NEW HYDROGEN (DEUTERIUM) BOHR ORBITS IN QUANTUM CHEMISTRY AND COLD FUSION PROCESSES

Jean-Pierre Vigier
Gravitation et Cosmologie Relativistes
Université Paris VI - CNRS/URA 769
Tour 22 = 4ème étage, Boîte 142
4, place Jussieu, 75005 Paris

ABSTRACT

It is suggested that recent confirmation of the existence in dense matter of very small quantities of fusion "ashes" both in electrolysis and glow-discharge experiments [1], can be heuristically interpreted (within the frame of conventional Quantum Mechanics and Nuclear theory) if one combines screening (i.e. tunneling) and the introduction of spin-spin and spin-orbit couplings with the usual effects of the Coulomb Potential in atoms and molecules.

The new Quantum Chemistry associated with the corresponding new tight Bohr orbits in dense matter explains [2] the observed excess heat [3] (above break even) and predicts the existence of fusion processes which become dominant at high energy current input [4].

As we shall now see, the formation of a new stable tight phase $\tilde{H}_2^+$ and $\tilde{D}_2^+$ of H_2^+ and D_2^+ can be justified, within the frame of present quantum theory (i.e. quantum chemistry), as a consequence of the introduction of spin-spin and spin-orbit forces (which always exist but cancel out in free-space due to random spin orientations) when they resonate with the surrounding electron plasma oscillations.

The existence of such new "tight" states is now supported by two facts: The exothermic formation [5] of the corresponding states which could correspond to resonance phenomena within the cathode (such as resonances within the electron clouds in internal regions suggested by Preparata). Their de-exitation (also corresponding to quantum jumps from one new Bohr orbit to another) leads to soft X-ray spectra... and X-rays have been observed in such experiments [1].

The formation of the new "tight" states $\tilde{H}_2^+$ and $\tilde{D}_2^+$ is not necessarily tied to the existence of the input current. Even when cut it can be supported by internal (ionization) currents or internal voltage differences carried by the Pd or Nickel... so that one could explain in this way, the existence of the "heat after death" phenomena discovered by Fleischmann and Pons [5]. The excess heat depends on the number of $\tilde{H}_2^+$ and $\tilde{D}_2^+$ (in light and heavy water) i.e. on the loading of the capillaries contained in the electrode. It is created only when they are formed, i.e. not necessarily immediately since individual capillary situations change with the metal. The corresponding binding energies have been shown [5] to be of the order of ≈50 kev instead of the usual ≈5 ev of quantum chemistry. The corresponding heat is ≈4 times as big for $\tilde{D}_2^+$ as for $\tilde{H}_2^+$.

As first basis for the new phenomena one can add (following a suggestion of Barut [6]) to the Coulomb Potential (utilized in Hydrogen and Deuterium) spin-spin and spin-orbit interactions. Usually neglected, they manifest themselves when $\vec{L},\ \vec{M}_1,\ \vec{M}_2$ are oriented (parallel) by internal electromagnetic interactions when H and D are in various types of electrodes. Indeed for two charged particles e_1, e_2 with magnetic moments $\vec{M}_1$ and $\vec{M}_2$ the usual quantum Schrödinger Hamiltonian is given by

$$H = \frac{1}{2m_1}\left(\vec{P}_1 - e_1\,\vec{M}_2 \times \frac{(\vec{r}_2 - \vec{r}_1)}{(r_1 - r_2)^3}\right)^2 + \frac{1}{2m_2}\left(\vec{P}_2 - e_2\,\vec{M}_4 \times \frac{(\vec{r}_2 - \vec{r}_1)}{(r_1 - r_2)^2}\right)^2 + \frac{e_1\,e_2}{(r_1 - r_2)} - M_1 \cdot M_2 \cdot S_{12}\,(r_1 - r_2) \qquad (1)$$

where S_{12} is the usual dipole-dipole interaction tensor* and r their distance, i.e.

$$S_{12}\,(\vec{r}) = \frac{3\sigma_1 \cdot r_1 \cdot \sigma_2\, r - \sigma_1 \cdot \sigma_2}{r^3} + \frac{8\pi}{3}\,\vec{\sigma}_1 \cdot \vec{\sigma}_2\,\delta(\vec{r}) \qquad (2)$$

