Relaxation toward equilibrium

PLASMONS ENHANCE FUSION

M. BALDO† and R. PUCCI‡,*

† Istituto Nazionale di Fisica Nucleare, Sezione di Catania
   Corso Italia 57-95129 Catania-ITALY

‡ Dipartimento di Fisica e G.N.S.M., Unità di Catania
   Corso Italia 57-95129 Catania-ITALY

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* Author to whom correspondence has to be sent
Abstract.

It is shown that the coupling of hydrogen (or deuterium) nuclei with the collective plasmon excitations inside a metal produces an attractive nucleus-nucleus interaction. This interaction greatly reduces the distance where the Coulomb repulsion starts to dominate, in comparison with free deuterium molecules. Consequently the fusion reaction rate of deuterons in palladium is strongly enhanced. A simple estimate gives a fusion rate comparable with the experimental one reported by S.E.Jones et al. [Nature, 338, 737 (1989)].

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By using careful experimental techniques, S.E.Jones et al.\textsuperscript{1} have detected an emission of about 0.4 neutrons/sec when a current was passed through palladium or titanium electrodes immersed in an electrolyte of deuterated water and various metal salts. This interesting observation, recently confirmed under rather different experimental conditions\textsuperscript{2-4}, could be evidence of deuteron (d) fusion within the metal lattice. The fusion reaction rate is dramatically higher than expected for free deuterium molecules. The latter has been estimated by C.DeW.Van Siclen and S.E.Jones\textsuperscript{5}, and found to be nearly fifty order of magnitude smaller. In Ref. 1 it was pointed out that such an enhancement can be obtained by assuming an electron effective mass a few times larger than the bare one, since in this case the bond distance of the deuterium molecule is then accordingly reduced. However localization at distances of about 0.1 Å requires electron momenta several times larger than the Fermi momentum, and electrons with these momenta are expected to be essentially free. We also believe that pressure effects cannot play a relevant role, since there is no evidence of large decrease of the d - d bond distance in solid deuterium under pressure\textsuperscript{9}. Except for the possible influence of cosmic rays \textsuperscript{7,8}, it seems clear that the presence of the metal lattice must be at the origin of the observed effect.

In this paper we show the relevance of the deuteron interaction with the collective plasmon excitations of the metal, which produces a strong attractive d - d potential. Let us first consider a single deuteron interacting with the electron gas of the metal. The problem of the d self-energy can be studied along the same lines as the one of a positron in an electron gas, which was considered in detail by the authors \textsuperscript{9,10} on the basis of the dielectric function formulation of many-body theory \textsuperscript{11}. To lowest order in the d - electron interaction, the d self-energy $\Sigma$ is given by the first graph indicated in Fig. 1a

$$
\Sigma_d(k) = i\nu_{ed}(\bar{k}_1)\epsilon^{-1}(\bar{k}_1)G_d(k + \bar{k}_1)
$$

(1)

where $\nu_{ed}$ is the bare d - electron interaction, $\epsilon$ is the electron dielectric function, $G_d$ the d Green's function, $k = (\bar{k}, \omega)$ and barred variables are integrated over. In Refs. 10,12 it
was found that the main contribution to the positron energy is given by its coupling with the plasmon excitations, which essentially saturate the oscillator sum rule. Considering one plasmon contribution, one gets ($\hbar = c = 1$)

$$\Sigma_d (k) = - \frac{e^2 \omega_p^2}{\pi} \int_0^{k_c} \frac{d(\vec{q})}{\omega_1(\vec{q})} \left[ \frac{(\vec{q} - \vec{k})^2}{2M_d} + \omega_1(\vec{q}) - \omega + \mu \right]^{-1}$$

(2)

where $\omega_1(\vec{q})$ is the plasmon energy at momentum $\vec{q}$, $\omega_p$ the plasma frequency, $k_c$ the plasmon momentum cutoff, $M_d$ the deuteron mass and $\mu$ the deuteron chemical potential. It has to be stressed that the inclusion of incoherent electron particle - hole contribution would not affect the treatment and the validity of our considerations. For a bare particle of charge $Z$ this expression has to be multiplied by $Z^2$. This is in agreement with the elementary fact that, to the lowest order in $Z$, the total energy of a particle in a medium is proportional to the square of its charge. It follows immediately that when two deuterons are very close to each other their energy is four times the energy of a single d, and thus they must feel a net attraction. This can be seen more closely by considering the first graph indicated in Fig. 1b, which describes the exchange of a single plasmon between two deuterons. If we let two deuterons to approach each other this graph gives their interaction energy, and when they are very close, it reduces to a self-energy diagram and gives the above mentioned factor of four. The dependence on the distance of this interaction is determined by the Fourier transform of the plasmon propagator.

