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Cold fusion in metals

(deuterons/palladium)

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ABSTRACT **A simple model of a metal containing deuterons is considered. The example of palladium is treated in detail. It is shown that the effect of screening of Coulomb fields by conduction electrons is sufficient to allow deuteron pairs to fuse at rates of 10^{-30} sec^{-1}, seven orders of magnitude smaller than those reported by Jones *et al.* [Jones, S. E., Palmer, E. P., Czirr, J. B., Decker, D. L., Jensen, G. L., Thorne, J. M., Taylor, S. F. & Rafelski, J. (1989) *Nature (London)* 388, 737–740].**

The recent reports of cold fusion in metals, both at high levels (1) and at much lower levels (2), have stimulated great interest and considerable skepticism (3, 4). In this note, we propose a simple model which suggests that cold fusion of deuteron pairs occurs at a rate of 10^{-30} sec^{-1}, 7 powers of 10 smaller than the lower level (2) but 17 orders of magnitude larger than the upper limit of ref. 4. The model makes use of the fact that screening of Coulomb fields in a metal, a collective effect involving many conduction electrons, may be much more effective than the screening of Coulomb fields by valence electrons in a molecule.

We consider the possibility of cold fusion of deuterons in palladium metal, which has a face-centered-cubic lattice with cube edge $L = 3.879$ Å. Any four nearest-neighbor Pd atoms form the vertices of a regular tetrahedron whose edge length is $\frac{1}{2}\sqrt{2}L$ (= 2.743 Å). The center of the tetrahedron is $\frac{1}{12}\sqrt{3}L$ (= 0.5599 Å) distant from any of its faces, and $\frac{1}{4}\sqrt{3}L$ (= 1.6797 Å) from any vertex. There are two such cages for every Pd atom. In addition, there is a larger octahedral cage for every Pd atom. We will first consider the possibility of deuterons being trapped in such a cage.

In palladium metal, the outermost 10 4*d* electrons furnish the metallic binding. We make the approximation of treating all 10 such electrons per atom on the same footing, considering them to be conduction electrons with some effective mass. According to the jellium model of a metal (5), the Fermi energy E_F is related to the longitudinal velocity of sound s by the relation

$$E_F = \tfrac{1}{2}Ms^2, \qquad [1]$$

where M is the atomic mass per conduction electron. For s, we take a weighted rms average of the velocities (6) associated with the three symmetry directions, making use of the fact that there are three (100) directions, six (110) directions, and four (111) directions. Thus

$$s = \{\rho^{-1}[c_{11} + \tfrac{14}{13}(c_{12} + 2c_{44})]\}^{1/2} = 7.0781 \times 10^5 \text{ cm/sec},$$

where $\rho = 11.40$ g/cm^3 is the mass density and the c_{ij} are the elastic constants. We now have

$$E_F = 8.3473 \text{ eV}. \qquad [2]$$

(1 eV = 1.60×10^{-19} J.)

It might be objected that 10 conduction electrons per atom is too many, 2 or 4 might be more appropriate, these being the two accepted valences of Pd. But with these smaller numbers, we would obtain unreasonably large values of E_F, especially for a band built primarily out of *d* electrons. MacDonald *et al.* (7) have calculated a 4*d* bandwidth in Pd of 6.26 eV.

The density of conduction electrons is

$$n_0 = 4 \times 10/(3.879 \text{ Å})^3 = 0.68533 \text{ Å}^{-3}. \qquad [3]$$

In the free-electron model of a metal, $E_F = (p_F^2/2m^*)$, $n_0 = (3\pi^2)^{-1}(p_F/\hbar)^3$, p_F being the Fermi momentum and m^* the effective mass. We then have

$$(m^*/m) = \tfrac{1}{2}(3\pi^2)^{2/3}(n_0 a_0^3)^{2/3}(E_0/E_F) = 3.3958. \qquad [4]$$

Here m is the electronic mass, a_0 is the Bohr radius, and the Hartree energy E_0 is

$$E_0 = (\hbar^2/ma_0^2) = (e^2/a_0) = 27.21 \text{ eV}.$$

The Debye screening length in a metal, λ_D, obtained by linearizing the Thomas–Fermi method (for a comprehensive review of the Thomas–Fermi method, see ref. 8), is

$$\lambda_D = (E_F/6\pi n_0 e^2)^{1/2} = 0.21183 \text{ Å}. \qquad [5]$$

A deuteron will experience a potential energy minimum at the center of a trap. Assuming a uniform conduction electron density n_0, the potential energy in the vicinity of the center will be $U_1 = \frac{1}{2}\kappa r^2$, where the effective spring constant

$$\kappa = \tfrac{4}{3}\pi n_0 e^2 = \tfrac{2}{9}(E_F/\lambda_D^2) = 41.441 \text{ eV/Å}^2. \qquad [6]$$

