Theoretical Hypothesis of a Double Barrier Regarding the D-D Interaction in a Pd Lattice: A Possible Explanation of Cold Fusion Experiment Failures

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ABSTRACT

During the past 15 years, disputable experimental evidence has built up for low energy nuclear reaction phenomena (LENR) in specialized heavy hydrogen systems [1-4]. Actually, we cannot say that a new branch of science is beginning. In spite of experimental contributions, the real problem is that there is no theoretical explanation for LENR. In this work, we analyze the deuteron-deuteron reactions within palladium lattice by means of the coherence theory of nuclear and condensed matter [5] and, using this general theoretical framework accepted from ‘cold fusion scientists’, we will show the low occurrence probability of fusion phenomena. In fact, in the coherence approach, the D-D potential exhibits double barrier features and, in this way, the D-D fusion is inhibited.

1. Introduction

The Coherence Theory of Condensed Matter represents a general theoretical framework accepted by most of the scientists who work on cold fusion phenomena. In the coherence theory of condensed matter [5], it is assumed that the electromagnetic (e.m.) field due to elementary constituents of matter (i.e. ions and electrons) plays a very important role in a dynamic system. In fact, considering the coupling between e.m. equations, due to charged matter, and the Schrödinger equation of field matter operator, it is possible to demonstrate that, in proximity of e.m. frequency $\omega_0$, the matter system shows a coherence dynamics. For this reason, it is possible to talk about coherence domains whose length is about $\lambda_{CD}=2\pi/\omega_0$. Of course, the simplest model of matter with coherence domain is the plasma system. In the usual plasma theory, we must consider the plasma frequency $\omega_p$ and the Debye length that measures the Coulomb force extension, i.e. the coherence domain length. For a system with $N$ charge $Q$ of $m$ mass within a $V$ volume the plasma frequency can be written as:

$$\omega_p = \frac{Q}{\sqrt{m}} \sqrt{\frac{N}{V}}$$

(1)
In this work, we will study the “nuclear environment”, that is supposed to exist within the palladium lattice D₂-loaded at room temperature as predicted by Coherence Theory. In fact, when the palladium lattice is loaded with deuterium gas, some people declared that it is possible to observe traces of nuclear reactions [1,2,3]. For this reason, many physicists talk about Low Energy Nuclear Reactions (LENR).

The more robust experiments tell us that, in the D₂-loaded palladium case, the more frequent nuclear reactions are [3,4]:

1.) \( D + D \rightarrow ^3H + p + 4.03MeV \)  

2.) \( D + D \rightarrow ^4He + 23.85MeV \)

In this work we also propose a “coherence” model by means of which we can explain the occurrence of reactions 1 and 2 and their probability according to the more reliable experiments. First, we will start from the analysis of the environment; i.e. of plasmas present within palladium (d-electron, s-electron, Pd-ions and D-ions) using the coherence theory of matter. Finally, we will use the potential reported in ref. [6,7] adding the role of lattice perturbations by means of which we compute the D-D tunneling probability.

2. The plasmas present within unloaded palladium

According to the Coherence Theory of Condensed Matter, in a palladium crystal at room temperature the electron shells are in a coherent regime within coherent domains. In fact, they oscillate in tune with a coherent e.m. field trapped in the coherent domains. For this reason, in order to describe the lattice environment, we must take into account the plasma of s-electron and d-electron.

a) The plasma of the d-electrons

The plasma is formed by electrons of palladium d-shell. We start by computing:

\[
\omega_d = \frac{e}{\sqrt{m}} \sqrt{\frac{n_e N}{V}}
\]  

(3)

as d-electrons plasma frequency. But, according to the coherence theory of matter, we must adjust this plasma frequency by a factor 1.38. We can understand this correction observing that the formula (3) is obtained assuming a uniform d-electron charge distribution. But, of course, the d-electron plasma is localized in a shell of radius R (that is about 1Å), so the geometrical contribution is:

\[
\frac{\sqrt{6}}{\sqrt{\pi}} = 1.38
\]  

(4)
Labeled with $\omega_{de}$ the renormalized d-electron plasma frequency, we have [5]:

$$\omega_{de} = 41.5eV / h$$

(5)

and the maximum oscillation amplitude $\xi_d$ is about 0.5 Å.

