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Uncertainties of Conventional Theories and New Improved Formulations of Low-Energy Nuclear Fusion Reactions

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Abstract

We examine uncertainties of conventional theoretical estimates for low-energy nuclear fusion cross-section $\sigma(E)$ and fusion rate $\langle\sigma v\rangle$. Using new formulations based on the optical theorem and the radial distribution function, we derive new improved formulae for $\sigma(E)$ and $\langle\sigma v\rangle$. Our results of the optical theorem formulation for $\sigma(E)$ indicate that a near cancellation of the Gamow factor can occur if the imaginary part of the effective nuclear interaction in the elastic scattering channel has a very weak component with a long finite interaction range. Uncertainties of conventional estimates of the electron screening effect for $\sigma(E)$ are also examined and a new alternative formulation is proposed. Finally, based on a solution of three-body Schrödinger equation and the optical theorem formulation, we derive a new formula for three-body fusion cross-section and rate and compare its predictions with conventional estimates and also with the recent experimental data for three-deuteron fusion reaction.

1. Introduction

In this paper, we examine uncertainties of conventional theoretical estimates and propose new improved formulations of low-energy nuclear fusion reactions. Since the 1989 announcements of nuclear fusion at room temperature in palladium (Pd) [1] and titanium (Ti) [2] electrolytic cells using heavy water (D_2O), there have been persistent claims of observing the cold fusion phenomena. Most of the reported experimental results are not reproducible at a desirable level of 100% [3]. However, there are a few experimental results which appear to be 100% reproducible [4,5]. There have been many theoretical models proposed to explain the cold fusion phenomena. Most of those theoretical models claiming to have explained the phenomena appear far from having accomplished their claims [6,7].

In section 2, we present a new alternative theoretical formulation of low-energy nuclear fusion reactions based on the optical theorem [8], which is much less model-dependent than previous theoretical approaches. In section 3, we describe and compare our new improved formula with the conventional one for the fusion cross-section. In section 4, we show that some of the cold fusion phenomena may be justified theoretically if the imaginary part of the effective nuclear interaction in the elastic channel has a very weak component with a long finite interaction has a component with a long finite range. A new modified general formula for nuclear fusion rate in high-density plasma is derived in section 5. In section 6, we discuss uncertainties of the conventional theoretical estimates of low-energy fusion rates due to electron degrees of freedom. We propose an alternative formulation for investigating the electron screening effect, which avoids this difficulty. In section 7, we show that there is a very serious difficulty associated with non-square integrability in the conventional formula. In section 8, we describe a derivation of a new formula for three-body fusion cross-section and rate, and compare its predictions with the conventional estimates and also with the recent experimental data for $D+D+D \rightarrow p+n+{}^4\mathrm{He}$ reaction [5]. Section 9 contains a summary and conclusions.

2. Optical Theorem Formulation of Fusion Reactions

For the elastic scattering cross-section $\sigma^{(e\ell)}(E)$, we introduce the partial wave expansion $\sigma^{(e\ell)}(E) = \sum_\ell (2\ell+1)\sigma_\ell^{e\ell}$ where $\sigma^{(e\ell)}$ is related to the elastic partial wave scattering amplitude $f_\ell^{(e\ell)}$ by $\sigma_\ell^{(e\ell)} = |f_\ell^{(e\ell)}|^2$ where $f_\ell^{(e\ell)} = f_\ell^c + e^{2i\delta_\ell^c} f_\ell^{N(e\ell)}$ with $f_\ell^{N(e\ell)} = (S_\ell - 1)/2ik$ and the ℓth partial wave S–matrix given by S_ℓ. Hence, $\sigma_\ell^{(e\ell)}$ can be written as

$$\sigma_\ell^{(e\ell)} = |f_\ell^{(e\ell)}|^2 = \sigma_\ell^c + \sigma_\ell^{\mathrm{int}} + \sigma_\ell^{N(e\ell)} \tag{1}$$

where $\sigma_\ell^c = |f_\ell^c|^2 = 4\pi \sin^2\delta_\ell^c/k^2$ (Rutherford scattering), $\sigma_\ell^{\mathrm{int}} = -2\pi Re\ [(S_\ell - 1)(e^{2i\delta_\ell^c} - 1)]/k^2$ (interference term), and $\sigma_\ell^{N(e\ell)} = |f_\ell^{N(e\ell)}|^2 = \pi |S_\ell - 1|^2/k^2$ (nuclear scattering).