The deuteron (mass m_d) will oscillate with a characteristic frequency

$$\omega_0 = (\kappa/m_d)^{1/2} = 4.4560 \times 10^{14} \text{ sec}^{-1},$$

and the corresponding ground-state classical turning radius will be

$$\mathcal{R} = (\hbar\omega_0/\kappa)^{1/2} = 0.08413 \text{ Å}.$$

We have been considering a bare deuteron in the trap. What about a neutral deuterium atom? For an electron to bind to the deuteron, it is necessary (9) that $2(\lambda_D/a_0) > 1.6799$, clearly not satisfied here, where $(\lambda_D/a_0) = 0.3998$.

We are particularly interested in the situation where there are two deuterons in a trap. The Hamiltonian for this problem separates in terms of the center-of-mass coordinate $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ and the relative coordinate $\vec{r} = (\vec{r}_1 - \vec{r}_2)$. We have

$$H = H_R + H_r,\ H_R = -(\hbar^2/4m_d)\nabla_R^2 + \kappa R^2, \qquad [7]$$

$$H_r = -(\hbar^2/m_d)\nabla_r^2 + \tfrac{1}{4}\kappa r^2 + V_{eff}(r), \qquad [8]$$

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Abbreviations: E_F, Fermi energy; n_0, conduction electron density; a_0, Bohr radius; E_0, Hartree energy; λ_D, Debye screening length; ω_0, characteristic frequency; TFM, Thomas–Fermi–Mott.

where $V_{eff}(r)$ is the effective interaction between two deuterons in the presence of screening conduction electrons. The major problem of this paper is to calculate V_{eff}.

First we consider the additional potential resulting from the presence of a single deuteron in the metal. To this end, we make use of a modification of the Thomas–Fermi equation, which Mott (10) used to treat the potential resulting from a localized impurity in a metal.¶ This equation, which we refer to as the TFM equation, is

$$\nabla^2 V(\vec{r}) = -4\pi e^2[n(\vec{r}) - n_0],$$

$$n(\vec{r}) = (8\pi/3h^3)(2m^*)^{3/2}[E_F - V(\vec{r})]^{3/2}, \quad [9]$$

$$n_0 = (8\pi/3h^3)(2m^*E_F)^{3/2}.$$

Here h is the Planck constant, 6.63×10^{-34} J·sec. In the case we are considering, of spherical symmetry, it is convenient to express distances and energies in Thomas–Fermi units, distance measured in units of

$$a_F = \tfrac{1}{2}(\tfrac{3}{4}\pi)^{2/3}\,(m/m^*)a_0 = 0.88534(m/m^*)a_0$$

$$= 0.13797 \text{ Å},$$

energy in units of

$$(a_0/a_F)E_0 = 104.3671 \text{ eV}.$$

We write

$$V(\vec{r}) = -e^2 r^{-1}\phi(x),\ x \equiv (r/a_F). \quad [10]$$

The TFM equation becomes

$$(d/dx)^2\phi = x^{-1/2}(\phi + Dx)^{3/2} - D^{3/2}x, \quad [11]$$

where $D = 0.079980$ is the Fermi energy expressed in these new energy units.

Starting at $x = 0$ and subject to the boundary conditions $\phi(0) = 1$, $\phi'(0) = -m$, this equation was integrated numerically out to large values of x. The constant m was chosen such that $\phi(x)$ vanishes as $x \to \infty$. A variant of the Noumerov method (11) for integrating linear second-order differential equations was found to be quite efficient. At large distances, $\phi(x)$ becomes proportional to $\exp[-(a_F/\lambda_D)x]$. It is important to point out that the proportionality factor is *less than one*. At large distances, it appears that a charge smaller than unit charge is being screened out by the conduction electrons.

It is convenient for what follows that we have an accurate analytic approximation to $\phi(x)$. With an error of less than 0.2%, we can approximate $\phi(x)$ by the expression

$$\phi_{app}(x) = \sum_{i=1}^{5} A_i e^{-\alpha_i r}, \quad [12]$$

where A_i and α_i are listed in Table 1. This expression satisfies boundary conditions at $x = 0$ and $x \to \infty$.

Thus far, we have considered a single deuteron. Now consider a pair of deuterons. We make the approximation

¶It should be emphasized that the Thomas–Fermi approach is more accurate for determining the screening of a deuteron in a metal, where many electrons make partial contributions, than is the case for an isolated neutral deuterium atom, where only one electron is involved.

