Microscopic Calculation of the Molecular-Nuclear $d+d \rightarrow {}^3He+n \oplus {}^3H+p$ Reactions at Close to Zero Energies

T. Frederico#*
Department of Physics, University of Washington
FM-15, Seattle, Washington 98195, USA
and
J. J. de Groote† and J. E. Hornos
Instituto de Física e Química de São Carlos, Universidade de São Paulo
Caixa Postal 369, 13560 São Carlos, SP, Brasil
and
M. S. Hussein
Instituto de Física, Universidade de São Paulo
Caixa Postal 20516, 01498-970 São Paulo, SP, Brasil

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Microscopic calculations of the astropliysically interesting reaction $d+d \rightarrow {}^3He+n$ and $d+d \rightarrow {}^3H+p$ are performed using nuclear reaction theory and Born-Oppenheimer type molecular calculation of the d + d initial stage. The sensitivity of the fusion rate to the behaviour of the d + d wave function at close to zero separation is assessed. Relevance of the results to the cold fusion problem is discussed.

I - Introduction

Recently, interest has arisen in very low energy fusion reactions of the type

$$\begin{aligned} d+d &\longrightarrow n+ {}^3He \\ d+d &\longrightarrow p+ {}^3H \\ p+d &\longrightarrow {}^3He+\gamma \\ p+t &\longrightarrow {}^4He+\gamma \end{aligned}$$

Although the so-called ***cold fusion*** has not been fully verified[1-5], it is still of importance to study these reactions for their relevance to fusion energy application and for nuclear processes in the early solar system and early universe[6].

The fusion rate of two hydrogen nuclei in a diatomic molecule is invariably written as

$$\Lambda = A|\varphi_{dd}(\overset{0}{R}_{dd})|^2[s^{-1}], \qquad (1)$$

where φ_{dd} is the normalized wave function describing the relative molecular motion of the two nuclei; A is related to the low-energy behaviour of the fusion cross section[7] and is tabulated in ref.[8]. Finally $\overset{0}{R}_{dd}$ is the molecular distance fixed for the purpose of evaluating A, usually taken to be 10 fm. The values of A given in ref.[7] are extrapolations from low-energy fusion measurements to lower energies. In the evaluation of *(1)* $|\varphi_{dd}(\overset{0}{R}_{dd}\simeq 10)|^2$ is calculated from a molecular model for the two approaching hydrogen nuclei and A is taken from ref.[8].

The purpose of the present paper is to calculate **A** and accordingly A from a fully microscopic model that utilizes known low-energy behaviour of the observables of these few body systerns. The aim here is not so much the absolute value of the fusion rate but rather to have at hand a model through which the sensitivity of A to the short distance (SD) behaviour of the radial $d+$ d wave function. In the context of cold fusion, the effect of the enviroment in which the d + d system is implanted, is simulated here by a change in the SD behaviour of $\varphi_{dd}(r)$.

The paper is organized as follows. In section II a three-body model is proposed to treat the d + d interaction. In section III the results of the calculation is presented and in section IV we present our conclusions and discussion.

II. The Model

We consider the process $d+d \longrightarrow {}^3He+n$ as being

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that of the break-up of one of the deuterons and subsequent interaction (or fusion) of the participant proton with the other deuteron nucleus.

The corresponding amplitude can be written down as[9,10]

$$T = <^3 He, k_n|V_{np} + V_{nd}|\Psi^{(+)}>, \quad (2)$$

where $\Psi^{(+)}$ describes the three-body $n-p-d$ system, $\vec{k}_n$ is the outgoing momentum of the spectator neutron and V_{np} and V_{nd} are the n – p and n – d interaction potentials respectively. Note that the amplitude for the process d + d $\longrightarrow$ $^3He + p$ can be written as $<^3 H, K_p|V_{np} + V_{pd}|\Psi^{(+)}>$. We write the three-body Schrodinger equation as