**b) The plasma of delocalized s-electrons**

The s-electrons are those that, in the lattice, neutralize the adsorbed deuterons ions. They are delocalized and their plasma frequency depends on the loading ratio (D/Pd percentage) by means of the following formula (5):

$$\omega_{se} = \frac{e}{\sqrt{m}} \left( \frac{N}{V} \right)^{1/2} \sqrt{\frac{x}{\lambda_a}}$$

(6)

where

$$\lambda_a = \left[ 1 - \frac{N}{V} V_{pd} \right]$$

(7)

and $V_{pd}$ is the volume effectively occupied by the Pd-atom. As reported in reference [5] we have:

$$\omega_{se} \approx x^{1/2} 15.2eV / h$$

(8)

For example, for $x=0.5$, we have $\omega_{se} \sim 10.7 \text{ eV}/h$.

**c) The plasma of Pd-ions**

Finally, we must consider the plasma due to palladium ions that forms the lattice structure. In this case, it is possible to demonstrate that the frequency is [5]:

$$\omega_{pd} = 0.1eV$$

(9)

3. **The plasmas present within D$_2$-loaded palladium**

We know that the deuterium is adsorbed when placed near a palladium surface. This loading can be enhanced using electrolytic cells or vacuum chambers working at opportune pressure [8,9]. By means of Preparata’s theory of Condensed Matter it is assumed that, according to the ratio $x=D/Pd$, three phases concerning the D$_2$-Pd system exist:

1) $\alpha$ phase

for $x<0.1$
2) β phase for $0.1 < x < 0.7$
3) γ phase for $x > 0.7$

In the α-phase, the D$_2$ is disordered and not in a coherent state (D$_2$ is not charged!). Regarding the other phases, we must remember that on the surface, due to lattice e.m., the following ionization reaction takes place:

$$D_{\text{lattice}} \rightarrow D^+ + e^-$$

Then, according to the loading percentage $x = D/Pd$, the deuterium ions can enter octahedrical sites (Fig. 1) or in the tetrahedral (Fig. 2) in the (1,0,0)-plane. In the coherence theory, the deuterons plasma in the octahedral site can be called β-plasma, whereas those in the tetrahedral one can be called γ-plasma.
Regarding to $\beta$-plasma, it is possible to affirm that the plasma frequency is given by [5]:

$$\omega_\beta = \omega_\beta^0 (x + 0.05)^{1/2}$$  \hspace{1cm} (11)$$

where

$$\omega_\beta^0 = \frac{e}{\sqrt{m_D}} \left( \frac{N}{V} \right)^{1/2} \frac{1}{\lambda_a^{1/2}} \frac{0.15}{\lambda_a} \ eV / \hbar$$ \hspace{1cm} (12)$$
For example, if we use $\lambda_a=0.4$ and $x=0.5$ it is obtained $\omega_B=0.168 \, eV/\hbar$. In the tetrahedral sites the D$^+$ can occupy the thin disk that encompasses two sites (Fig. 3). The D$^+$ ions form a barrier.

Note that the electrons of the d-shell oscillate past the equilibrium distance $y_0$ (about 1.4 Å), thus embedding the ions in a static cloud of negative charge (which can screen the coulomb barrier). So, as reported in [5], we have:

$$\omega_\gamma = \sqrt{\frac{4Z_{\text{eff}} \alpha}{m_p y_0^2}} \approx 0.65 \, eV/\hbar$$

(13)

Of course, this frequency depends also on the chemical condition of palladium (impurities, temperature etc…)

Due to a large plasma oscillation of d-electrons, in the disk-like tetrahedral region (where the $\gamma$-phase D$^+$s are located) a high density negative charge condenses, giving rise to a screening potential $W(t)$ whose profile is shown in Fig. 4.
We emphasize that the $\gamma$-phase depends on $x$ value and that this new phase has been experimentally observed [11].