Table 1. Parameters for the analytic representations of ϕ and $\bar{\phi}$; $Z = 1$ case

i	α_i	A_i	C_i	D_i
1	0.651324	0.6485306	0.3521383	0.1369708
2	1.261690	0.0924173	0.1542122	0.0053880
3	2.234930	0.2000000	0.3742368	0.0446986
4	5.602250	0.0459964	0.0933864	0.0059263
5	29.910950	0.0130557	0.0260263	0.0025492

that the one-electron potential associated with the pair is simply the sum of the potentials associated with each deuteron by itself—i.e.,

$$V(\vec{r}) = V_1(\vec{r}) + V_1(\vec{r} - \vec{R}),$$

$$V_1(\vec{r}) = -r^{-1}\phi(r). \quad [13]$$

(We are still measuring distance and energy in Thomas–Fermi units.) Here we have one deuteron at $\vec{r} = 0$, the other at $\vec{r} = \vec{R}$. This approximation, if anything, will *underestimate* the screening when the two deuterons are close. We will return to this point later. The electrostatic interaction energy of the two screened deuterons can be broken into three pieces. The Coulomb interaction energy of the screening electrons is

$$\tfrac{1}{2}\int \{V(\vec{r}) + r^{-1} + |\vec{r} - \vec{R}|^{-1}\}\,\{n(\vec{r}) - n_0\}d^3r,$$

where

$$n(\vec{r}) - n_0 = -(4\pi)^{-1}\nabla^2 V(\vec{r}).$$

The factor of $\tfrac{1}{2}$ is to correct for double counting. The Coulomb interaction between deuteron nuclei and screening electrons is

$$-\int \{r^{-1} + |\vec{r} - \vec{R}|^{-1}\}\,\{n(\vec{r}) - n_0\}d^3r.$$

The Coulomb interaction between the deuteron nuclei is $+R^{-1}$. Thus the total electrostatic interaction energy is

$$V_E(R) = +R^{-1} - I_1 - I_2, \quad [14]$$

where, after some algebra,

$$I_1 \equiv (4\pi)^{-1}\int r^{-2}[1 + \phi(r)]\phi''(r)d^3r$$

$$= \int_0^\infty dr[1 + \phi(r)]\phi''(r), \quad [15]$$

$$I_2 \equiv (4\pi)^{-1}\int (rr')^{-1}[1 + \phi(r)]\phi''(r')d^3r$$

$$= (2R)^{-1}\int_0^\infty dr[1 + \phi(r)][\phi'(r + R) - \phi'(r - R)]. \quad [16]$$

(We are using the notation $\vec{r}' \equiv \vec{r} - \vec{R}$.) I_1, being a constant independent of R, may be dropped by redefining the zero

of energy. Making use of the analytic expression for $\phi(r)$, we get

$$V_E(R) = +R^{-1} - I_2 = R^{-1}\bar{\phi}(R), \quad [17]$$

$$\bar{\phi}(R) \equiv \sum_{i=1}^{5} (C_i - D_i R)e^{-\alpha_i R}, \quad [18]$$

$$C_i \equiv A_i(1 - \tfrac{1}{2}B_i), \quad [19]$$

$$B_i \equiv \sum_{j\neq i}^{5} 2A_j(\alpha_j^2 + \alpha_i^2)(\alpha_j^2 - \alpha_i^2)^{-1}, \quad [20]$$

$$D_i \equiv \tfrac{1}{2}\alpha_i A_i^2. \quad [21]$$

Note that $\Sigma_i C_i = 1$. The values of C_i and D_i are listed in Table 1. It can be seen that $C_1 < A_1$, whereas $C_i > A_i$ for $i \geq 2$. This means that $V_E(r)$ is much more sharply peaked at the origin than is $V_1(r)$; i.e., the barrier of the former is narrower. $V_E(r)$ is the desired $V_{eff}(r)$ of Eq. **8**. It may be considered the interaction between two identical composite particles, our composite particle being a bare deuteron plus the associated screening cloud of conduction electrons.

The total effective potential for a deuteron pair in a trap, expressed in Thomas–Fermi units, is

$$U(x) = x^{-1}\bar{\phi}(x) + \kappa' x^2, \quad [22]$$

where $\kappa' \equiv 0.0018896$. This has a minimum at $x = 2.7331$. The characteristic frequency of zero-point oscillations about this minimum is $\omega_0 = 1.1545 \times 10^{15}$ sec^{-1}, and the energy of this state

$$E_T = U_{min} + \tfrac{1}{2}\hbar\omega_0 = 0.018210.$$

The inner classical turning point of this state, x_c, is close to $x = 2.27$.

