Proc. Natl. Acad. Sci. USA
Vol. 87, pp. 8652–8654, November 1990
Physics

Cold fusion in palladium: A more realistic calculation

(deuterons/Thomas–Fermi–Mott)

R. H. PARMENTER[†‡] AND WILLIS E. LAMB, JR.[†‡§]

[†]Department of Physics, [‡]Arizona Research Laboratories, and [§]Optical Sciences Center, University of Arizona, Tucson, AZ 85721

Contributed by Willis E. Lamb, Jr., July 16, 1990

ABSTRACT **The Thomas–Fermi–Mott equation is modified to take account of the fact that conduction electrons in a metal may be considered to have an effective mass at wavenumbers comparable with or less than the inverse Debye screening length, but they should be considered to have the free-electron mass at much larger wavenumbers. This modification allows for a more realistic calculation of the fusion rate of deuteron pairs in palladium, this rate being 10^{-23} sec^{-1}, comparable with some experimental results. The Oppenheimer–Phillips process enhances the rate by a factor of 2.262.**

In a recent article (1), we calculated the fusion rate of a pair of deuterons in an interstitial trap in palladium metal, obtaining a rate $\lambda = 10^{-18}$ sec^{-1}. This rate was determined by treating each deuteron as a composite particle, a bare deuteron plus the associated screening cloud of excess conduction electrons. The electrostatic repulsion energy of the composite pair is the barrier through which quantum mechanical tunneling must take place for fusion to occur. Prior to calculating this repulsion energy, one must determine the additional one-electron potential energy in the metal resulting from the presence of the two deuterons. This was calculated via the Thomas–Fermi–Mott (TFM) equation, a variant of the Thomas–Fermi equation, invented by Mott (2) to obtain the potential resulting from a localized impurity in a metal. In calculating the additional potential associated with a pair of deuterons, we made the approximation that the potential associated with the pair is simply the sum of the localized potentials associated with each deuteron by itself. The rate calculation was carried through with each of two different choices for the single-deuteron potential: (*i*) the potential associated with a single deuteron ($Z = 1$); (*ii*) *one-half* of the potential associated with a single α particle ($Z = 2$). For reasons discussed in ref. 1, we believe the $Z = 2$ choice is the more accurate approximation for purposes of calculating the fusion rate.

In the present paper we repeat the calculation of ref. 1 with one important change. Rather than use the TFM equation, we use what we believe to be a more accurate equation for the present problem. We refer to this as the modified Thomas–Fermi–Mott (MTFM) equation, the development of which we now describe.

As in ref. 1, the basic input is the density of conduction electrons, $n_0 = 0.67917$ Å^{-3}, and the asymptotic Debye screening length, $\lambda_D = 0.14270$ Å; this latter is obtained from the measured low-temperature electronic contribution to the specific heat. In ref. 1 we took a simple model of 10 conduction electrons per atom in a single band with a Fermi energy $E_F = 3.75371$ eV and an effective mass ratio $(m^*/m) = 7.50601$. In reality, there are 5 different 4d bands, each with the same E_F, but with an effective mass ratio $(m^*/m) = 5^{-2/3}(7.50601) = 2.56702$, each band containing 2 conduction electrons per atom. The former model is simpler, the latter model is more realistic.[¶] They would have given identical results in the previous paper employing the TFM equation.

In using the TFM equation, the implicit assumption is made that the conduction electrons can be treated as having a constant effective mass independent of wavenumber. At wavenumbers comparable with or smaller than $K_D \equiv \lambda_D^{-1}$, the inverse of the asymptotic screening length, it seems reasonable to treat the screening electrons as having an effective mass. At wavenumbers much larger than K_D, however, it seems most reasonable to treat the electrons as having the free electron mass. The MTFM approach that we now propose is still simple but sufficiently realistic to automatically achieve this variation of effective mass with wavenumber.