The new phase $\gamma$ is very important in the LENR investigation. In fact, many “cold fusion scientists” declare that the main point of cold fusion protocol is that the loading D/Pd ratio must be higher than 0.7, i.e. the deuterium must take place in the tetrahedral sites.

4. The D-D potential

In reference [6], it was shown that the phenomena of fusion between nuclei of deuterium in the crystalline lattice of a metal is conditioned by the structural characteristics, by the dynamic conditions of the system, and also by the concentration of impurities present in the metal under examination.

In fact, studying the curves of the potential of interaction between deuterons (including the deuteron-plasmon contribution) in the case of three typical metals (Pd, Pt and Ti), a three-dimensional model showed that the height of the Coulomb barrier decreases on varying the total energy and the concentration of impurities present in the metal itself.

The potential that takes into account the role of temperature and impurities is given by the expression [6]:

$$V(r) = k_0 \frac{q^2}{r} \cdot M_d \left( V(r)_M - \frac{J \cdot k \cdot T \cdot R}{r} \right)$$  \hspace{1cm} (14)
In (14), $V(r)_M$, the Morse potential, is given by:

$$V(r)_M = \left( \frac{J}{\zeta} \right) \left\{ \exp \left( -2\phi \left( r - r_0 \right) \right) - 2 \exp \left( -\phi \left( r - r_0 \right) \right) \right\} \quad (15)$$

Here parameters $\phi$, $r_0$ depend on the dynamic conditions of the system, $\zeta$ is a parameter depending on the structural characteristics of the lattice, i.e. the number of “d” band electrons and the type of lattice symmetry, varying between 0.015 and 0.025.

Of course the Morse potential is used in the interval that includes the inner turning point $r_a$ and continues on towards $r=0$, that is strictly linked to the coulomb potential (Fig 5).

![D-D potential features using a Morse potential](image)

In reference [6] by means of the following formula ($\alpha$ is the zero crossing $r$-value of potential):

$$|P|^2 = \exp \left( -2 \int_0^{\alpha} K(r)dr \right) \quad (16)$$

where:

$$K(r) = \sqrt{2\mu [E-V(r)]/\hbar^2} \quad (17)$$

This is obtained (using for the nuclear rate the reasonable value of $10^{21}$ min$^{-1}$) a fusion probability normalized to the number of events per minute of $10^{25}$ for $\alpha=0.34 \text{ Å}$, $E=250$ eV, $T=300 \text{ K}$ and $J=0.75$ (a case of high impurities). Many experiments confirmed these fusion rate values regarding reaction (1 and 2) in Ref. [10].
In this work, according to the coherence theory of condensed matter, we will study the role of potential (14) in the three different phases: $\alpha$, $\beta$ and $\gamma$.

So, in this theoretical framework we need to clarify:

1) What is $K_T$?
2) What is the role of electrons, ions plasma?

Regarding the first point, according to the different deuteron-lattice configurations, $K_T$ can be:

i) the lattice temperature, if we consider the deuterons in the $\alpha$-phase

ii) $\omega_\beta$, if we consider the deuterons in $\beta$-phase

iii) $\omega_\gamma$, if we consider the deuterons in the $\gamma$-phase

The second point raises a more complicated question.

In fact, the lattice environment is a mixing of coherent plasmas (ion Pd, electron and deuterons plasma) at different temperatures, due to different masses. Thus, describing an emerging potential is a very hard office. The method that in this work we propose is the following: considering the total contribution of lattice environment at D-D interaction (i.e. $V_{tot}$) as random potential $Q(t)$. So, in this model we can write:

$$V_{tot}(t) = V(r) + Q(t)$$

(18)

Of course we assume that:

$$\left\langle V_{tot}(t) \right\rangle, \neq 0$$

(19)

that is, we suppose that $Q(t)$ (a second order potential contribution) is a periodic potential (the frequency will be labeled by $\omega_Q$) that oscillates between the maximum value $Q_{max}$ and 0.