The probability per unit time that two deuterons in a trap will fuse is given by (12)

$$\lambda = A|\psi(R_n)|^2, \quad [23]$$

where $\psi(R_n)$ is deuteron–deuteron wave function at a separation distance R_n equal to the range of the nuclear interaction. We take $R_n = 3.22F$, twice the experimentally observed rms radius of the α particle. The constant A is

$$A = S(0)(\pi\alpha\mu c)^{-1} = 1.478 \times 10^{-16} \text{ cm}^3/\text{sec},$$

where α is the fine structure constant, c the velocity of light, μ the reduced mass, and $S(0) = 106$ keV·barn (13) is the low energy limit of the nuclear S-factor for d–d fusion (1 barn = 10^{-28} m^2). Using the quantum mechanical WKB (Wentzel–Kramers–Brillouin) approximation,

$$|\psi(R_n)|^2 = Fe^{-2\pi\eta}, \quad [24]$$

where $\exp(-2\pi\eta)$ is the Gamow penetration factor and

$$F = (16\,\pi^{3/2})^{-1}\,(k_2/k_1)^2(k_1R_n)[1 - \exp(-k_1R_n)]^2R_n^{-3}. \quad [25]$$

Here we are defining k_1 and k_2 such that $(\hbar^2k_1^2/2\mu) = U(R_n)$, $(\hbar^2k_2^2/2\mu) = \frac{1}{2}\hbar\omega_0$, so that

$$(k_1R_n) = [(\mu/m)(R_n/a_0)]^{1/2},$$

$$(k_2/k_1) = [(\tfrac{1}{2}\hbar\omega_0/E_0)(R_n/a_0)]^{1/2}.$$

We have approximated $U(x)$ by $U(R_n)$ for $x \leq R_n$.

Table 2. Parameters for the analytic representations of ϕ and $\bar{\phi}$; $Z = 2$ case

i	α_i	A_i	C_i	D_i
1	0.651324	0.5315000	0.2166725	0.0919970
2	1.547610	0.2470066	0.3481617	0.0472116
3	2.922640	0.1602994	0.3122658	0.0375500
4	7.906130	0.0546916	0.1099179	0.0118243
5	61.319420	0.0065024	0.0129821	0.0012963

We have

$$2\pi\eta = K\int_{R_n}^{x_c} [U(x) - E_T]^{1/2}dx,$$

$$K = 2[(m_d/m)(a_F/a)]^{1/2} = 61.868, \quad [26]$$

we find $2\pi\eta = 104.796$, $F = 2.269 \times 10^{28}$ cm^{-3}, so that

$$\lambda = 1.0304 \times 10^{-33} \text{ sec}^{-1}. \quad [27]$$

As already mentioned, the approximation embodied in Eq. **22** will tend to underestimate the screening when the two deuterons are close. Electrons much farther away from the origin than the two deuterons will find themselves in the screened field of an impurity of charge $Z = 2$. This suggests the alternative approach of letting $V_1(\vec{r})$ be *one-half* the solution to the TFM equation for a single α particle, rather than the solution for a single deuteron. Such an approximation, if anything, probably slightly *overestimates* the screening when the two deuterons are well separated. However, it is the behavior when the deuterons are close together that plays a crucial role in determining the size of the Gamow factor.

We have solved Eq. **11** for the case $Z = 2$, and we have analytically fitted one-half of the resultant $\phi(x)$ in the same manner as before. The various parameters are listed in Table 2. The resultant $U(x)$ has a minimum at $x = 2.5381$, the classical turning point is close to $x_c = 2.08$, the characteristic frequency is $\omega_0 = 1.1638 \times 10^{15}$ sec^{-1}, and the energy is $E_T = 0.016378$. We find $2\pi\eta = 97.232$, $F = 2.287 \times 10^{28}$ cm^{-3}, so that the pair fusion rate is

$$\lambda = 2.003 \times 10^{-30} \text{ sec}^{-1}. \quad [28]$$

This number is smaller by a factor of 10^7 than the observations of Jones *et al.* (2). It should be mentioned that they were using titanium, not palladium. Eq. **28** is in agreement with the calculations of Kondo (14), who determined the parameters of his theory by a somewhat different procedure.

Leggett and Baym (4) claim that the maximum possible value of λ is 3×10^{-47} sec^{-1}. It may or may not be coincidental that we calculate $\lambda = 1.27 \times 10^{-47}$ sec^{-1} by disregarding any harmonic oscillator potential (i.e., setting $\kappa = 0$) and by keeping only the asymptotic screening at large distances (i.e., by making the only nonvanishing A_i be $A_1 = 1$).

We recognize that, rather than using either of the two approximations involving Eq. **13**, it would be preferable to solve Eq. **9** directly for the case of two deuterons separated by a distance R, and from the results calculate $V_E(R)$. The numerical difficulties involved are considerable.

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