In this picture the deuteron screening due to the particle - holes is not considered. This can be included in the approximation scheme\textsuperscript{10}. However it is expected to have little effect on the energy, and there are evidences that the deuterons behave as unscreened particles inside transition metals\textsuperscript{13,14} and in Nb – V alloys\textsuperscript{14}.

In the following we take $\omega = \mu + k^2/2M_d$ in Eq. (1), and we identify the corresponding self-energy $\Sigma$ with the energy of a single deuteron. This is equivalent to the lowest order term in the Rayleigh - Schrödinger expansion\textsuperscript{15} of the interaction energy of the charged particle in the medium.
Due to the large mass of the deuteron the recoil energy \((\vec{q} - \vec{k})^2/2M_d - k^2/2M_d\) is negligible with respect to the plasmon energy. This allows to treat the deuteron as a fixed particle and to introduce the d - d interaction potential as a function of their relative distance \(R\).

A similar procedure can be used to calculate the two plasmon contribution \(E^{(2)}_d\) to the single d energy, indicated in the second graph of Fig. 1a, and the result is

\[
E^{(2)}_d = - \left( \frac{e^2\omega_p}{\pi} \right)^2 \int \int_{0}^{k_0} \frac{d(|\vec{q}|)}{\omega_1(\vec{q})^2} \frac{d(|\vec{k}|)}{\omega_1(\vec{k})^2} \left[ \omega_1(\vec{q}) + \omega_1(\vec{k}) \right]^{-1}
\]  \tag{3}

This term is proportional to \(Z^4\). Again for two deuterons the second (two plasmon exchanges) and the third (vertex corrections) graphs of Fig. 1b give their interaction energy, and they reduce to self - energy diagrams when the two deuterons are close to each other. One then gets the correct second order self - energy for a \(Z = 2\) particle. Notice that in Fig. 1b we have only indicated the structure of the graphs, and not all the 14 graphs which occur in this case.

The interaction energy calculated along these lines can be used as an adiabatic potential acting between the two deuterons. The validity of the adiabaticity assumption can be checked in each specific application.

The physical situation is similar to the one encountered in fusion reactions between heavy ions, where the role of the plasmons is played by the internal degrees of freedom of the two nuclei, and indeed in some cases the adiabatic limit is also the appropriate one\(^16\).

We have applied the model to the case of deuterium in palladium. For this metal at least three peaks in the energy loss spectra have been identified as due to bulk plasmon excitations\(^17\), at 7.5, 26.5 and 33.8 eV. The last one can be attributed to the simultaneous excitation of the first two. Thus we have introduced only the first two plasmon excitations in the model. The above described treatment can be easily generalized to the case of two plasmons, provided the oscillator sum rule is fulfilled

\[
\int_{0}^{+\infty} \omega d\omega \text{Im}(\epsilon^{-1}(\vec{k}, \omega)) = -2\pi^2 e^2 n/m
\]  \tag{4}
where \( n \) is the total electron density and \( m \) the electron mass. This condition is satisfied if

\[
\omega_{p_1}^2 + \omega_{p_2}^2 = 4\pi e^2 n/m
\]

(5)

which is approximately verified in palladium\(^{17}\). A further characteristic of palladium is that the lowest plasmon is essentially dispersionless\(^{18}\). Since this plasmon gives the main contribution, for simplicity we have assumed both plasmons as dispersionless. Then the d-d potential \( V(R) \) assumes a very simple form

\[
V(R) = V_1(R) + V_2(R)
\]

\[
V_1(R) = -2\frac{e^2}{\pi}(k_1 I(x_1) + k_2 I(x_2))
\]

\[
V_2(R) = -2 \left(\frac{e^2}{\pi}\right)^2 k_1 \left[ \frac{k_1}{2\omega_{p_1}} (3I(x_1)^2 + 4I(x_1)) + \frac{k_2}{\omega_{p_1} + \omega_{p_2}} (3I(x_1)I(x_2) + 2I(x_1) + 2I(x_2)) \right]
\]

\[
-2 \left(\frac{e^2}{\pi}\right)^2 k_2 \left[ \frac{k_2}{2\omega_{p_2}} (3I(x_2)^2 + 4I(x_2)) + \frac{k_1}{\omega_{p_1} + \omega_{p_2}} (3I(x_1)I(x_2) + 2I(x_1) + 2I(x_2)) \right]
\]

(6)

where \( k_1, k_2 \) are the cutoff momenta of the two plasmons, \( x_1 = k_1 R, x_2 = k_2 R \) and

\[
I(x) = \frac{1}{x} \int_0^x \frac{\sin(y)}{y} dy
\]

(7)

is essentially the Fourier transform of the plasmon propagator in the dispersionless case.