For reaction cross-section, we have $\sigma^{(r)} = \sum_\ell (2\ell+1)\sigma_\ell^{(r)}$ where $\sigma_\ell^{(r)} = \pi(1 - |S_\ell|^2)/k^2$. Using $\sigma_\ell^{(r)} + \sigma_\ell^{N(e\ell)} = 2\pi(1 - ReS_\ell)/k^2$, and $Imf_\ell^{N(e\ell)} = (1 - ReS_\ell)/2k$, we obtain the optical theorem for two-potential scattering case as

$$Imf_\ell^{N(e\ell)} = \frac{k}{4\pi}\left(\sigma_\ell^{(r)} + \sigma_\ell^{N(e\ell)}\right) \tag{2}$$

which is a rigorous result.

For low energies, $f_\ell^{N(e\ell)} \propto e^{-2\pi\eta}/k$ and hence $\sigma_\ell^{N(e\ell)} = |f_\ell^{N(e\ell)}|^2 \propto e^{-4\pi\eta}/k^2$. Since $\sigma_\ell^{(r)} \propto e^{-2\pi\eta}/k^2$, we have $\sigma_\ell^{(r)} >> \sigma_\ell^{N(e\ell)}$ at low energies, and hence we can write eq. (2) as

$$Imf_\ell^{N(e\ell)} \approx \frac{k}{4\pi}\sigma_\ell^{(r)} \tag{3}$$

which is still a rigorous result at low energies. We note that eqs. (2) and (3) are for non–radiative nuclear reactions and need to be modified for radiative nuclear reactions.

In terms of the partial wave T–matrix, T_ℓ, the elastic nuclear scattering amplitude, $f_\ell^{N(e\ell)} = (S_\ell - 1)/2ik$, can be written as

$$f_\ell^{N(e\ell)}(E) = -\frac{2\mu}{\hbar^2 k^2}\langle\psi_\ell^c|T_\ell|\psi_\ell^c\rangle \tag{4}$$

where ψ_ℓ^c is the ℓth partial wave regular Coulomb function and μ is the reduced mass. Using the low energy optical theorem eq. (3) with eq. (4), we obtain the ℓth partial-wave (fusion) reaction cross-section $\sigma_\ell(E)(=\sigma_\ell^{(r)}(E))$ as

$$\sigma_\ell(E) \approx \frac{4\pi}{kE}\int_0^\infty \psi_\ell^c(r)U_\ell(r,r')\psi_\ell^c(r')drdr' \tag{5}$$

where $E = \hbar^2k^2/2\mu$ and $U_\ell(r,r') = -Im\langle r|T_\ell|r'\rangle$ with T_ℓ representing the ℓth partial wave contribution of the T-matrix operator. The total cross-section $\sigma(E)$ is given by $\sigma(E) = \sum(2\ell+1)\sigma_\ell(E)$. It is important to note that our optical theorem formulation of nuclear reactions, eq. (3), can be applied to both non-resonance and resonance reactions using the T-matrix given in eq. (4). In reference [8], we have shown that $U(r,r')$ has a separable form for the case of two open channels (elastic and fusion).

3. New Fusion Cross-Section Formula and the Effective Potential Range

It is shown in reference [8] that $Im\langle r|T_\ell|r'\rangle$ for $\ell = 0$ case and hence $U_0(r,r')$ in eq. (5) are separable for the two-channel case. Therefore, for estimating the S-wave cross section, $\sigma_0(E)$, for the two-channel case, we can parameterize $U_0(r,r')$ in eq. (5) by two parameters λ (strength/length) and β^{-1} (range) in a separable form as

$$U_0(r,r') = \lambda g(r)g(r') \tag{6}$$

where λ is expected to be a slowly varying function of E for the non-resonance case. (For the case of resonance reactions the energy dependence of λ can be parameterized by the Breit-Wigner expression.) For $g(r) = e^{-\beta r}/r$, the integral in eq. (5) can be carried out analytically using eq. (6) and the exact form $\psi_0^c(r) = C_0(\eta)M_{i\eta,\frac{1}{2}}(2ikr)/2i$, where $C_0^2(\eta) = 2\pi\eta/(e^{2\pi\eta}-1)$ and $M_{i\eta,\frac{1}{2}}'$ is the Whittaker function. The result is

