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A THEORETICAL STUDY OF COLD NUCLEAR FUSION USING BARRIER PENETRATION APPROACH *

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ABSTRACT

The cold nuclear fusion process is investigated in terms of barrier penetration calculations by considering both the deuteron-molecule and colliding deuteron-deuteron atoms. Atomic collisions with strongly screened interatomic potential and the resonant state formation can bring agreement with present experimental results. Analysis of the data in terms of the reaction rates is also discussed.

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For d-d fusion at room temperature, experimentally, rates of 10^{-19}-10^{-23} fusions/sec/dd pair have been reported [1)-5)] at present. Theoretically, fusion of a deuterium molecule was studied earlier by Van Siclen and Jones [6)] who estimated $\Lambda \approx 10^{-70}$-10^{-79} sec^{-1}. These rates, however, are far below the recent experimental data. Rafelski et al. [7)] carried out a parametric study of the observed cold fusion rates by incorporating effective charge and mass of the electron and confinement of the d-d motion. It is rather difficult to get any justification of these effects, say, on the basis of condensed matter physics. Also, there exist exotic explanations by Shaw et al. [8)] based on the anti-diquark catalysis and Barut [9)] having an additional minimum in the potential energy surface of the d-d-e system.

In this letter, we present for the first time a thorough study of the barrier penetration calculation for the cold fusion problem, using a formulation similar to that of Van Siclen and Jones [6)]. We consider that inside a deuterium-saturated metal, instead of deuterium molecule formation, (neutral) deuterium atoms collide with each other. We refer to this process in the following as "atomic fusion". In such a process, the barrier to be penetrated by the d-d atoms, with their electrons coupled to spin zero, is thinner as compared to that for the molecule. Furthermore, formation of the d-d atom resonant state at such small collision energies would result in additional enhancement of fusion rates due to multiple collisions. Our calculations show that "atomic fusion" enhances the calculated fusion rates considerably but to achieve fusion rates comparable with present experiments we need additional screening of the interatomic Coulomb potential. For comparisons, the barrier penetration calculations for deuteron molecule in its ground state are also carried out (termed "molecular fusion" in the following).

<u>Molecular fusion</u>: For the motion of deuterons in a molecular potential V(r), Van Siclen and Jones [6)] have derived the WKB penetrability (for zero relative angular momentum)

$$P = \exp\left(-2 \int_{r_n}^{r_a} \left\{ \left| \frac{2\mu}{\hbar^2} [E-V(r)] - \frac{1}{4r^2} \right|^{1/2} - \frac{1}{2r} \right\} dr \right) \qquad (1)$$

where r_a and r_n are the first and second turning points, respectively *). Then, for a deuteron molecule, the fusion rate is

$$\Lambda = K_0 \, \Omega^{-1} \, P \qquad (2)$$

where Ω^{-1} gives the normalization of the molecular ground state wave function ($= 2.1 \times 10^{24}$ cm^{-2}, as deduced from Ref.6) and K_0 is the nuclear reaction constant ($= 0.74 \times 10^{-16}$ cm^3 sec^{-1}, obtained by matching to the measured KeV $^2D(d,n)^3He$ cross-sections [6),7),10)].

We have used in our work, the realistic potential, obtained for $0.40 \leq r \leq 10$ a.u. by Kolos and Wolntewicz (KW) [11)] in a self-consistent variational procedure for the $^1\Sigma_g^+$ state of hydrogen molecule. For $r < 0.40$ a.u., in contrast to the procedure of Ref.6 of joining the molecular potential to the Coulombic potential at some arbitrary point, we have matched the KW molecular potential at $r = \rho = 0.40$ a.u. to the normally adopted screening functions $\chi(r)$ with the Coulombic potential

$$V(r) = \frac{1}{r}\chi(r) \qquad \text{for } r \leq \rho \qquad (3)$$

We have used here [12)]

$$\chi(r) = e^{-Ar} \qquad \text{(Bohr's screening function)} \qquad (4)$$

and

$$\chi(r) = \frac{1}{1+Br} \qquad \text{(Kerner's screening function)} \qquad (5)$$