As above, we assume 5 bands, with each band having 2 conduction electrons per atom. The total conduction electron density is

$$n_0 = 5 \times 2 \times \frac{4}{3}\pi(p_F/h)^3 = (5/3\pi^2)k_F^2, \qquad [1]$$

where $p_F = \hbar k_F$ is the Fermi momentum. As already stated, we take the numerical value of n_0 used in ref. 1. However, we now assume each band has a *nonparabolic* energy-versus-wave-vector curve. For values of k much larger than K_D, we want the energy $E(k)$ to be parabolic with a free-electron mass. For values of k comparable with or smaller than K_D, we want $E(k)$ to be approximately parabolic with an effective mass m^*. We take

$$E(k) = [\hbar^2k^2/2m^*(k)], \qquad [2]$$

$$m^*(k) = m\{1 - (1 - \alpha)[1 + (\alpha k/K_D)^2]^{-1}\}^{-1}, \qquad [3]$$

where α is a parameter to be determined such that $0 < \alpha < 1$. Note that

$$m^*(0) = m\alpha^{-1}, \quad m^*(\infty) = m. \qquad [4]$$

The ratio of effective masses at $k = K_D$ and $k = 0$ is given by

$$R(\alpha) \equiv [m^*(K_D)/m^*(0)] = (1 + \alpha^2)(1 + \alpha)^{-1}. \qquad [5]$$

We have chosen the dependence of $m^*(k)$ upon the parameter α so that $m^*(k)$ will be relatively insensitive to the value of k in the range $0 \le k \le K_D$. We see that $R(0) = R(1) = 1$, while the *minimum* value of $R(\alpha)$ occurs at $\alpha_1 \equiv (\sqrt{2} - 1)$ and has the value

$$R_{min} = R(\alpha_1) = 2\alpha_1 = 0.828427. \qquad [6]$$

The publication costs of this article were defrayed in part by page charge payment. This article must therefore be hereby marked "*advertisement*" in accordance with 18 U.S.C. §1734 solely to indicate this fact.

Abbreviations: TFM, Thomas–Fermi–Mott; MTFM, modified Thomas-Fermi-Mott; OP, Oppenheimer–Phillips.

[¶]In order that n_0 and λ_D be the same in both models, it is necessary that $E_F = (p_F^2/2m^*)$ be the same but the Fermi momentum p_F be smaller by a factor of $5^{1/3}$ in the 5-band model, so that m^* must be smaller by a factor of $5^{2/3}$.

In other words, $m^*(K_D)$ never gets smaller than about (5%)$m^*(0)$. Fig. 1 shows a plot of $m^*(k)/m$ versus k/K_D, for the value of $\alpha = 0.3804356$ as obtained in Eq. **19**.

The total number of allowed states per unit volume (including spin degeneracy) in all 5 bands having energy less than $E(k)$ is given by

$$n(k) = (5/3\pi^2)k^3. \quad [7]$$

The total number of allowed states per unit energy per unit volume at energy $E(k)$ is

$$N(k) = (dn/dk)(dE/dk)^{-1}. \quad [8]$$

The parameter α will be chosen, as in equation **6** of ref. 1, to ensure that

$$\lambda_D^{-2} = K_D^2 = 4\pi e^2 N(k_F), \quad [9]$$

As already stated, we take the numerical value of λ_D used in ref. 1.

We define

$$\Gamma \equiv (a_0/\lambda_D) = 3.708479, \quad [10]$$

where $a_0 = 0.5292$ Å is the Bohr radius, and

$$E_D \equiv (\hbar^2 K_D^2/2m) = \frac{1}{2}\Gamma^2 E_0 = 187.1071 \text{ eV}, \quad [11]$$

where $E_0 = (\hbar^2/ma_0^2) = (e^2/a_0) = 27.21$ eV is the Hartree energy. At this point it is convenient to express distance in units of λ_D, and (temporarily) energy in units of E_D. In these units,

$$\lambda_D = 1, \quad n_0 = 1.97356 \times 10^{-3}. \quad [12]$$

Eqs. **1**, **7**, and **8** remain unchanged. Eq. **9** becomes

$$N(k_F) = (\Gamma/8\pi), \quad [13]$$

while Eqs. **2** and **3** become

$$E(k) = k^2\{1 - (1 - \alpha)(1 + \alpha^2 k^2)^{-1}\}. \quad [14]$$

Inverting this, we have

$$k^2 = (2\alpha)^{-1}\left\{(\alpha E - 1) + \sqrt{(\alpha E - 1)^2 + 4E}\right\}. \quad [15]$$

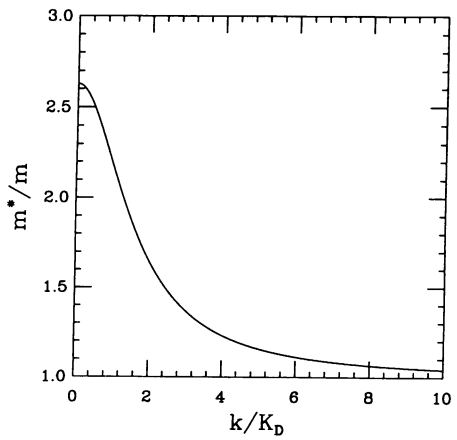

FIG. 1. Plot of $m^*(k)/m$ versus k/K_D.