$$(E - K_n - K_p - K_d - V_{np} - V_{pd} - V_{nd})\Psi = 0, \quad (3)$$

where K is the kinetic energy operator. Then one can define the three Faddeev wave function Ψ_{np}, Ψ_{nd}, Ψ_{pd}, where $\Psi = \Psi_{np} + \Psi_{nd} + \Psi_{pd}$, are given by

$$\begin{aligned} \Psi^{(+)}_{np} &= G^{(+)}_0 V_{np}\Psi^{(+)} \\ \Psi^{(+)}_{nd} &= G^{(+)}_0 V_{nd}\Psi^{(+)} \\ \Psi^{(+)}_{pd} &= G^{(+)}_0 V_{pd}\Psi^{(+)} \\ G^{(+)}_0 &\equiv (E - K_n - K_p - K_d + i\epsilon)^{-1}. \end{aligned} \quad (4)$$

Since $\Psi_{np} + \Psi_{nd} = G^{(+)}_0(V_{np} + V_{nd})\Psi^{(+)}$, we can write for the amplitude

$$\begin{aligned} T &= <^3 He, k_n|G^{(+)^{-1}}_0|\Psi^{(+)}_{np}> \\ &+ <^3 He, k_n|G^{(+)^{-1}}_0|\Psi^{(+)}_{nd}>= \\ &= <^3 He, k_n|V_{pd}|\Psi^{(+)}_{np}> \\ &+ <^3 He, k_n|V_{pd}|\Psi^{(+)}_{nd}> \\ &\approx <^3 He, k_n|V_{pd}|\Psi^{(+)}_{np}> \end{aligned} \quad (5)$$

where the approximation $<|\Psi_{nd}> \ll <|\Psi_{np}>$ is made since $\Psi^{(+)}_{np}$ is the most dominant of the three Faddeev components as it contains the incident d – d channel. Further we have used the identity $<^3$He, $k_n|G^{(+)^{-1}} = <^3$He, $k_n|(E - K_n - K_p - K_d) =$ $<^3$ He, $k_n|(E - K_n - K_p - K_d - V_{pd}) + V_{pd} = <^3 He, k_n|V_{pd}$.

A DWBA treatment of $\Psi^{(+)}_{np}$ is now in order such that

$$\Psi^{(+)}_{np} \approx |\varphi^{N+M}_{dd}\phi_d>, \quad (6)$$

where ϕ_d is the intrinsic wave function of the active deuteron and φ^{N+M}_{dd} is the molecular+nuclear distorted wave function that describes the relative motion of the two deuterons. We remove the short-range nuclear distortion from φ^{N+M}_{dd} and apply it to the outgoing neutron plane wave $< k_n|$ which then becomes an appropriate distoried wave $<\varphi^{(-)}_{kn}|$. We thus write finally

$$T = < G_{^3He}, \varphi^{(-)}_{kn}|\varphi^{M(+)}_{dd}\phi_d>, \quad (7)$$

where $G_{^3He}$ is the vertex function of ^3He,

$$|G_{^3He}> \equiv V_{pd}|^3He>.$$

The reaction (fusion) rate, Λ' in units of fm^3 s^{-1} is then calculated according to the expression

$$\Lambda' \equiv \sigma v = \frac{1}{4\pi}\frac{K_n\mu_{n-^3He}}{\hbar^3}\int d\Omega_{k_n}|T|^2 \quad (8)$$

where σ is the angle integrated cross-section, v is the relative incident velocity and μ_{n-^3He} is the reduced $n-^3He$ mass. The value of $k_n = 0.3438$ fm^{-1} is fixed by that of the Q-value for the reaction d + d $\longrightarrow$ n + ^{3}He.