The role of potential $Q(t)$ could increase or decrease the barrier. In Fig. 6 we show the plot of potential $V_{tot}$ for two different values of $Q(t)$. 


This means that, according to \( \omega_Q \) and to the energy of particles incoming to the barrier, we can have the following main cases:

1) the particle crosses the barrier in the point \( \alpha \)
2) the particle crosses the barrier in the \( \alpha' \)

For this reason, we can talk about scenario 2 as the worst case to have high tunneling probability, and scenario 1 as the best case.

To determine the model parameters, we must make some hypothesis regarding \( Q(t) \) and \( \omega_Q \). In this work, we will limit ourselves to approximate \( Q(t) \) as the screening potential \( W(t) \) due to d-electrons reported in Fig. 5.

This means that \( \omega_Q \sim \omega_d \).

Of course, there is a strong dependence between the scenario and the deuteron phase since \( Q(t) \) is, at first order, only the d-electrons screening potential.

To summarize, we can have the following cases in a palladium lattice according to loading ratio:

i) **\( \alpha \)-phase**

In the phase \( \alpha \) the deuterons are in a molecular state and the thermal motion is about:

\[
0.02 \, eV < \hbar \omega_\alpha < 0.2 \, eV
\]

This phase takes places when \( x \) is less than 0.1, and since \( W(t) \) is zero, the D-D potential is:
Expression (20) has been partially evaluated in a previous paper [6] but, in that case, we were interested only in the dependence of tunneling probability on impurities present within lattice. In this work, we will examine the correlation between potential features and loading ratio. In paragraph 6, we will show some numerical results.

**ii) β-phase**

When $x$ is bigger than 0.1 but less 0.7, the phase β happens. The interaction takes place between deuteron ions that oscillate between the following energy values:

$$0.1 \text{ eV} < \hbar \omega_\beta < 0.2 \text{ eV}$$

In this case $W(t)$ is zero, so the potential is given by the expression (21):

$$V(r) = const \frac{q^2}{r} \cdot M_d \left( V_M(r) - \frac{\hbar \omega_\beta R}{r} \right)$$

(21)

Comparing expressions 20 and 21, it clearly seems that the weight of impurities is more important in the β-phase. Of course, this conclusion is in accordance with the previous papers [6,7] where we had studied the role of temperature on tunneling effect.

**iii) γ-phase**

Finally, when the loading ratio is higher than 0.7, the deuteron-palladium system is in the γ-phase. According to the synchronism between phase oscillations of deuteron and d-electron plasmas, we must consider the following two cases:

**Case 1: $Q(t)=0$**

In this case the potential is a natural extension of formula (14), than it can be written as:

$$V(r) = const \frac{q^2}{r} \cdot M_d \left( V_M(r) - \frac{\hbar \omega_\gamma R}{r} \right)$$

(22)
Case 2: $Q(t) \neq 0$

This is the more interesting case. It happens when $\omega_\gamma$ is about $\omega_Q$ and, of course, when the respective oscillations are in phase. The deuterons undergo the screening due to d-electrons shell, so we suppose that the D-D potential must be computed assuming that the well present in potential (14), due to Morse contribution, disappears. In fact, if we use a classical plasma model where the $D^+$ ions are the positive charge and the d-electrons the negative one, it is very reasonable to suppose that we must use the following potential:

$$V(r,t) = \text{const} \frac{q^2}{r} \cdot M_d \left( \frac{\alpha}{|\vec{r}|} e^{-\frac{|\vec{p}|}{\lambda_{D}}} - \frac{J\hbar \omega_\gamma R}{r} \right) + Q(t) \tag{23}$$

Where

$$V_c(\vec{r}) = \frac{\alpha}{|\vec{r}|} e^{-\frac{|\vec{p}|}{\lambda_{D}}} \tag{24}$$

And $\lambda_D$ is the Debye length of this classical plasma.