This 2-body problem with magnetic forces is separable, like the 2-body Coulomb problem. With

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \qquad R = \frac{m_2\,\vec{r}_1 + m_2\,\vec{r}_2}{M_0} \qquad \vec{p} = \vec{p}_1 + \vec{p}_2$$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \qquad P = \frac{m_2\,\vec{P}_1 - m_1\,\vec{P}_2}{M_0} \qquad M_0 = m_1 + m_2 \qquad (3)$$

still utilizing Barut's rotations [13] we obtain after some calculation

$$H = \frac{1}{2M_0}\,P^2 + \frac{1}{2\mu}\,p^2 - \vec{p} \cdot \frac{\vec{a} \times \vec{r}}{r^3} - \frac{\vec{P} \cdot \vec{b} \times \vec{r}}{r^3} + \frac{A}{r^4} + \frac{e_1\,e_2}{r} - M_1 \cdot M_2\,S_{12}\,(\vec{r}) \qquad (4)$$

where

$$\vec{a} = \frac{e_1}{m_1} \cdot \vec{M}_2 + \frac{e_2}{m_2}\,\vec{M}_1\ ,$$

$$\vec{b} = \frac{e_1}{m_1 + m_2}\,\vec{M}_2 - \frac{e_2}{m_1 + m_2}\,\vec{M}_1\ ,$$

$$A = \frac{e_1^2}{m_2}\,M_2^2 + \frac{e_2^2}{m_2}\,M_1^2\,.$$

In the center of mass frame ($\vec{P} = 0$) we have

$$H_{relative} = \frac{1}{2\mu}\,p^2 - \vec{p} \cdot \frac{\vec{a} \times \vec{r}}{r^3} + \frac{A}{r^4} + \frac{e_1\,e_2}{r} - M_1 \cdot M_2 \cdot S_{12}\,(\vec{r}) \qquad (5)$$

Using $\quad -\vec{p} \cdot (\vec{a} \times \vec{r}) = \vec{p} \cdot (\vec{r} \times \vec{a}) = (\vec{p} \times \vec{r}) \cdot \vec{a} = -\vec{a} \cdot (\vec{r} \times \vec{p}) = -\vec{a}$

we see that the second term corresponds to a charge-dipole potential, and the last term to a dipole-dipole potential.

In the special case $m_2 >> m_1$, $M_1 = 0$ hence $\vec{a} = \frac{e_1}{m_1} M_2$, $\vec{b} = 0$, $A = \frac{e_1^2}{m_1} M_2^2$, we have the simpler

Hamiltonian
$$H_{relative} = \frac{1}{2\mu} p^2 + \frac{e_1 e_2}{r} - \frac{e_1 M_2}{m_1} \frac{\vec{\sigma} \vec{L}}{r^3} + \frac{e_1^2 M_2^2}{m_1} \cdot \frac{1}{r^4} \tag{6}$$

We now try to solve exactly the eigenvalue problem $H\Psi = E\Psi$ with H given in equation (6). For simplicity we take the spin of the particle 2 to be 1/2.

As we shall see, following de Broglie [7], they are given by the relation
$$\frac{M^2 \hbar^2}{m_1 r^3} + \frac{\delta V(r)}{\delta r} = 0 \tag{7}$$

where r denotes their radius and M an integer quantum number, multiplied by r^5 yields the relation:
$$\left(\frac{m^2 \hbar^2}{m_1} + B \right) r^2 = A r^3 + C r + D \tag{8}$$

which can be written in the form $r^3 + a_2 r^2 + a_1 r + a_0 = 0$ (9)

Introducing $Q = (1/3) a_1 + (1/g) a_2^2$ and $R = (1/6) (a_1 a_2 - 3 a_0) - (1/27) 0_2^3$ we see that
-- with $Q^2 + R^2 > 0$ there is one real root and a pair of complex conjugate roots
-- with $Q^2 + R^2 = 0$ all roots are real and at least two are equal
-- with $Q^2 + R^2 < 0$ all roots are real.