In the calculation below we consider all relative motions to be in the S-waves states. With this assumption it is then possible to write T as

$$\begin{aligned} T &= 8\pi^2\int_0^\infty dR_{pd}R^2_{pd}dR_{np}R^2_{np}G_{^3He}(R_{pd}) \\ &\times\phi_d(R_{np})\theta(R_{pd}, R_{np}), \end{aligned} \quad (9)$$

where

$$\begin{aligned} &\theta(R_{pd}, R_{np}) = \\ &= \int_{-1}^1 d\cos\theta\varphi^{(-)^*}_{kn}\left(\left|\vec{R}_{np} - \frac{2}{3}\vec{R}_{pd}\right|\right) \\ &\times\varphi^M_{dd}\left(\left|\vec{R}_{pd} - \frac{\vec{R}_{np}}{2}\right|\right) \end{aligned} \quad (10)$$

and $\vec{R}_{pd}$ and $\vec{R}_{np}$ are the p – d and n – p relative coordinates, respectively and $\cos\theta = \vec{R}_{np}\cdot\vec{R}_{pd}/R_{np}R_{pd}$.

The vertex for the ^3He nucleus is approximated by that of ^3H in order to avoid dealing with Coulomb problems. Using separable two-body potentials with Yamaguchi form factors it can be shown[11] that the vertex function that represents ^3H is given by

$$\begin{aligned} &G_{^3He}(R_{pd}) \approx G_{^3He}(R_{pd}) = \\ &= \frac{3}{4}\sqrt{\frac{3\mu_{pd}}{2\pi}}C^T_S(\mu^2_{pd} - \beta^2_{pd}) \\ &\times\frac{e^{-\beta_{pd}R_{pd}}}{R_{pd}}, \end{aligned} \quad (11)$$

where $\beta_{pd} = 0.9086$ fm^{-1}, $\mu = 0.4485$ fm^{-1} and $C^T_S = 1.82$ is the asymptotic normalization of ^3He [12].

The deuteron bound-state wave function $\phi_d(R_{np})$ is also constructed with a separable Yamaguchi potential and is given by[13]

$$\phi_d(R_{np}) = \sqrt{\frac{\mu_d}{2\pi}}C_d\left(\frac{e^{-\mu_dR_{np}}}{R_{np}} - \frac{e^{-\beta_dR_{np}}}{R_{np}}\right) \quad (12)$$

where $C_d = 1.3$ is the asymptotic normalization of the deuteron, $\mu_d = 0.2316 fm^{-1}$ and $\beta_d = 1.45 fm^{-1}$. The distorted wave function of the outgoing neutron (distorted by the field of ^3He), with the same Yamaguchi recipe, is given by[13]

$$\varphi_{kn}^{(-)}(R_n) = \frac{\sin k_n R_n}{k_n R_n} + \frac{S_0 - 1}{2ik_n} \times \left(\frac{e^{ik_nR_n} - e^{-\beta_n R_n}}{R_n}\right) \quad (13)$$

with $S_0 = \eta_0 e^{2i\delta_0}$, $\eta_0 = 0.5$ [14], $\delta_0 = -55°$ [14] and $\beta_n = 1\ fm^{-1}$ [15]. In (13) R_n is the relative distance of the outgoing neutron with respect to the center of mass of ^3He.

III. Results

The molecular wave function φ_{dd}^M of Eq. (5) should, in principle, be found by solving the four- and three-body Coulombic problem for D_2 and D_2^+, respectively. However, as usually done, we adopt the Born-Oppenheimer approximation. The $d-d$ effective potential is reasonably well accounted for by the following expression[7]

$$V_{eff}(r) = \frac{e^2}{r} - C \quad (14)$$

where $C \simeq 51.8$ eV for D_2 and 20.4 eV for D_2^+. Tlien the WKB approximation gives for the radial φ_{dd}^M the following expression

$$\varphi_{dd}^M(r) = \left(\frac{\alpha}{2\pi}\right)^{1/2} \frac{r}{\sqrt{a}} \exp\left[-\int_r^{r_0} \sqrt{\frac{2\mu}{\hbar^2}(V_{eff}(r') - E))}dr'\right] \quad (15)$$

in the classically forbidden region (Note that φ_{dd} of Eq. (1) is $\frac{1}{\sqrt{4\pi}}\varphi_{dd}^M/r$). The parameter $a = (M_N/m_e)/\omega/\hbar$ [fm^2] where M_N is the nucleon mass, m_e is the electron inass and $\hbar\omega$ is the vibrational frequency of the molecule. Finally r_0 is the classical turning point. The integral in Eq. (15) can be obtained in closed form if Eq. (14) is used, and is given by