Eq. **7** gives

$$n(E) = (2\alpha)^{-3/2}(5/3\pi^2)\left\{(\alpha E - 1) + \sqrt{(\alpha E - 1)^2 + 4E}\right\}^{3/2}. \quad [16]$$

Eq. **8** gives

$$N(k) = (dn/dE)$$

$$= (2\alpha)^{-1/2}(5/4\pi^2)\left\{1 + \frac{(\alpha E - 1 + 2\alpha^{-1})}{\sqrt{(\alpha E - 1)^2 + 4E}}\right\}$$

$$\times \left\{(\alpha E - 1) + \sqrt{(\alpha E - 1)^2 + 4E}\right\}^{1/2}$$

$$= (5/2\pi^2)k\left\{1 - (1 - \alpha)(1 + \alpha^2 k^2)^{-2}\right\}^{-1}. \quad [17]$$

Eqs. **13** and **17** give

$$(1 - \alpha) = (1 + \alpha^2 k_F^2)^2\{1 - (20/\pi)(k_F/\Gamma)\}. \quad [18]$$

Eq. **1** gives $k_F = 0.226934$, Eq. **18** gives

$$\alpha = 0.3804356. \quad [19]$$

Thus

$$[m^*(0)/m] = \alpha^{-1} = 2.628566,$$

$$[m^*(K_D)/m^*(0)] = (1 + \alpha^2)(1 + \alpha)^{-1} = 0.82925,$$

$$E_F = E(k_F) = 1.982821 \times 10^{-2} \quad [20]$$

(this last being equivalent to 3.71000 eV).

For a spherically symmetric problem, Poisson's equation in conventional units is

$$\nabla^2 V = r^{-1}(d/dr)^2(rV)$$

$$= -4\pi e^2[n(E_F - V) - n_0],$$

where

$$V = -e^2 r^{-1}\phi.$$

In terms of the dimensionless units we have been using, these become

$$(d/dr)^2\phi = 4\pi r[n(E_F - V) - n_0], \quad [21]$$

$$V = -(2/\Gamma)r^{-1}\phi. \quad [22]$$

Define

$$G_1 \equiv (20/3\pi)\Gamma^{-3/2} = 0.297142706$$

$$G_2 \equiv (\Gamma/2\alpha) = 4.873990454$$

$$G_3 \equiv (2\Gamma/\alpha^2) = 51.24641308$$

$$G_4 \equiv 4\pi n_0 = 2.480049092 \times 10^{-2}$$

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

Case	i	α_i	A_i	C_i	D_i
$Z = 1$	1	1.0	0.5257392	0.1876645	0.1382009
	2	2.4258593	0.3982298	0.6464533	0.1923548
	3	5.1761412	0.0739773	0.1617771	0.0141636
	4	101.402959	0.0020537	0.0041051	0.0002138
$Z = 2$	1	1.0	0.4240103	0.0877642	0.0898924
	2	2.3613116	0.4775152	0.6938484	0.2692140
	3	4.9027188	0.0957208	0.2128855	0.0224605
	4	118.328328	0.0027537	0.0055019	0.0004486

$$D \equiv \frac{1}{2}\Gamma E_F = 3.676625963 \times 10^{-2} \quad [23]$$

and

$$\psi \equiv \phi + Dr. \quad [24]$$

Using Eqs. **16** and **21**, along with these definitions, we find after some algebra the working MTFM equation

$$(d/dr)^2\psi = G_1 r^{-1/2}\left[(\psi - G_2 r) + \sqrt{(\psi - G_2 r)^2 + G_3 r\psi}\right]^{3/2} - G_4 r. \quad [25]$$

The right-hand side of this equation vanishes when $\phi = 0$, since

$$G_4 = G_1\left[-(G_2 - D) + \sqrt{(G_2 - D)^2 + G_3 D}\right]^{3/2}. \quad [26]$$

In numerically evaluating the right-hand side of Eq. **25**, there is considerable partial cancellation, leading to loss of significant figures. This is why the values in Eqs. **23** contain a large number of significant figures.

