Muon catalyzed fusion in solid deuterium

L. I. Menshikov
Kurchatov Institute Russian Research Center, 123182 Moscow, Russia
V. V. Fliftenkov
Joint Institute for Nuclear Research, 141980 Dubna, Russia

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1. INTRODUCTION. THE “STANDARD” THEORY OF THE

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2. CALCULATION OF THE $d\mu$ MOLECULE FORMATION RATE IN SOLID DEUTERIUM

Let us write the resonance condition for reaction (1) in a solid:

$$\epsilon_{ddp}=\epsilon_{d}+\Delta E,$$

where $\Delta E=E_f-E_i$ and $E_i$ and $E_f$ are the lattice energies in the initial and final states, respectively. In the initial state the lattice Hamiltonian has a form

$$\hat{H}_{i}=\sum_{\alpha}p_{\alpha}^{2}/2M+U.$$

where $M$ is the $D_2$ molecule mass, the summation is made over $D_2$ molecules ($a=1,2,...$), and $U$ is the lattice potential energy.

Strictly speaking, one should assume that the $dp$ atom interacts with the whole lattice and forms an intermediate complex $C$ with it, i.e., one should take into account the effect of coherent formation of the $dp$ molecule on a lattice. However, this effect is negligible. The reason is the smallness of the overlap integral of the wave functions of the $dp$ atoms joined to the neighboring $D_2$ molecules. So let us distinguish one $D_2$ molecule, label it zero, and assume that the $dp$ atom interacts with it only. The $ddp$ formation rate calculated in this manner should be multiplied by the total number of the $D_2$ molecules in a lattice. In the following calculations we put the coordinate origin in the equilibrium position of the zero molecule.

In the final lattice state the mass of the zero molecule is changed, $M\rightarrow M^c$, so

$$\hat{H}_{F}=\sum_{a} \frac{\hat{p}_{0}}{2M} + \frac{\hat{p}_{0}^{2}}{2M} + U=\hat{H}_{I} + \hat{V}_{L},$$

$$\hat{V}_{L}=\frac{1}{2} \sum_{a} \frac{1}{M_{a}} \hat{p}_{a}^{2}.$$

It follows from the expression for $\hat{H}_{I}$ and $\hat{H}_{F}$ that the characteristic parameter of the problem is $\xi=(M_{p}^{-1}M_{D})^{-1/2}$ (either $M_{p}$ or $M$ may be in the denominator).

Hence, $\hat{H}_{I} \neq \hat{H}_{F}$. This is indicated by the tilde in the notation for the energy of the final lattice state (see Eq. (6)). It follows from Eqs. (3), (4), and (5) that one can neglect the $dp$ atom energy in Eq. (6), which is very small in comparison with $|\epsilon_{I}|$. Hence, the simplified resonance condition is

$$\Delta E=\epsilon_{I},$$

If $\epsilon_{I}>0$ holds, then, according to Eq. (7), we have $\Delta E<0$, that is, phonons of energy $-\epsilon_{I}$ are absorbed. However, at the lowest energies the number of such phonons is exponentially small, $e^{-\epsilon_{I}/kT}$. That is why one can neglect the transitions (3) and (4) for the experimental conditions of Refs. 1, 2 and should consider only the transition (5), which goes with an escape of the even phonon numbers (the last circumstance is obvious from the form of $\hat{V}_{L}$). Besides, as follows from the previous consideration, one can neglect the existing lattice phonons, that is, one can consider the initial lattice state as vacuum: $\hat{H}_{I}(0)=\hat{E}_{I}(0)$.

The distance between the $D_2$ molecules in a lattice is large ($\sim 6$ a.u.) compared with the size of the molecule, so one can consider $dp$, $D_2$, and $C$ to be point-like, and the interaction operator which is responsible for the transition (1) can be written in the form

$$\hat{H}=A\hat{v}(\epsilon),$$

where $A$ is a constant which will be obtained later, $\epsilon=r_{D}-U_{0}$, $r_{D}$ are the $dp$ atom coordinates, $U_{0}$ is the displacement of the $D_2$ molecule from the equilibrium point. To obtain the value of $A$ let us first calculate the $ddp$ molecule formation rate in the double-collision approximation (1) with $\epsilon_{I}>0$.