Unfortunately the values of the cutoff momenta are not known experimentally, at least to our knowledge, so we have chosen the value extracted from the corresponding \( \omega_p \) in the free electron approximation, which gives \( k_1 = 0.92 \) and \( k_2 = 1.41 \text{ Å}^{-1} \). In Fig. 2 are reported the bare Coulomb potential \( e^2/R \) between the two deuterons (dash-dotted line), the total potential as given by Eq. (6) (dotted line) and the sum of the two (full line). The deuterons are strongly attracted and only at a distance \( R \approx .2 \text{ Å} \) the Coulomb repulsion takes over. The long attractive tail is due to our assumption of undamped plasmon. In a more realistic treatment the potential would tend more rapidly to zero. This is irrelevant for our considerations. Furthermore the potential can be considered adiabatic to a very good approximation. In fact the adiabatic parameter \( \hbar(1/V(R))(dV(R)/dt) \leq .1 \text{ eV} \), which
is much smaller than the plasmon energies (or other typical electron excitation energy).

To have an estimate of the consequence of this result on the d - d fusion rate, let us model the deuterons inside palladium as a classical gas interacting through the total conservative potential depicted in Fig. 2 (full line), at a temperature T. Then the number of fusion per second $N_f$ in a gas of N deuterons at a density $\rho$ can be written

$$N_f \simeq N \rho \langle v \sigma \rangle \simeq N \frac{4 \pi \rho \hbar}{M_d} \langle \frac{1}{k} \rangle \simeq P$$

(8)

where $v$ is the relative velocity, $\sigma$ is the fusion cross section and $P$ the penetration factor through the potential barrier for s - wave and low energy scattering. The latter can be estimated in the WKB approximation\(^9\)

$$P \approx \exp \left[ - \int_0^{R_0} \left( 2 \sqrt{M_d(V(R) + \frac{e^2}{R}) - \frac{1}{4R^2}} - \frac{1}{R} \right) dR \right]$$

(9)

where $R_0$ is the distance at which the total potential passes through zero. For a Boltzmann distribution the order of magnitude of $N_f$ is given by $N_f \approx 10^{35} \rho T^{\frac{1}{2}} P$, if one measures the density in $\text{Å}^{-3}$, T in eV and $N \approx 10^{23}$. At room temperature and for a Pd/d ratio of order one, one gets $N_f \approx 10^{-14} \text{\,sec}^{-1}$, which is 37 order of magnitude larger than for a gas of free deuterium molecules. In view of the uncertainty in the plasmon cutoff momenta, we tried also other values of the cutoffs, and we found that for $k_1 = k_2 = 1.6 \text{ Å}^{-1}$ it is possible to reproduce the fusion rate reported in Ref. 1. These cutoff values seem not unreasonable, and the corresponding total d - d interaction potential is reported in Fig. 2 (dashed line). We also considered the case of titanium, and found a similar situation, provided one includes also the surface plasmon\(^{20}\).

In conclusion we have shown that d - d fusion rate can be greatly enhanced by the interaction of the deuterons with the plasmons of the metal, in which they are immersed. The model here presented is based on well established many-body theory of solids. Some cautions have to be considered as regards the convergence of the expansion we used for the d - d energy, since the second order contribution is larger than the first order one.

\[ e^2 = 14.4 \, eV \times \text{Å} \]
However our calculations clearly show that the plasmon contribution must play a crucial role in the d - d interaction inside metals, and the described interaction mechanism is a good candidate for the explanation of the surprising high d - d fusion rate, observed by S.E. Jones et al.¹. Moreover our results suggest that the d - d fusion should increase in those metals which can load a large number of d nuclei and which possess low-energy plasmon excitations. Finally we note that it appears interesting to explore the implications of the model for the deuteron dynamics.
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Figure Captions

Fig. 1 First and second order graphs for the self-energy (a) and plasmon exchanges (b). Full lines indicate deuterons and wiggly lines plasmons.

Fig. 2 Interaction potentials (in eV) used in the calculations as functions of the deuteron - deuteron separation distance $R$ (in Å): bare Coulomb potential (dash-dotted line), plasmon contributions to the deuteron - deuteron interaction (dotted line) for palladium with plasmon cutoff momenta $k_1 = .92$ and $k_2 = 1.41\,\text{Å}^{-1}$, the sum of the two (full line) and the corresponding one for $k_1 = k_2 = 1.6\,\text{Å}^{-1}$ (dashed line).