$$\sigma_0(E) = \frac{4\pi\lambda}{kE}\left[\int_0^\infty dr\psi_0^c(r)e^{-\beta r}/r\right]^2 = \frac{4\lambda\pi^2}{E}R_B\frac{(e^{-2\phi\eta}-1)^2}{(e^{2\pi\eta}-1)}e^{4\phi\eta} \tag{7}$$

which for the low-energy case reduces to

$$\sigma_0(E) = \frac{\tilde{S}_0(E)e^{4\phi\eta}}{E}\, e^{-2\pi\eta} \tag{8a}$$

with

$$e^{4\phi\eta} = \exp\left[4\alpha\frac{\mu c^2}{\hbar c}\left(\frac{Z_aZ_b}{k}\right)\tan^{-1}\left(\frac{k}{\beta}\right)\right] \tag{8b}$$

where $\phi = \tan^{-1}(k/\beta)$ and $\tilde{S}_0(E) = 4\pi^2\lambda R_B$ with $R_B = \hbar^2/(2\mu Z_aZ_be^2)$. Since the energy dependence of V_0 and β is expected to be weak, $\tilde{S}_0(E)$ depends weakly on energy. Numerical results of eq. (8b) will depend on the unknown range parameter β^{-1}, which needs to be determined either from experimental data or from reliable microscopic calculations.

The use of $g(r) = e^{-\beta r}$ leads to

$$\sigma_0(E) = \frac{4\pi^2\lambda}{ER_B}\left(\beta^2 + k^2\right)^{-2}\left(e^{2\pi\eta} - 1\right)^{-1} e^{4\phi\eta} \tag{9}$$

while, for $g(r) = re^{\beta r}$, we obtain

$$\sigma_0(E) = \frac{4\pi^2\lambda}{ER_B^3}\left[(2R_B\beta + 1)^2/\left(\beta^2 + k^2\right)^4\right]\left(e^{2\pi\eta} - 1\right)^{-1} e^{4\phi\eta}\,. \tag{10}$$

The use of a more general form for $g(r) = e^{-\beta r}\left(\Sigma_{i=0}^{N} c_i r^i\right)$ in eq. (6) also leads to the same enhancement factor $e^{4\phi\eta}$. Therefore, the enhancement factor $e^{4\phi\eta}$ is independent of shape of the separable function $g(r)$ used in eq. (6). The enhancement factor $e^{4\phi\eta}$ can be applied to both light nuclei reactions (small Z_a and Z_b) but also to heavy ion reactions (larger Z_a and Z_b) such as sub-barrier heavy ion fusion where $e^{4\phi\eta}$ can be very large.

Our derivation of eq. (8a) is the first derivation of the Gamow factor based on the optical theorem, and is much more rigorous than other previous derivations, most of which are based on the barrier transmission coefficient derived in the WKB approximation. Our new extra exponential factor, $e^{4\phi\eta}$, eq. (8b), in eq. (8a) is obtained together with the Gamow factor from our derivation and can be regarded as a modification of the Gamow factor affecting it only at low energies, or as a part of the S-factor if we still wish to keep the conventional formula eq. (11). In any case, the new exponential factor has a sound theoretical foundation as the above nearly model-independent derivation clearly shows. Furthermore, the energy dependence of this new extra exponential factor depends on the range parameter, inverse of beta (β^{-1}). If the range is small, this factor is nearly energy independent as experimental data for some low-energy reactions show. If the range is longer, the new extra exponential factor can provide an enhancement of the "S-factor" or the cross-section over the conventional values at low energies, and thus could give a reasonable explanation of the experimental data referred to below [9-12]. Therefore, it is important to determine the range of the imaginary part of the effective potential in the elastic channel for each nuclear reaction from experiment and/or from reliable microscopic calculations.