with parameters $A = 2.6109$ and $B = 4.6039$. In the following we denote these potentials as Bohr's weak screening potential (BWSP) and Kerner's weak screening potential (KWSP). In order for these functions to screen the Coulombic potential strongly, we must match them to the molecular potential at $\rho \gg 0.4$ a.u. Choosing $\rho = 0.75$ a.u. we obtain $A = 5.3753$ and $B = 73.7925$ which characterize, respectively, the Bohr strongly screened potential (BSSP) and the Kerner strongly screened potential (KSSP).

*) We use atomic units throughout for r and E. 1 a.u. $(r) = 0.52918$ A° and 1 a.u. $(E) = 27.21$ eV. For d-d system $2\mu/\hbar^2 = 3666$ a.u.

Taking the turning points $r_n = 10^{-4}$ a.u. ($= 5.29$ fm) [13)] and $r_a = 1.20$ a.u. (at this distance KW potential has $E = -0.1649$ a.u.) we have calculated the Λ-values for all the four potentials mentioned above. Our results are given in Table 1. We notice that for the weakly screened potentials $\Lambda \approx 10^{-61}$-10^{-63} sec^{-1}, whereas it increases to $\sim 10^{-54}$ and 10^{-34} sec^{-1} for the strongly screened potentials BSSP and KSSP, respectively. This means, we obtain an increase in fusion rates over Ref.6 by at least eight orders of magnitude and our penetrability P depends strongly on the nature of screening function. A close look at the calculations shows that the spatial region lying between 0.40 and 0.75 a.u. contributes maximum to the penetrability integral in Eq.(1). Comparing our results with experimental data, we notice that even for the most favourable screening function (KSSP), the calculated Λ value falls short of experiments by about ten orders of magnitude. Hence the "molecular fusion" seems to be inadequate to explain the present cold fusion experiments.

Atomic fusion: The deuterium atoms having energies of the order of an eV can undergo collisions inside a deuterium-saturated metal or on its interface. Such energies can arise due to the acceleration of d atoms towards the electrode. For such a situation we evaluate the penetrability P in Eq.(1) at $E = 0.023664$ a.u. ($= 0.644$ eV) which occurs in the KW potential at $r = 0.75$ a.u. Choosing the other turning point again at $r_n = 10^{-4}$ a.u. and taking $\Omega^{-1} = 1.16 \times 10^{23}$ cm^{-3}, which corresponds to normalizing two d atoms in a sphere of typical radius $R = 1.6$ A°, we have calculated Λ-values (Eq.(2)) for all the four potentials of the previous section. The results are given in Table 1. (The $^1\Sigma_g^+$ potential would be seen by the colliding dd atoms in $\frac{1}{4}$ collisions only. This factor due to spin is not included in our calculations.) We notice that even for the weak screening potentials there is a considerable gain in going from molecular to atomic picture (compare $\Lambda \sim 10^{-61} - 10^{-63}$ sec^{-1} with $10^{-53} - 10^{-55}$ sec^{-1}). On the other hand, comparing with experiments, though BSSP still gives too small a Λ value ($\sim 10^{-43}$ sec^{-1}) but KSSP predicts $\Lambda \sim 10^{-22}$sec^{-1} which is close to experiments.

Due to multiple collisions in the resonance state of lifetime τ and impinging frequency ν, the enhanced fusion rate $\Lambda_{\nu\tau>1}$ will be given as

$$\Lambda_{\nu\tau>1} = \Lambda \nu\tau \tag{6}$$

For the KW potential well depth of $\sim$0.2 a.u.(= 5.4 eV) and size of $\sim$3 a.u. (= 1.6 A^{o}), the collision velocity $v = 2.28 \times 10^{6}$ cm sec^{-1}, which gives the assault frequency $\nu(= v/R) = 1.43 \times 10^{14}$ sec^{-1} for the d-d atoms. Further, assuming a typical lifetime of the atomic state $\tau = 10^{-8}$ sec, we get the enhancement factor of Eq.(6), $\nu\tau = 1.43 \times 10^{6}$. Our calculated $\Lambda_{\nu\tau>1}$ values are also given in Table 1, which again shows that only KSSP describes the experimental data. The KSSP here gives a kind of upper limit required on the screening function for explaining the present cold fusion experiments.