The wave functions of the initial and the final state are

$$\Psi_{I}=\phi_{0}(r),$$

$$\Psi_{F}=\Psi_{dp}(r),$$

where $\Psi_{dp}(r)$ is the wave function of the bound state of the $dp$ atom and the $D_2$ molecule, that is the wave function of the complex $C$. In first order of perturbation theory with respect to the operator $\hat{V}$, we have ($h=1$, the normalized volume is chosen equal to unity)

$$A_{ddp}=\int_{0}^{\infty} J_{1}(|\epsilon|)d\epsilon 2\pi |\epsilon|^{1/2} \phi_{0}(\epsilon)|\Psi_{dp}|^{2}=2\pi \eta_{0} \phi_{I}(\epsilon_{I})B,$$

where $\eta_{0}$ is the number of deuterium nuclei in a unit volume, $\epsilon_{I}>0$. From this and Eqs. (3) and (5) for $K_{I}=1$ and $K_{F}=1$ one obtains $B=5\times 10^{-12}$ a.u. From this and Eqs. (3) and (5) for $K_{I}=1$ and $K_{F}=0$ one determines

$$B=5.5\times 10^{-12} \text{ a.u.}$$

It follows from the expression for $\hat{H}_{I}$ and $\hat{H}_{F}$ that the characteristic parameter of the problem is $\xi=(M_{p}^{-1}M_{D})^{-1/2}$ (either $M_{p}$ or $M$ may be in the denominator).
3. DISCUSSION

In the present paper it has been shown that in the limit $T \to 0$ the value of the $d \mu \mu$ molecule formation rate $\lambda_{d\mu\mu}$ approaches a constant, and the estimate (15) is obtained for the value of $\lambda_{d\mu\mu}$ in solid deuterium. This has been done on the basis of the pseudopotential method, which originates from the work of E. Fermi and N. N. Bogoliubov. As in these papers, the formula for $\lambda_{d\mu\mu}$ is rigorous because a comparison with the rigorous calculation was used in obtaining the value for $A$ in it. Doubt may arise whether the formulas (9) and (11) are applicable in our consideration. They coincide in form with the Fermi golden rule of perturbation theory, but in our case the problem parameter is not small ($\xi \ll 1$). However, as has been shown in, this fact is indeed too coincidental. The validity of these formulas is not ensured by the smallness of $\Delta$, but is due to the following circumstances.

a) The smallness of the width $\Gamma_{\nu}$ decay of the complex $C$ via the elastic channel:

$$\Gamma_{\nu} \ll \omega_{C}, \quad \Gamma_{\nu} \ll \omega_{C},$$

(16)

where $\omega_{C}$ is the vibrational quantum of the complex $C$.

b) The short-range character of the interaction of the neutral $d \mu \mu$ atom with the nuclei of the $D_{2}$ molecule.

In its entirety, the $d \mu \mu$ molecule formation process is written as

$$d \mu + D_{2} \xrightarrow{\lambda_{d\mu\mu}} C,$$

where $\lambda_{d\mu\mu}$ is the DD fusion reaction rate in the $d \mu \mu$ molecule. The products of this reaction are detected in experiments. That is why the observed muonic molecule formation rate is indeed the effective rate

$$\lambda_{d\mu\mu} = \omega_{C} \lambda_{d\mu\mu}, \quad \omega_{C} = \lambda_{C}(\lambda_{C} + \Gamma_{C}).$$

According to Ref. 7, $\omega_{C}=0.3$ holds for positive resonance energies $\epsilon > 0$. In our case these energies satisfy $\epsilon < 0$, so the complex cannot decay into the initial state of the $d \mu \mu + D_{2}$ system where the $d \mu \mu$ atom spin is $F=3/2$. However, it can decay into the state with $F=1/2$. As follows from Ref. 7, the back decay rate is $\Gamma_{b} \ll 10^{-3}$ s$^{-1}$, i.e., condition (16) is satisfied.

Another possible channel of the complex decay is the transition from its bound state with $K_{F}=0$ to the decay state with $K_{F}=1$ due to inelastic scattering on the $D_{2}$ molecule (in

Let us now calculate the value of $\lambda_{d\mu\mu}$ for a lattice. In this case

$$\Psi_{r} = e^{i\epsilon_{r} r}, \quad \Psi_{f} = \Psi_{f}(r) |r\rangle,$$

where $\epsilon_{r}$ is the $d \mu$ atom momentum in the lattice rest frame and $\langle r \rangle$ is the vector of the lattice final state $H_{f}\langle r \rangle = E_{f}\langle r \rangle$.