$$\varphi_{dd}^M(r) = \left(\frac{\alpha}{2\pi}\right)^{1/2} \frac{r}{\sqrt{a}} \exp\left(\sqrt{\frac{2M_N r_0}{\hbar^2}}\left[\frac{-(r_0/r - 1)^{1/2}}{(r_0/r)} + \tan^{-1}(r_0/r - 1)^{1/2}\right]\right), \quad (16)$$

where a = 0.53 Å is the Bohr radius. Notice that the factor r multiplying the exponential above arise from the inclusion of the term $\hbar^2/4r^2$ in the effective potential[16]. This repulsive term represents what might be called the semiclassical zero point centrifugal energy. Since $r_0 \sim 0.58Å$ for D_2 and $0.9Å$ for D_2^+, in the r $\sim$ few fm's region, we may expand the exponent and find

$$\varphi_{dd}^M(r) \simeq \left(\frac{\alpha}{2\pi}\right)^{1/2} \frac{r}{\sqrt{a}} \exp\left[-\sqrt{\frac{2M_N r_0}{\hbar^2}} + \frac{\pi}{2}\right] \exp\left[-\sqrt{\frac{2M_N r_0}{\hbar^2}}\left(\frac{r}{r_0}\right)^{3/2}\right]. \quad (17)$$

Notice that $\varphi_{dd}^M(r)$ given by Eq.(15) is normalized and $\int_0^\infty |\varphi_{dd}^M(r)|^2 dr = 1$. The above discussion about the small distance behaviour of $\varphi_{dd}(r)$ is fully justified from a recent extensive numerical solution of the D_2^+ problem using the hyperspherical method[17].

Before proceeding, we give the values of a for D_2 and D_2^+ respectively, $\alpha(D_2) = 1.0 \times 10^{-8} fm^{-2}$ and $\alpha(D_2^+) = 0.55\times 10^{-8} fm^{-2}$. These values were obtained from the relation $a = (M_N m_e)\omega/\hbar$ with $\hbar\omega(D_2) = 0.38$ eV and $\hbar\omega(D_2^+) = 0.23$ eV[18].

With Eq.(16) for $\varphi_{dd}^M(r)$, the integrals in Eq. (9) for the T-matrix are then easily evaluated. The calculation of A from Eq. (2) is then performed and we find $\overset{0}{R}_{dd}$= 10 fm after multiplying Eq. (8) by the factor 4 to account for the p and n channel and the bosonic nature of the two deuterons, A = 66.7 x $10^{-16} cm^3 s^{-1}$. This value is about 1.5 orders of magnitude larger than the extracted value[7] $1.5 \times 10^{-16} cm^3 s^{-1}$. Note that the neutron- and proton-cliannel cross sections are different by as much as $\sigma_n/\sigma_p \sim 1.2$ [6] but we have ignored this difference here.

The reason behind the rather large value of A obtained in our model calculation may be the neglect of other processes besides the ones considered here namely $d+d \longrightarrow p+n+d \longrightarrow p+^3He$ and $d+d \longrightarrow p+n+d \longrightarrow n+^3He$, which might interfere destructively. Further work is needed to clarify the situation. We should remind the reader that the value 1.5 x 10^{-16} crn^3 s^{-1} was extracted from nuclear reaction studies in the KeV region.

The fusion rate A for D_2 was found to be 5.3 x $10^{62}\ s^{-1}$, larger than the value obtained by Koonin and Nauenberg[7] (3 x $10^{-64}\ s^{-1}$). Similar calculation was performed for D_2^+ and we found A = 4 x $10^{-79}\ s^{-1}$.

Of course our calculation was performed assuming free space. However the recent intensive interest in cold fusion, which now has considerably subsided, prompts us to investigate within our model the possible influence of a, e.g. crystal environment on A and A. We decided to look into effects which may change the short distance behaviour of φ_{dd}^M(r). We therefore arbitrarily assumed that $\varphi_{dd}^M(r)$ behaves like r^n where n is a certain number decided upon by the type of enviroment in which the D_2 or D_2^+ molecule is found.