We emphasize that $Q(t)$ is not known as a perturbative potential. About it, we can only say that:

$$\langle Q(t) \rangle_t \approx \frac{W_{\text{max}}}{\sqrt{2}} \tag{25}$$

As previously said, we suppose that it is the screening potential due to d-electron and its role that reduces the repulsive barrier.

5. The barrier crossing treatment

Now we proceed to discuss how we can handle the crossing of barrier in the $\gamma$-phase and for $Q(t)$ different to zero. The starting point in any case is the Scrödinger equation:

$$\frac{\hbar^2}{2\mu} \Psi''(r) \left[ E - V_{\text{tot}}(r,t) \right] \Psi'(r) = 0 \tag{26}$$

but solving this problem is very difficult.
So, to handle in a very simple way this topic, we can start observing that when we use \( V_{tot}(r,t)=V(r)+W_{max}/\sqrt{2} \), the main energy values that interest our problem are four (see Fig. 7) \( E_1, E_2, E_3 \) and \( E_4 \) and the problem is equivalent to the treating of a double barrier case.

From reference [12] we know that:

\[
E_1 = \text{a few eV};
\]

\[
E_2 = -D \left( 1 - \frac{\gamma h}{\sqrt{2\mu D}} \left( \mu + \frac{1}{2} \right) \right)^2
\]

\[
E_3 \sim \left( \frac{m_2}{M_N} \right) E_1 \sim \frac{1}{1000} \text{eV}
\]

\[
E_4 = D'
\]

\( \gamma \) is the constant of metal anharmonicity and \( \nu \) the vibrational constant. Another important quantity is \( D' \) that is the depth of the potential well. According to the Morse potential (15) it is \( J/\zeta \).

Now we can build an energy tensor \( E_{ij} \):
\[ E_{11}=E_1, \ E_{22}=E_2, \ E_{33}=E_3, \ E_{44}=E_4, \ E_{ij}=E_i-E_j, \ E_{ij}=-E_{ji} \]

So, in this way, we can define a square quadratic energy value:

\[
\langle E \rangle = \sqrt{\frac{\text{tr}E_jE_j}{4}}
\]  

(31)

and a dispersion:

\[
\sigma = \sqrt{\frac{\sum_{i \neq j} E_{ij}E_{ij}}{4}}
\]  

(32)

If we neglect the term \( Q(t) \) and consider only the random characteristic of deuteron energy, a reasonable value of \( K(r) \) can be:

\[
K(r) = \frac{1}{\hbar} \sqrt{2\mu \left[ V(r) - \left( \frac{\text{tr}E_rE_r}{4} \pm \sigma \right) \right]}
\]  

(33)

And finally:

\[
P(\alpha) = \exp \left( -2 \int_0^\alpha K(r) \, dr \right)
\]  

(34)

But according to statistical treatment we can observe that:

\[
P = P(\alpha, \langle E \rangle, \sigma)
\]  

(35)

where we remember that in the \( \gamma \)-phase

\[
\alpha = \alpha[Q(t)]
\]  

(36)

Since we supposed that the greater contribution to \( Q(t) \) is due to the screening effect of d-electrons (i.e. of random potential) in the \( \gamma \)-phase, we can limit ourselves to consider the two following cases (i.e. double barrier approximation):

3) \( Q(t) = 0 \rightarrow \alpha = 0.34 \text{ Å} \).
4) \( Q(t) \neq 0 \rightarrow \alpha = 0.16 \text{ Å} \)
Of course, case 4 is the more advantageous to obtain high tunneling probability.

6. Result and Discussion

Now we will present the D-D fusion probability normalized to the number of events per minute for the D-D interaction in all different phases. More exactly, we will compare the fusion probability in the $\alpha$, $\beta$ and $\gamma$ phases using a reasonable square average value of 200 eV and 50 eV.

