]. For Barut, Gryzinsky, and Vigier, the analysis is predicated on very unlikely precise symmetry. The electron must be exactly the same distance on a line between the two d's. The tightness of the orbit violates the uncertainty principle for a Coulomb potential, but may not violate it with stronger potentials. Although a non-relativistic analysis may be warranted for the large mass H isotopes around the electron, a non-stationary electron will require a relativistic treatment because it will attain a velocity close to the velocity of light due to its small mass. Perhaps a full relativistic calculation including spin-spin and spin-orbit coupling may save this model, but this has not been presented as yet.

4. Rigorous Bound for the Binding Energies of H_2^+ and D_2^+

Recently, Kim and Zubarev[13] have shown a rigorous bound of –16.39 eV for the binding energies of H_2^+ and D_2^+, which poses a more serious difficulty for the tightly bound D_2^+ models[10,11,12].

The non-relativistic Hamiltonian for D_2^+ (or H_2^+) is

$$\begin{aligned} H = & -\frac{\hbar^2}{2M_1}\nabla^2_{R_1} - \frac{\hbar^2}{2M_2}\nabla^2_{R_2} - \frac{\hbar^2}{2m_e}\nabla^2_{r_e} \\ & - \frac{e^2}{|\vec{r}_e - \vec{R}_1|} - \frac{e^2}{|\vec{r}_e - \vec{R}_2|} + \frac{e^2}{|\vec{R}_1 - \vec{R}_2|} \end{aligned} \tag{13}$$

where m_e and M_i (i =1 or 2) are the masses, and $\vec{r}_e$ and $\vec{R}_i$, are laboratory coordinates of the electron and deuteron, respectively. In terms of the center of mass coordinate $\vec{R}_c = \left(m_e\vec{r}_e + M_1\vec{R}_1 + M_2\vec{R}_2\right)/\left(m_e + M_1 + M_2\right)$, the internuclear coordinate $\vec{R} = \vec{R}_1 - \vec{R}_2$, and the relative electron coordinate $\vec{r} = \vec{r}_e - \left(\vec{R}_1 + \vec{R}_2\right)/2$, the Hamiltonian reads

$$H = -\frac{\hbar^2}{2M_t}\nabla_{R_c}^2 - \frac{\hbar^2}{2M}\left(\nabla_R + \frac{\gamma}{2}\nabla_r\right)^2 - \frac{\hbar^2}{2\mu}\nabla_r^{\ 2} - \frac{e^2}{|\vec{r}_e - \vec{R}_1|} - \frac{e^2}{|\vec{r}_e - \vec{R}_2|} + \frac{e^2}{R} \tag{14}$$

where $M_t = m_e + M_1 + M_2$, $M = (M_1 M_2)/(M_1 + M_2)$, $\mu = m_e(M_1 + M_2)/(m_e + M_1 + M_2)$, and $\gamma = (M_1 - M_2)/(M_1 + M_2)$. After separating the motion of the center of mass, one has the following Schrödinger equation

$$\mathcal{H}\psi(\vec{r},\vec{R}) = E\psi(\vec{r},\vec{R}) \tag{15}$$

where

$$\mathcal{H} = -\frac{\hbar^2}{2M}\left(\nabla_R + \frac{\gamma}{2}\nabla_r\right)^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{|\vec{r}_e - \vec{R}_1|} - \frac{e^2}{|\vec{r}_e - \vec{R}_2|} + \frac{e^2}{R}. \tag{16}$$

The operator

$$-\frac{\hbar^2}{2M}\left(\nabla_R + \frac{\gamma}{2}\nabla_r\right)^2 = \frac{1}{2M}\left(\vec{P}_R + \frac{\gamma}{2}\vec{p}_r\right)^2 \tag{17}$$

where $\vec{P}_R = \frac{\hbar}{i}\vec{\nabla}_R$ and $\vec{p}_r = \frac{\hbar}{i}\vec{\nabla}_r$, is positive. Note that $\gamma = 0$ for $M_1 = M_2$. Therefore

$$\mathcal{H} \geq \tilde{H}. \tag{18}$$

or

$$\langle\psi|\mathcal{H}|\psi\rangle \geq \langle\psi|\tilde{H}|\psi\rangle\ , \quad \langle\psi|\psi\rangle = 1 \tag{19}$$

where

$$\tilde{H} = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{|\vec{r}_e - \vec{R}_1|} - \frac{e^2}{|\vec{r}_e - \vec{R}_2|} + \frac{e^2}{R}\ . \tag{20}$$

But $\tilde{H}$ is separable in confocal elliptic coordinates[14], and hence the exact numerical solution of the Schrödinger equation,

$$\tilde{H}\zeta_R(\vec{r}) = E(R)\zeta_R(\vec{r}) \tag{21}$$

is well known to be[14]

$$\tilde{H} > E_{min}(R) = -16.39\ \text{eV}\ . \tag{22}$$

Since $\mathcal{H} \geq \tilde{H}$, we have for any $|\psi\rangle$ with $\langle\psi|\psi\rangle = 1$

The spin-orbit and spin-spin interactions are not expected to change the above bound of

$$\langle\psi|\mathcal{H}|\psi\rangle > E_{min} = -16.39 \text{ eV} \qquad (23)$$

–16.39 eV, eq. (23), dramatically.

5. Summary

We have examined several models which purportedly explain the results of Cold Fusion, and found each to be lacking in some respect. Models in which the electron is tightly bound to the hydrogen or deuterium nucleus were found to have serious qualitative or quantitative defects, and models in which it is claimed that an unusual electron resonance occurs are likely to be spurious. Finally, a lower bound for the binding energies of H_2^+ and D_2^+ was found which is considerably higher than the claimed binding energies in "superbound" models of the two H isotope molecules.

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