As in the case of the double collision (1), one obtains in the first order of perturbation theory

$$\lambda_{d\mu\mu} = n_{d}\sum_{q} \int \frac{d^{4}q}{(2\pi)^{4}} 2\pi \delta(q_{2} + q_{1} - q) e^{-i\epsilon_{1}} e^{-i\epsilon_{2}},$$

(11)

where $\langle q \rangle$ is the distribution of the $d \mu$ atoms in their momentum $q$, $e_{r} = q^{2}/2\mu_{r}$ is the mesatom kinetic energy (which we neglect according to expression (7)), $\epsilon_{1} = E_{f} - E_{g}$, $\epsilon_{2} = E_{g} - E_{f}$, $\omega_{r} = 1/3$ is the statistical weight of the para-deuterium, and

$$Q(\omega) = \sum_{q} \left| \langle q | \exp(iq_{a}u_{a}) | 0 \rangle \right|^{2} \delta(\omega - E_{f} + E_{g}),$$

(12)

Here we put $\exp(iq_{a}u_{a}) \neq 1$ neglecting the small terms in the expression for $\lambda_{d\mu\mu}$, which are $\sim T\omega_{r}$, where $\omega_{r}=100$ K is the Debye frequency for solid deuterium. It follows from Eqs. (11) and (12) that for $T \ll \omega_{r}$, the value of $\lambda_{d\mu\mu}$ does not depend on temperature, which agrees with the experiments.\(^\text{1,2}\)

The physical meaning of the term $Q$ is clear. Let the mesomolecular complex $C$ be formed at $t=0$ in the collision of a $d \mu$ atom with a $D_{2}$ molecule. Then at $t=0$ an instantaneous change in the lattice Hamiltonian occurs: $H_{f} \to H_{f}$, that is a "shaking". For $t \to 0$, the lattice was in the vacuum state $|0\rangle$. So the probability of being in the state $|\tilde{r}\rangle$ is $P_{\tilde{r}} = |\langle \tilde{r} | 0 \rangle|^{2}$. It follows from this that the probability of finding the lattice in the states with energies in the interval $(\omega_{r}+\Delta \omega)$ is $d\omega$. Equation (12) provides the necessary condition

$$\int_{-\infty}^{\infty} Q(\omega) d\omega = 1.$$

(13)

One should add that $Q(\omega)$ differs from zero only for $\omega > 0$ (as can also be seen from Eq. (12)).

At $\xi \ll 1$ the term $Q(\omega)$ coincides with $\delta(\omega)$. In this case there is no energy transfer to the lattice. For $\xi \neq 0$, the term $Q(\omega)$ differs from zero in the whole interval $(0,+\infty)$. At $\xi \ll 1$, it concentrates mainly in the region of frequencies $\omega = \omega_{a}$ characteristic of this problem. Taking into account $\langle \epsilon_{1} \rangle = \omega_{a}$, from this and from Eq. (13) we obtain an estimate

$$\langle \epsilon_{1} \rangle \sim \Delta \omega \sim 5 \times 10^{3} \text{ a.u.}$$

(14)

Rigorous calculation of $Q(\omega)$ will be performed later. Unfortunately, it can be done only numerically.

In obtaining the estimate (14) we neglected the difference between the values of $\epsilon_{1}$ and $\epsilon_{2}$. This difference can be easily estimated from perturbation theory using the Debye phonon model:

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our case of solid deuterium, this occurs by means of phonon absorption. Since the rate of this process is proportional to \( \exp(-\Delta E/7) \), where \( \Delta E \) is the transition energy, it is small.

Thus, in the case considered we have \( w_f = 0.3 \) (according to Ref. 7), and

\[ \lambda_{ddp} = 10^9 \text{ s}^{-1}. \]

It follows from this that the mechanism considered for \( ddp \) molecule formation with lattice excitation can play an essential role in solid deuterium.

The important role of many-particle effects and transitions with \( \varepsilon_0 < 0 \) was first pointed out in Ref. 15, where the reaction (1) was considered involving a third particle (in our case it is the \( D_2 \) molecule) carrying away the excess energy. This mechanism turned out to be efficient for the \( d+t \) fusion cycle at low temperature but not for a pure deuterium. But if one understands it more broadly, just the same process is realized in a solid deuterium where multiphonon phenomena take place.

In conclusion we would like to mention that there is a possibility of directly checking the results of the present work. For this one should measure the \( ddp \) molecule formation rate with solid deuterium in the pure orthostate, which is the natural equilibrium state for the lowest temperatures. Since in solid orthodeuterium practically all \( D_2 \) molecules are in the rotational state with \( K_f = 0 \), one should expect a sharp decrease of \( \lambda_{ddp} \) in comparison with the nonequilibrium deuterium usually used in experiments. Note that measurements with orthodeuterium would also be important in liquid and gaseous deuterium. It would allow one to examine the theory of resonant \( ddp \) molecule formation in a full measure.