For non-resonance reactions, it is customary to extract the S-factor, $S(E)$, from the experimentally measured $\sigma(E)$ using the following formula

$$\sigma_G(E) = \frac{S(E)}{E} e^{-2\pi\eta(E)} \tag{11}$$

where $\eta(E) = Z_a Z_b e^2/\hbar v$, $e^{-2\pi\eta(E)}$ is the Gamow factor representing the probability of bringing two charged nuclei to zero separation distance, and $S(E)$ is expected to be a slowly varying function of E. Recent results for $\sigma(E)$ from laboratory beam experiments for nuclear reaction involving light nuclei at low energies (> 3 keV) show that the extracted $S(E)$ increases toward lower energies instead of being a constant extrapolated from higher energy data, indicating a possibility of the importance of the electron screening. However, recent theoretical calculations [13,14] of the electron screening effect yield limiting values which are much smaller (by $\sim 1/2$) than those extracted from the experimental data for reactions ^{3}He$(d,p)^4$He [9,10], ^{6}Li$(p,\alpha)^3$He, ^{6}Li$(d,\alpha)^4$He, ^{7}Li$(p,\alpha)^4$He [11], ^{10}B$(p,\alpha)^7$Be, and ^{11}B$(p,\alpha)^7$Be [12]. This discrepancy between the experimental data and the theoretical estimate for the electron screening effect is not understood at present. Because of the importance of accurate low-energy cross-sections for bare nuclei needed for astrophysical problems, it is very important to understand and resolve the discrepancy. If we identify $\tilde{S}_0(E)$ in eq. (8a) as $S(E)$ in eq. (11), $e^{4\phi\eta}$ in eq. (8a) is a new enhancement factor for S-factor $S(E)$ in eq. (11).

Since $\phi = \tan^{-1}(k/\beta) = \pi/2$ and $e^{4\phi\eta} = e^{2\pi\eta}$ in the limit of $\beta \to 0$, a (near) cancellation of the Gamow factor $e^{-2\pi\eta}$ can occur if the interaction range β^{-1} is large (or β is small). Therefore, it is important to investigate a possibility that the interaction range is finite but large (i.e., long finite range). One example is a long range potential which can arise from Coulomb interaction as an electric polarization potential in the real part of the effective potential in the elastic scattering channel at low energies due to the electric polarizability of the target [15-19].

The effective potential V for scattering of a charged projectile from a target with an extended charge distribution can be written as

$$V = V^S + V^C + V^{pol} \tag{12}$$

where V^C and V^S are Coulomb and strong interactions, respectively. The polarization potential in the adiabatic approximation is given by

$$V^{pol}(r) \approx \frac{\alpha_e e^2}{2R_B r^4}, \quad r >> R_B \tag{13}$$

where α_e is the electric polarizability of the target and R_B is the Bohr radius of the target plus the projectile, $R_B = \hbar^2/(2\mu Z_a Z_b e^2)$. If we denote the S-factor, S, corresponding to the case of no polarization potential ($V^{pol} = 0$, and $V = V^S + V^C$) and the polarization S-factor, S_p, for the case including V^{pol} ($V = V^S + V^C + V^{pol}$), perturbation calculations [15-18] yield $|S_p/S - 1| < 10^{-3}$, and show that V^{pol} has negligible effects for fusion reactions involved in stellar nucleosynthesis [19]. Even though V^{pol} has a long range, it is the real part of the effective potential, and hence it does not contribute to the enhancement factor $e^{4\phi\eta}$ in eq. (8a) which is due to a finite range interaction in the imaginary part of the effective potential.

Using the observed value of the deuteron polarization $\tilde{\alpha} = \alpha_e/R_B = 0.63$ fm^3 [19], we can show that $V^{pol}(R_B) \approx 10$ eV. To obtain an upper bound of $|S_p/S - 1|$, we can use the following expression

$$\left|\frac{S_p(E)}{S(E)} - 1\right| < \left|e^{2\pi(\eta(E+V_{pol}(R_B)) - \eta(E))} - 1\right|. \tag{14}$$

For the $d+d$ reaction with $E = 2$ keV, eq. (14) yields $|S_p(E)/S(E) - 1| < 10^{-2}$. In laboratory beam experiments, the electron screening effect needs to be taken into account using the screening energy, which is known to be larger than $V^{pol}(R_B) \approx 10$ eV. Therefore, the effect of the polarization potential may be negligible for low-energy fusion reactions. This example shows that the contribution of the real part of the effective potential to the reaction cross-section behaves drastically different from that of the imaginary part of the effective potential.