Fig. 1 shows our results for A as a function of n for two different values of $\overset{0}{R}_{dd}$, 10 fm and 15 fm. It is clear that there is a strong dependence both on n and $\overset{0}{R}_{dd}$. We should of course stress that whatever n is,

$\varphi_{dd}^{M}(r)$ must be properly normalized. If the enviroment is represented by an effective degree of freedom (besides r) which makes $\varphi_{dd}^{M}(r)$ behaves as r^n with n > 0, the fusion rate is lowered.

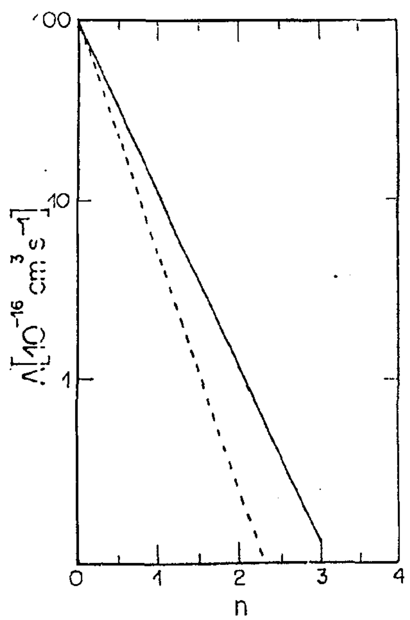

Figure 1: Calculated nuclear fusion rate constant, A (multiplied by 1.5) vs. n (Here n specifies the form of $\varphi_{dd} = (R_{dd} \to 0)$ $(\approx R_{dd}^n)$). The solid curve was obtained for $R_{dd}^0 = 10$ fm and the dashed curve corresponds to $R_{dd}^0 = 15 fm$. See text for details. The full curve can be represented by **100.4** $e^{-2.17n}$ and the dashed curve by **100.4** $e^{-2.88n}$.

For n < 0, A is increased, following the exponential dependence shown in the figure (linear on a log scale). In fact the dependence on n was found to be $63.2\, e^{-2.17n}$ at $\overset{0}{R}_{dd}= 10$ fm and $63.2\ e^{-2.88n}$ at $\overset{0}{R}_{dd}= 15$ fm. For $n = -0.5$, $A = 213.7 \times 10^{-1}\ cm^3\ s^{-1}$ for $\overset{0}{R}_{dd}= 10$ fm and $320.3 \times 10^{-16}\ cm^3\ s^{-1}$ for $\overset{0}{R}_{dd}= 15$ fm. For $n = -1.0$ we obtain $A = 922.2 \times 10^{-16}\ cm^3\ s^{-1}$ for $\overset{0}{R}_{dd}= 10$ fm and $2075.8 \times 10^{-16}\ cm^3\ s^{-1}$ for $\overset{0}{R}_{dd}= 15$ fm.

Finally a comment about the nuclear S-factor. At zero energy it is given by[8]

$$S(E=0) = \frac{\pi\alpha}{c}\left[\frac{M_N}{2}c^2\right]A \quad , \quad \alpha = (137)^{-1} \qquad (18)$$

which gives the value 4.45 MeV^{-1} barns, compared to the "experimental" value $1.1 \times 10^{-1} MeV^{-1}$ barns. The "experimental" value is of course an extrapolated one from the measured value in the KeV's energy region.

IV. Conclusions

In conclusion, we have performed here a microscopic calculation of the $d+d$ fusion rate, A, in free space using a three-body model for the nuclear process. The nuclear rate constant A has also been calculated in free space. The effect of the enviroment on A has been assessed in a simple way by modifying the short distance behaviour of the $d+d$ initial wave function. It was found that if $\varphi_{dd}^{M}(r)$ behaves like r^n with n > 0 the nuclear rate is reduced while for n < 0 an appreciable increase in the rate was found. In a future work we shall apply our three-body model to discuss the data on $d+d$ fusion at KeV energies, recently reported in the literature[6]. For this purpose higher partial waves have to be considered.

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