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ABSTRACT

Microscopic calculations of the astrophysically interesting reaction D+D $\longrightarrow$ ^{3}He+n and D+D $\longrightarrow$ ^{3}H+p are performed using nuclear reacton 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

$$d + d \longrightarrow n + {}^3He$$
$$\longrightarrow p + {}^3H$$
$$p + d \longrightarrow {}^3He + \gamma$$
$$p + t \longrightarrow {}^4He + \gamma \; .$$

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

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

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

The purpose of the present paper is to calculate Λ and accordingly A from a fully microscopic model that utilizes known low–energy behaviour of the observables of these few body systems. 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 Λ 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 $\Psi_{dd}(r)$.

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 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 then be written down as

$$T \;=\; \langle {}^3He, k_n | V_{np}+V_{nd} | \Psi^{(+)} \rangle \tag{2}$$

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. We write the three–body Schrodinger equation as

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

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

$$\begin{aligned} \Psi^{(+)}_{np} &= G^{(+)}_0 V_{np}\, \Psi^{(+)} \\ \Psi^{(+)}_{nd} &= G^{(+)}_0 V_{nd}\, \Psi^{(+)} \\ \Psi^{(+)}_{pd} &= G^{(+)}_0 V_{pd}\, \Psi^{(+)} \end{aligned} \tag{4}$$

$$G^{(+)}_0 \equiv (E - K_n - K_p - K_d + i\varepsilon)^{-1} \; .$$

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

$$\begin{aligned} T \;=\; & \langle {}^3He, k_n | G^{(+)^{-1}}_0 | \Psi^{(+)}_{np} \rangle + \langle {}^3He, k_n | G^{(+)^{-1}}_0 | \Psi^{(+)}_{nd} \rangle \;= \\ =\; & \langle {}^3He, k_n | V_{pd} | \Psi^{(+)}_{np} \rangle + \langle {}^3He, k_n | V_{pd} | \Psi^{(+)}_{nd} \rangle \;\approx\; \langle {}^3He, k_n | V_{pd} | \Psi^{(+)}_{np} \rangle \end{aligned} \tag{4}$$

where the approximation $\langle | \Psi_{nd} \rangle \ll \langle | \Psi_{np} \rangle$ is made since $\Psi^{(+)}$ is the most dominant of the three Faddeev components as it contains the incident d–d channel. Further we have used the identity $\langle {}^3He, \; k_n | G^{(+)^{-1}}_0 = \langle {}^3He, \; k_n | (E - K_n - K_p - K_d) = \langle {}^3He, k_n | (E - K_n - K_p - K_d - V_{pd}) + V_{pd} = \langle {}^3He, k_n | V_{pd}$.

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

$$\psi^{(+)}_{np} \;\approx\; | \varphi^{N+M}_{dd} \; \phi_d \rangle \tag{6}$$

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 describe 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 $\langle k_n |$ which then becomes an appropriate distorted wave $\langle \varphi^{(-)}_{kn} |$. We thus write finally

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

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

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

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

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

where σ is the angle integrated cross–section, v is the relative incident velocity and $\mu_{n-{}^3He}$ 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 $d+d \rightarrow n+{}^3He$.

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

$$T = 8\pi^2 \int_0^\infty dR_{pd}\, R_{pd}^2\, dR_{np}\, R_{np}^2\, G_{{}^3He}(R_{pd})\, \phi_d(R_{np})\, \theta(R_{pd}\, R_{np}) \quad , \qquad (9)$$

where

$$\theta(R_{pd}, R_{np}) = \int_{-1}^{1} d\cos\theta\, \varphi_{kn}^{(-)*}\left[|\vec{R}_{np} - \tfrac{2}{3}\vec{R}_{pd}|\right] \varphi_{dd}^{M}\left[|\vec{R}_{pd} - \tfrac{\vec{R}_{np}}{2}|\right] \qquad (10)$$