It is now convenient to redefine the units of energy. We express energy in units of

$$(2/\Gamma)E_D = \Gamma E_0 = 100.90772 \text{ eV}, \quad [27]$$

so that Eq. **22** becomes

$$V(r) = -r^{-1}\phi(r) \quad [28]$$

and

$$D = E_F. \quad [29]$$

Note that all the constants G_i and D still have the numerical values given in Eqs. **23**. Eqs. **24** and **25** remain unchanged.

From this point on, the procedure of the present paper is completely equivalent to that of ref. 1, so that there is no need to repeat the details. The MTFM equation is solved numerically for both cases $Z = 1$ and $Z = 2$. The resulting values of $\phi(r)$ are fitted accurately by a sum of four exponentials, using the constants α_i and A_i listed in Table 1. The constants α_i, C_i, and D_i are used in fitting the related quantity $\bar{\phi}(r)$. The fusion rate of a pair of deuterons in palladium can be written in the form

Table 2. Pair fusion rate and related quantities

	Case	$2\pi\eta$	F, cm^{-3}	λ, sec^{-1}
$Z = 1$	Without OP	87.0036	2.8110×10^{28}	0.06813×10^{-24}
	With OP	85.0483	0.8999×10^{28}	0.15413×10^{-24}
$Z = 2$	Without OP	82.9736	2.9747×10^{28}	4.0564×10^{-24}
	With OP	81.0184	0.9523×10^{28}	9.1757×10^{-24}

$$\lambda = AFe^{-2\pi\eta}, \quad [30]$$

where $A = 1.478 \times 10^{-16}$ cm^3/sec, F, as defined in equation **29** of ref. 1, is a quantity of the order of 10^{28} cm^{-3}, and $e^{-2\pi\eta}$ is the Gamow penetration factor. The quantities $(2\pi\eta)$, F, and λ are listed in Table 2, calculated both ignoring and considering the Oppenheimer–Phillips (OP) process (3), whereby the potential barrier is lowered somewhat at separation distances of the order of 10^{-12} cm because of the mutual polarization of the two deuterons. Note that for both $Z = 1$ and $Z = 2$ the OP process enhances λ by a factor of 2.262 and somewhat increases the $^3H/^3He$ branching ratio associated with the deuteron–deuteron nuclear reaction. The most accurate value of λ is believed to be the case $Z = 2$ including the OP process. This value of $\lambda = 0.918 \times 10^{-23}$ sec^{-1} is five powers less than the value obtained in ref. 1, but this value does agree with the experimental values of Jones *et al.* (4).

The calculations reported here may be viewed by some as a vain attempt on the part of the authors "to revive a dead horse," in view of the recent outpouring of negative publicity concerning cold fusion and the sometimes vicious attacks on its proponents. Nevertheless, we feel obligated to report that our calculations suggest that the results of Jones *et al.* (4) can be explained without invoking any physics more esoteric than that of screening of positive charges by conduction electrons. The Thomas–Fermi approach that we have used is much 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. Unlike the atom, the screening in the metal at large distances is given correctly, where the conduction electrons behave as having an effective mass. At the same time, at distances appreciably smaller than the asymptotic screening length λ_D, the screening results from electrons with a free-electron mass. An important part of our treatment is the recognition that the barrier to be penetrated by quantum mechanical tunneling is that associated with a pair of composite particles, each particle being a bare deuteron plus an associated screening cloud of electrons. On the basis of our calculations, we conclude that it would be wrong to say that the fusion phenomenon is impossible.

1. Parmenter, R. H. & Lamb, W. E. (1990) *Proc. Natl. Acad. Sci. USA* **87**, 3177–3179.
2. Mott, N. F. (1936) *Proc. Cambridge Philos. Soc.* **32**, 281–290.
3. Oppenheimer, J. R. & Phillips, M. (1935) *Phys. Rev.* **48**, 500–502.
4. 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)* **338**, 737–740.