Interaction range of the imaginary part of the effective potential in the elastic channel for nuclear fusion reactions at low energies has not been investigated previously, although there are some examples of the imaginary part of the effective potential with a long finite interaction range involving Coulomb excitation. When inelastic channels due to Coulomb excitation of the target nucleus to excited states become open at higher energies, a dynamic polarization potential results from the long-range Coulomb potential. For the case of a quadrupole excitation, the dynamic polarization potential has an imaginary part with an asymptotic behavior of r^{-5} at large distances [20]. For nuclear fusion reactions involving charged nuclei, rearrangement or fusion is involved in the exit channel, and hence it may be reasonable to expect that a long range interaction may result as an imaginary part of the effective potential due to the long-range Coulomb potential involved in nuclear fusion reactions. Therefore it is suggestive that the imaginary part may also have a component with a long finite range interaction for some nuclear systems at low energies. If the imaginary part of the effective potential or $g(r)$ in eq. (6) has a form

$$g(r) = e^{-\beta_1 r}/r + \Lambda e^{-\beta r}/r \tag{15}$$

with $\beta < \beta_1$, the second term could be dominant over the first term even if $\Lambda << 1$. In the limit of $\beta \rightarrow 0$, $\phi = \tan^{-1}(k/\beta) = \pi/2$ and $e^{4\phi\eta} = e^{2\pi\eta}$ which can cancel the Gamow factor $e^{-2\pi\eta}$ in eq. (8a). Although at present we have not succeeded to prove theoretically the existence of a long finite interaction range ($\beta \approx 0$) for $\Lambda e^{-\beta r}$ from our quantum mechanical derivation of the imaginary part of the effective potential [8], the possibility of the existence of term $\Lambda e^{-\beta r}$ with $\beta \approx 0$ and hence a near cancellation of the Gamow factor at low energies cannot be ruled out theoretically. A near cancellation of the Gamow factor at low energies may provide an explanation for anomalous fusion products (new isotopes and enhanced isotope abundances) reported in some recent experiments [3]. Therefore, it is important to investigate both theoretically and experimentally the possibility of existence of the long finite range ($\beta \approx 0$) interaction for the imaginary part of the effective potential.

4. Possible Scenarios for Cold Fusion

Since we cannot rule out the possibility of (near) cancellation of the Gamow factor $e^{-2\pi\eta}$ by the enhancement factor $e^{4\phi\eta}$ in eq. (8a), we investigate possible scenarios for cold fusion based on such hypothetical near cancellation of the Gamow factor. We examine $d+d$, $d+Pd$, and $p+Pd$ as examples in this section.

For the observed neutron counting rate of $(4.1 \pm 0.8) \times 10^{-3}\text{s}^{-1}$ claimed by Jones et al. [2], the fusion rate is 0.41 s^{-1} after neutron detection efficiency of $\sim$ 1% is taken into account for 3 g of Ti. Since the Ti density is 4.5 g/cm^3 and its molar weight is 47.9 g/mole, the observed fusion rate is

$$R^J_{\text{exp}} = 0.615/\text{sec} - \text{cm}^3(\text{deuterons}) \approx 1.0/\text{sec} - \text{cm}^3(d's) \tag{16}$$

where we have assumed the deuteron density n_D to be $n_D = n_{Ti}/2 = 2.83 \times 10^{22}/\text{cm}^3 \approx 3 \times 10^{22}/\text{cm}^3$. The observed fusion rate claimed by Fleischmann and Pons is larger than R^J_{exp} by a factor of $\sim 10^{10}$,

$$R^{FP}_{\text{exp}} \approx 1.0 \times 10^{10}/\text{sec} - \text{cm}^3(\text{deuterons}) \ . \tag{17}$$

To include the electron screening effect, we assume $E = E_{sc}$ where E_{sc} is the screening energy given by Thomas–Fermi model [21]

$$E_{sc} = 30.7 Z_a Z_b \left(Z_a^{2/3} + Z_b^{2/3}\right)^{1/2} \text{ eV} \ . \tag{18}$$