Of course each real root denotes an infinite set (with m=1,2,...) of Bohr orbits. Introducing the two auxiliary quantities $S_1 = [R + (Q^3 + R^2)^{½}]^{⅓}$ and $S_2 = [R - (Q^3 + R^2)^{½}]^{⅓}$ one gets for these roots (which define three sets of Bohr orbits) the expressions

$$\begin{cases} r_1 = (S_1 + S_2) - \frac{a_2}{3} = f_1(m) \\ r_2 = -\frac{1}{2}(S_1 + S_2) - \frac{a_2}{3} + \frac{i\sqrt{3}}{2}(S_1 - S_2) = f_2(m) \\ r_3 = -\frac{1}{2}(S_1 + S_2) - \frac{a_2}{3} - \frac{i\sqrt{3}}{2}(S_1 - S_2) = f_3(m) \end{cases} \tag{10}$$

which satisfy three constraints, i.e.:

$$\begin{cases} r_1 + r_2 + r_3 = -a_2 \\ r_1 r_2 + r_1 r_3 + r_2 r_3 = a_1 \\ r_1 r_2 r_3 = -a_0 \end{cases} \tag{11}$$

According to the distance r one sees immediately
-- that when $A/r > (½) \cdot B/r^2 + (⅓) \cdot C/r^3 + (¼) \cdot D/r^4$ i.e. $Ar^3 > Br^2 + Cr + D$
one has a set of radii which varies like m^2 i.e. which corresponds to Bohrs initial orbits when $\theta = \pi/2$.

-- that when $C/3r^3 > A/r + (½) \cdot B/r^2$ i.e. $Cr > Ar^3 + D$ then $r \simeq C\, m_1 / m^2 \hbar^2$.

This set varies like $1/m^2$ and corresponds to a set of "tight" orbits never discussed by Bohr.
-- that when $(¼) \cdot D/r^4 > (⅓) \cdot C/r^3 + (½) \cdot B/r^2 + A/r$
then $r \simeq (D\, m_1 /m^2 \hbar^2)^{½} = (D\, m_1)^{½}/m\hbar$ a set which also yields a new set of "tight" Bohr orbits unknown in the literature.

Since a detailed analysis of the corresponding new Bohr energy levels is in preparation (and will shortly be published) we will now limit ourselves to the following remarks. The existence of these new "deep" Bohr levels depend, of course, on the relative spin (and spin-orbit) orientations, i.e. they can only be excited in special physical situations where they are determined by their surroundings. This appears now to be the case when Hydrogen-Deuterium, etc. are imbedded in dense media.

When one utilizes D_2 or other types of fusion material, the creation of excess heat by the tight D_2^+ states is generally accompanied by some real fusion processes: since an electron (when located by ions) behaves (within the deeper potential due to spin-spin and spin-orbit forces) as if it had acquired a heavier "effective" mass [4]. Indeed smaller Bohr orbits facilitate tunneling through the Coulomb barrier. Moreover, "heavier" electrons also explain some types of observed regular collective motions (i.e. cluster formations) which can contain triangular, tetrahedral, cubic ... configurations which move collectively and have been observed to have strongly enhanced cross sections (by many orders of magnitude) with individual particles. This configuration naturally arises when the Ampère force cuts the current into beads in a capillary since the situation of the ions then resembles what happens to fast going cars which crash successively into each other during a slowdown (accident) on a modern highway.

This situation is very different from the usual quantum mechanical interpretation of chemical phenomena, i.e. of the normal states of H_2^+ and D_2^+ which are assumed (according to the Born-Oppenheimer approximation) to correspond to the rapid motion of the electron in the field of two almost fixed nuclei. If one first neglects the spin and considers two masses M (with charges z) rotating at a distance r from a mass (charge z) i.e.

Fig. 1 z ———————— z
M r m r M

this gives the Hamiltonian $$H = \frac{2P^2}{2M} + \alpha\left(\frac{2Zb}{r} + \frac{Z^2}{2r}\right) \qquad (12)$$

which yield when quantized by the usual Bohr-Sommerfeld method ($\int pdq = n\hbar$)
with ($\hbar = C = 1$); Energy levels $E_n = -(¼)\{M\, \alpha^2/n^2\}\, Z^2\, (2z + Z/2)^2$ i.e.

-- For the He atom this yields $E_0 = 6{,}12$ Ryd close to the observed value ≈ 5,69 Ryd.