Finally, in the case of atomic collisions, the event rate will perhaps be better described by the reaction rates than the radio-active-decay-like formula used by the experimentalists to extract the Λ-values. For the collisions to occur inside the volume V of the electrode with deuteron density n cm^{-3}, the yield (event rate) will be

$$Y = \frac{1}{2} n^2 V \sigma v \tag{7a}$$

or

$$\sigma v = \frac{Y}{\frac{1}{2} n^2 V} \quad \text{(volume)} \tag{7b}$$

This equation gives our deduced σv (volume) values in Table 1 for experiments of Refs.1, 3 and 4. Alternatively, if the fusion process takes place on the surface of electrode, the yield will then be [7)]

$$Y = n \frac{I_d}{I_0} \sigma v \quad \text{(surface)} \tag{8}$$

Here I_d and I_0 are, respectively, the deuteron current and the current of a single particle. Table 1 gives the σv (surface) deduced from the experimental data of Ref.1. For other experiments, the relevant data is not known.

Theoretically,

$$\sigma v = \Omega \Lambda_{\nu\tau>1} = K_0 P \nu\tau \tag{9}$$

which has the clear advantage of being independent of the choice of normalization constant Ω. Our calculated σv-values are also given in Table 1, which again stresses that agreement with present experiments is only possible for the strongly screened Kerner screening potential (KSSP). Furthermore, it is apparent that the fusion yield will be higher for the higher density d-d atomic collisions, which at present is provided by the host Pd/Ti metal. Such high densities of d-atoms could perhaps be generated also by other experimental means.

Concluding, we have shown that a considerable enhancement in barrier penetrability results if, instead of a deuterium molecule, the colliding dd atoms are studied. For being able to explain the present measurements of d-d fusion rates, our calculations demand an additional strong screening of the Coulombic potential. This result, however, needs to be justified by a further microscopic calculation of the interatomic potential. Probably, the physical situation will be more close to the weakly screened potential (BWSP or KWSP), which could then mean a complete non-observance of the cold nuclear fusion phenomenon at our present stage of experimentation ability.

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13) The authors of Ref.6 have shown that the WKB penetrability is almost independent of the choice of r_n value lying in the range 0-10^{-5} a.u.

Table 1

Calculated and experimental d-d cold fusion rates

Potential	Molecular Fusion	Atomic Fusion ($v\tau = 1$)	Atomic Fusion ($v\tau = 1.43 \times 10^6$)	Expts. Λ(sec^{-1})	Refs.
Calculated fusion rates Λ (sec^{-1})					
BWSP	1.69×10^{-63}	3.02×10^{-55}	4.33×10^{-49}	$\sim 10^{-19}$ (volume)	1
KWSP	1.80×10^{-61}	2.95×10^{-53}	2.95×10^{-47}	$\sim 10^{-23}$ (volume)	3
BSSP	6.96×10^{-54}	5.07×10^{-43}	7.27×10^{-37}	$\sim 10^{-20}$ (surface)	3
KSSP	8.93×10^{-34}	6.82×10^{-21}	9.77×10^{-15}	1.3×10^{-21} (volume)	4
Calculated reaction rates σv ($cm^3\ sec^{-1}$)				σv ($cm^3 sec^{-1}$)	
BWSP		2.61×10^{-78}	3.73×10^{-72}	1.3×10^{-40} (volume)	1
KWSP		2.55×10^{-76}	3.65×10^{-70}	4.4×10^{-38} (surface)	1
BSSP		4.37×10^{-66}	6.27×10^{-60}	1.2×10^{-46} (volume)	3
KSSP		5.86×10^{-44}	8.40×10^{-38}	2.7×10^{-44} (volume)	4

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