For $d+d$ reactions, $E_{sc} = 43.4$ eV, while $E_{sc} = 5.25$ keV for $d + Pd$ and $p + Pd$. Corresponding velocities, $(v/c) = \sqrt{2E/\mu} = \sqrt{2E_{sc}/\mu}$, are 0.3×10^{-3}, 2.4×10^{-3} and 3.3×10^{-3}, for $d+d$, $d+Pd$, and $p+Pd$ reactions, respectively. The observed fusion rate, R_{exp}, is related to the cross–section $\sigma(E)$ by $R_{\text{exp}} = n_a n_b \langle \sigma v \rangle/(1+\delta_{ab})$. For $E = E_{sc} = 43.4$ eV or 5.25 keV, $\langle \sigma v \rangle$ can be approximated by $\langle \sigma v \rangle = \sigma v$ and hence $R_{\text{exp}} \approx n_a n_b \sigma v/(1+\delta_{ab})$ or $\sigma \approx R_{\text{exp}}(1+\delta_{ab})/n_a n_b v$. Using $\sigma(E)$ given by eq. (8a), we obtain

$$\Lambda e^{4\phi\eta} e^{-2\pi\eta} \approx \frac{(1+\delta_{ab}) R_{\text{exp}} \mu c^2}{2 n_a n_b c \tilde{S}_0(E)} \left(\frac{v}{c}\right) \tag{19}$$

where we have used $g(r)$ given by eq. (15) with $\beta << \beta_1$. From the extrapolation of higher energy $d+d$ fusion data, $S(0)$ in eq. (23) is known to be $S(0) \approx 50$ keV–b for $D(d,p)^3$H or $D(d,n)^3$He reactions. For $d+d$ reactions with $\tilde{S}_0(E) \approx S(0) = 50$ keV–b, we obtain 0.2×10^{-30} and 0.2×10^{-20} for $\Lambda e^{4\phi\eta} e^{-2\pi\eta}$, with R^J_{exp} and R^{FP}_{exp}, respectively. For $d + Pd$ reaction, assuming $\tilde{S}_0(E) \approx 50$ keV–b, we obtain 1.6×10^{-30} and 1.6×10^{-20} for $\Lambda e^{4\phi\eta} e^{-2\pi\eta}$, with R^J_{exp} and R^{FP}_{exp}, respectively, while for $p + Pd$ reaction with the assumed value of $\tilde{S}_0(E) \approx 50$ keV–b, $\Lambda e^{4\phi\eta} e^{-2\pi\eta} = 1.2 \times 10^{-30}$ and 1.2×10^{-20}, respectively, for R^J_{exp} and R^{FP}_{exp}.

R^J_{exp} and R^{FP}_{exp} can be explained if we can assume large values of β^{-1}. The use of very small value of $\Lambda = 10^{-14}$ will preserve the conventional description of nuclear fusion reactions at higher energies greater than 1 keV for $d+d$ and greater than 1 MeV for $d + Pd$ and $p + Pd$. To obtain the claimed value of R^J_{exp} with $\Lambda = 10^{-14}$, we need $\beta^{-1} = 1633$ fm, 693 fm, and 686 fm, while $\beta^{-1} = 4275$ fm, 1881 fm, and 1845 fm for $d+d$, $d+Pd$, and $p+Pd$ fusion reactions, respectively, are needed to obtain R^{FP}_{exp}. Larger values of β^{-1} for $d+d$ case compared with smaller values of β^{-1} for $d+Pd$ and $p+Pd$ cases imply that $d+Pd$ and $p+Pd$ fusion reactions may be more favorable than $d+d$ fusion reaction. Another interesting aspect of $d+Pd$ and $p+Pd$ reactions is that the final fusion product can be unstable with a finite lifetime, which may help to explain "heat after death" phenomenon [22] and absence or lower level of X-rays and bremsstrahlung radiation.