-- For H_2^+ and D_2^+ the Bohr energy levels are approached by $E_n = -(9/16)\,(M\,\alpha^2/n^2)$ which correspond to ground states of 28.1 KeV for H_2^+ and D_2^+. The first stage of this model, i.e. the existence of excess heat in H or H_2O experiment (in the author's opinion) can be considered as already proven by a growing set of experiments [1,3]. These experiments show the existence of a non-fusion origin for presently observed excess heat and seems to exclude its interpretation in terms of virtual neutron exchange.

The second stage, i.e. the existence of new "tight" molecules such as H_2 or D_2, is in fact already suggested by the experiments of Mills et al. [6] which have detected by cryometry and mass spectrometry the existence of new tight states of H_2.

To quote the authors "an exothermic reaction is reported wherein the electrons of hydrogen atoms and deuterium atoms are stimulated to relax to quantized potential energy levels below that of the *ground state* via electrochemical reactants K^+ and K^+; Pd^2+ and Li^+, or Pd and O_2 of redox energy resonant with the energy hole which stimulates this transition. Calorimetry of pulsed current and continuous electrolysis of aqueous potassium carbonate (K^+/K^+ electrocatalytic couple) at a nickel cathode was performed. The excess power out of 41 watts exceeded the total input power given by the product of the electrolysis voltage and current by a factor greater than 8. The "ash" of the exothermic reaction is atoms having electrons of energy below the *ground state* which are predicted to form molecules. The predicted molecules were identified by lack of reactivity with oxygen by separation from molecular deuterium by cryofiltration, and by mass spectroscopic analysis [8].

The third stage, i.e. the prediction of H_2 or D_2 to explain excess heat at low energy input can also be considered as supported by the experiments of Miles, Bush et al. [10] which report ^{4}He (which they did not attempt to distinguish from D_2) and by the experiment of Yamaguchi and Nishioka [10] who have detected by mass spectroscopy (along with fusion "ashes" ^{3}He with an energy of 4-5-6 Mev and protons with an energy of 3Mev) ^{4}He accompanied (as it should in our model) by a heavier D_2 peak. Their input being dominant at low input. Further search for soft X-rays and also for the existence of H_2^+ in H or H_2O experiments would help to prove (or disprove) the proposed model.

Proof of the last stage, i.e. the possibility to add to the excess heat (generated by the new Bohr orbits) fusion energy generated by high energy input pulses is still in infancy [4] due to reluctance to accept the existence of the new phenomena.

REFERENCES

[1] Y.R. Kucherov et al., *PLA* 170 (1992) 265 and J. Dufour, *Fusion Technology*, vol 24 (1993), p 205.

[2] J.P. Vigier, Frontiers of Cold Fusion, Proc. of Third International Conference on Cold Fusion, Nagoya, Japan, Universal Acad. Press, H. Ikegami, Ed. (1993).

[3] For example see the contributions of Drs. McKubre, Takahashi, Kunimatsu and Storms in Frontiers of Cold Fusion, Universal Acad. Press Inc., Tokyo (1993) H. Ikegami, Ed.

[4] R. Antanasíjević, I. Lakicević, Z. Marić, D. Zević, and J.P. Vigier, *PLA* 180 (1993) 24.

[5] M. Fleischmann and S. Pons, see Proceedings ICCF4 in Hawaii (6-9 Dec. 1993).

[6] A. Barut, "Prediction of new tightly bound states of $H_2^+ (D_2^+)$ and `cold fusion experiments'," private communication (1992).

[7] L. de Broglie, "Non-linear Wave Mechanics," Elsevier, Amsterdam (1960). See also A.O. Barut and M. Basic, *Ann. Found. L. de Broglie*, vol 15 (1990), p 67.

[8] R.L. Mills, W.R. Good and R. Shanbach, "Dihydrino Molecule Identification," *Fusion Technology* (in press).

[9] See A. Takahashi et al., Proc. 2d Como Conference on Cold Fusion, The Science of Cold Fusion, Ital. Physical Soc. publ. (1992).

[10] E. Yamaguchi and T. Nishioka in Frontiers of Cold Fusion (see ref. 3) and M. Miles, B. Bush et al. in The Science of Cold Fusion (see ref. 8).