In order to cross the potential (14) in all four points $E_1$, $E_2$, $E_3$ and $E_4$. We will also consider the role of d-electron screening as perturbative lattice potential. This treatment, that interests us only the case where $Q(t)$ is different from zero, involves that we turn the time-dependent problem of a tunneling effect into a double barrier problem. To summarize, we can say that in the $\gamma$-phase the new ‘physics fact’ is the emerging of a double barrier. Note that the new phase $\gamma$ is invocated by cold fusion scientists, because the screening enhances the fusion probability. From an experimental point of view, in the cold fusion phenomenology it is possible to affirm that there are three typologies of experiments [13]:

1) Those that have given negative results.
2) Those that have given some results (faint evidence with respect to the background, fusion probability about 10^{-25}) using a very high loading ratio.
3) Those that have given clear positive results as Fleishmann and Pons experiments.

Nevertheless, we think that the experiment in category 3 are little accurate from an experimental point of view. For this reason, we believe that a theoretical model of controversial phenomenon of cold fusion can explain only the experiments in categories 1 and 2. In this case, the role of the loading ratio on the experimental results needs to be considered. Now, let us begin from $\alpha$-phase.

In Table 1 we show the results about the $\alpha$-phase. In this case, we can observe that the theoretical fusion probability is very low, less than 10^{-74}. It is possible to affirm that if we load the deuterium with a percentage $x < 0.2$ we do not observe any fusion events! The same absence of nuclear phenomenon is consistent with a loading ratio of about 0.7 (Table 2) since in this case the predicted fusion probability is less than 10^{-42}. These predictions, of course, are consistent with the experimental results. But for $x > 0.7$ a set of valid experiments do show some background spikes (for example see reference [10]).

The remarkable result of our model is that in the $\gamma$-phase, as shown in Table 3, we can really observe some background fluctuations, since we predict a fusion probability about 10^{-25} due to a very high loading ratio. This represents a new result compared to reference [6,7] since, in that case, the fusion probability was independent of loading ratio.
In order to predict very noteworthy nuclear evidence (about $10^{-17}$), we must have $\omega_\gamma$ comparable to $\omega_Q$ (Table 4). In fact, only in this condition the screening potential can enhance the tunneling probability, and the D-D interaction becomes a like-Debye potential.

The condition by means of which $\omega_\gamma$ is equal to $\omega_Q$ will be discussed in another paper, but in this work we will limit ourselves to observing that it is a very improbable condition!

To conclude, we show that the model proposed in this paper can explain some anomalous nuclear trace reactions in the solid state, but closes any hopes on the possibility of controlled fusion reactions in solid matter.

**Table 1.** For “Impure” Pd ($J \approx 0.75\%$), using the $\alpha$-potential (potential 20), has been computed the fusion probability normalized to the number of event/min for different values of energy ($\sigma = \pm 50$ eV).

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Table 2. For “Impure” Pd (J ≈ 0.75\%), using the β-potential (potential 21), has been computed the fusion probability P normalized to the number of event/min for different values energy (σ = ± 50 eV).

**Palladium J ≈ 0.75\% α ≈ 0.34 Å \langle E \rangle = 200eV**

<table>
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Table 3. For “Impure” Pd ($J \approx 0.75\%$), using the $\gamma$-potential with $Q(t) = 0$ (potential 22), has been computed the fusion probability normalized to the number of event/min for different values of energy ($\sigma = \pm 50$ eV).

**Platinum $J \approx 0.75\% \alpha \approx 0.34 \text{Å} \langle E \rangle = 200eV**

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Table 4. For “Impure” Pd ($J \approx 0.75\%$), using the Debye potential (potential 24), has been computed the fusion probability normalized to the number of event/min for different values of energy ($\sigma = \pm 50$ eV).

Palladium $J \approx 0.75\% \alpha \approx 0.16\,\AA\,\langle E\rangle = 200$ eV

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References