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[9] that the vertex function that represents ${}^3H$

$$G_{{}^3He}(R_{pd})\left[\approx G_{{}^3He}(R_{pd})\right] = \frac{3}{8}\sqrt{\frac{3M_T}{\pi}}\; C_S^T\, (\mu_{pd}^2 - \beta_{pd}^2) \times \frac{e^{-\beta_{pd}R_{pd}}}{R_{pd}} \quad , \qquad (11)$$

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

The deuteron bound–state wave function $\phi_d(R_{np})$ is also constructed with a separable Yamaguchi potential and is given by[10]

$$\phi_d(R_{np}) = \sqrt{\frac{\mu_d}{2\pi}}\; C_d \left[\frac{e^{-\mu_d R_{np}}}{R_{np}} - \frac{e^{-\beta_d R_{np}}}{R_{np}}\right] \qquad (12)$$

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[11]

$$\varphi_{kn}^{-*}(R_n) = \frac{\sin k_n R_n}{k_n R_n} + \frac{S_0 - 1}{2ik_n} \times \left[\frac{e^{ik_nR_n} - e^{-\beta_nR_n}}{R_n}\right] \qquad (13)$$

with $S_0 = \eta_0\, e^{2i\delta_0}$, $\eta_0 = 0.5$[12], $\delta_0 = -55^0$[11] and $\beta_n = 1\ fm^{-1}$[13].

III. Results

The molecular wave function φ^{M}_{d+d} 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])

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

where $c \simeq 51.8$ eV for D_2 and 20.4 eV for D_2^+. Then the WKB approximation gives for the radial φ^{M}_{dd} the following (note that Ψ_{dd} of Eq. 1 is $\frac{1}{\sqrt{4\pi}}\varphi^{M}_{dd}/r$)

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

in the classically forbidden region the parameter $\alpha = \frac{M_N\,\omega}{\hbar}$ [fm^2] with M_N the nucleon mass, m_e the electron mass and $\hbar\omega$ the vibrational frequency of the molecule. Finally r_0 is the classical turning point. The integral in Eq.(15) can be done in closed forms if Eq.(14) is used, giving (notice that $a = 0.53$ A, is the Bohr radius)

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

Notice that the r multiplying the exponential above arises from the inclusion of the term $\hbar^2/4r^2$ in the effective potential. This repulsive term represent what might be called the semiclassical zero point centrifugal energy. Since $r_0 \sim 0.58$ A for D_2 and 0.9 A for D_2^+,

in the $r \sim$ few fm's region, we may expand the expoent and find

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

Notice that $\varphi^{M}_{dd}(r)$, Eq.(15) is normalized, $\int_0^\infty |\varphi^{M}_{dd}(r)|^2\,dr = 1$. 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 casing the hyppersherical method[13]).

Before proceding, we give the values of α 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 $\alpha = M_N/\hbar\,\omega$ with $\hbar\omega(D_2) = 0.38$ eV and $\hbar\omega(D_2^+) = 0.23$ eV[14]).

With Eq.(16) for $\varphi^{M}_{dd}(r)$, 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 at $\mathring{R}_{dd} = 10$ fm after multiplying Eq.(8) by the factor 4 to account for the p and n channels and the bosonic nature of the two deuterons, $A = 66.7 \times 10^{-16}$ cm^3 s^{-1}. This value is about 1.5 orders of magnitude larger than the extracted value[7]) 1.5×10^{-16} cm^3 s^{-1}. Note that the neutron– and proton–channel cross sections are different by as much as $\sigma_n/\sigma_p \sim 1.2$ [6]). We have here ignored this difference.

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

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

Of course our calculation have all been done in free space. The recent itensive interest in could fusion, which now has considerably subsided, prompts us to investigate within our model the possible influence of a, e.g., crystal enviroment on Λ and A. We decided to look into effects which may change the short distance behaviour of $\varphi^M_{dd}(r)$. We therefore arbitrarily assumed that $\varphi^M_{dd}(r)$ 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 result for A as a function of n for two different values of $\mathring{R}_{dd}$, 10 fm and 15 fm. It is clear that there is a strong dependence both on n and $\mathring{R}_{dd}$. We should of course stress that whatever n is, $\varphi^M_{dd}(r)$ must be properly normalized. If the enviroment is represented by an effective degree of freedom (besides r) which makes $\varphi^M_{dd}(r)$ behaves as r^n with $n > 0$, the fusion rate is lowered.

For $n < 0$, Λ is increased, following the exponential dependence shown in figure (linear on a log scale). In fact the dependence on n was found to be $63.2\, e^{-2.17n}$ at $\mathring{R}_{dd} = 10$ fm and $63.2\, e^{-2.88n}$ at $\mathring{R}_{dd} = 15$ fm. For $n = -0.5$, $A - 213.7 \times 10^{-1}\ cm^3\ s^{-1}$ for $\mathring{R}_{dd} = 10$ fm and $320.8 \times 10^{-16}\ cm^3\ s^{-1}$ for $\mathring{R}_{dd} = 15$ fm. For $n = -1.0$ we obtain $A = 922.2 \times 10^{-16}\ cm^3\ s^{-1}$ for $\mathring{R}_{dd} = 10$ fm and $2075.8 \times 10^{-16}\ cm^3\ s^{-1}$ for $\mathring{R}_{dd} = 15$ fm.

Finally a comment about the nuclear S–factor at zero energy given by[8]

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

which gives the value 4.45 MeV^{-1} barns, compared to the "experimental" value 1.1×10^{-1} MeV 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, Λ, 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 changing the short distance behaviour of the d+d initial wave function. It is found that if $\varphi^M_{dd}(r)$ behaves like r^n with $n > 0$ the nuclear rate is reduced while for $n < 0$ an appreciable increase in the rate is 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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FIGURE CAPTIONS

Fig. 1: Calculated nuclear fusion rate constant, A vs. n (that specifies the form of $\varphi_{dd} = R^n_{dd}$). Full curve for $R^0_{dd} = 10$ fm and dashed curve for $R^0_{dd} = 15$ fm. See text for details. The full curve can be represented by $100.4\, e^{-2.17n}$ and the dashed curve by $100.4\, e^{-2.88n}$. Plotted is 3/2 A.

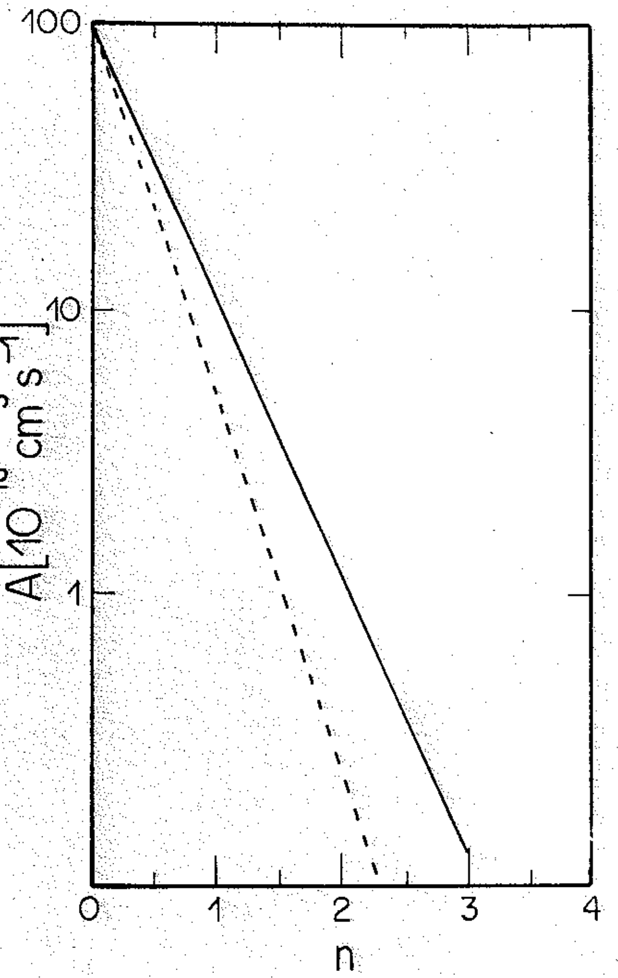

Fig. 1