The anomalous large ratio of T/n from $D(d,p)T$ and $D(d,n)^3$He claimed by many authors [3] can be explained by assuming that β^{-1} for the $D(d,p)T$ channel is larger than β^{-1} for the $D(d,n)^3$He channel. However, since bremsstrahlung radiation and other expected effects are not observed in many of the electrolysis fusion experiments [3], $D(d,p)T$ and $D(d,n)^3$He may not be occurring in these experiments. Other possibilities are now numerous, since our results with the electron screening effect using E_{sc} (eq. (18)) show a surprising result that the fusion cross-section for nuclei with larger values of Z can be comparable or much greater than that for nuclei with smaller Z, contrary to the commonly accepted belief otherwise. There are many possible candidate fusion reactions involving Pd with different Q values which produces no neutrons. For ${}^APd(d,p)^{A+1}Pd$, Q values are 5.21 MeV (A = 102), 1.48 MeV (A = 104), 7.72 MeV (A = 105), 3.71 MeV (A = 106), 7.27 MeV (A = 107), 6.88 MeV (A = 108), and 3.08 MeV (A = 110). For tritium producing ${}^APd(d,t)^{A-1}Pd$ reactions, Q values are 2.55 MeV (A = 105) and 0.32 MeV (A = 107). If X-rays and/or bremsstrahlung radiation are not observed or are at a very low level in the electrolysis experiments [3], all of the above fusion reactions involving Pd isotopes are ruled out except possibly ${}^{107}Pd(d,t)^{106}Pd$ reaction which have a small value of Q = 0.32 MeV, and hence we need to look for other candidate fusion reactions with small values of Q, including those involving impurity isotopes in electrolysis experiments. Examples of other possible fusion reactions with small Q values are ^{102}Pd(^{7}Li,^{6}Li)^{103}Pd (Q = 0.531 MeV), ^{108}Pd(^{14}N,^{15}N)^{107}Pd (Q = 0.102 MeV), ^{110}Pd(^{6}Li,^{5}Li)^{111}Pd (Q = 0.089 MeV), ^{110}Pd(^{10}B,^{12}B)^{108}Pd (Q = 0.254 MeV), and ^{110}Pd(^{19}F,^{21}F)^{108}Pd (Q = 0.136 MeV). Other possibilities with different sets of nuclei in the initial and final states are to be explored.

If the claimed results of excess heat with no accompanying radiation are confirmed at a level of $\sim$ 100% reproducibility, and if there are no candidate fusion reactions with Q values small enough to be consistent with the radiationless results, then we may need to investigate some unconventional mechanisms [3,6,7] involving collective excitations of Pd clusters and/or Pd crystals, in addition to the near cancellation of the Gamow factor discussed in section 3. The radiationless results may turn out to be independent of and decoupled from the mechanism described in this section and section 3.

5. New Modified Formula for High-Density Plasma Fusion

In this section, a new modified general formula for the high density nuclear fusion rate is described. For a given relative velocity $v = v_{ij} = |\vec{v}_i - \vec{v}_j|$ between the ith and jth particles and fusion cross-section $\sigma(v_{ij})$, the fusion rate per unit volume, R_f, is expected to be proportional to $P(\vec{r}_i,\vec{v}_i;\vec{r}_j,\vec{v}_j)v_{ij}\sigma(v_{ij})$ where P is the probability of finding the ith particle at $\vec{r}_i$ with $\vec{v}_j$ and the jth particle at $\vec{r}_j$ with $\vec{v}_j$. For a given one-body phase space (density) distribution, $\rho(q_\ell,p_\ell) = \rho(\vec{r}_i, m_i\vec{v}_i)$, one possible choice for P is, suppressing m_i, $P(\vec{r}_i,\vec{v}_i;\vec{r}_j,\vec{v}_j) = \rho(\vec{r}_i,\vec{v}_i)\rho(\vec{r}_j,\vec{v}_j)$ which is valid for a collisionless ideal or low-density gas but may not be valid for a high-density gas. The separability of the phase–space distribution $\rho(\vec{r}_i, \vec{v}_i) = n(\vec{r}_i)f(\vec{v}_i)$ is assumed, where $f(\vec{v}_i) = (m_i/2\pi kT)^{3/2}\exp(-m_i v_i^2/2kT)$ is the Maxwell–Boltzmann (MB) velocity distribution for a system in thermal equilibrium. With the above assumptions, we can write R_f as

$$\begin{aligned} R_f &= \frac{1}{(1+\delta_{ij})V_r^2}\int d^3r_i \int d^3r_i \int d^3v_i \int d^3v_j P(\vec{r}_i,\vec{v}_i;\vec{r}_j,\vec{v}_j)v_{ij}\sigma(v_{ij}) \\ &= \frac{1}{(1+\delta_{ij})V_r^2}\int d^3r_i \int d^3r_j \int d^3v_i \int d^3v_j n(\vec{r}_i)n(\vec{r}_j)f(\vec{v}_i)f(\vec{v}_j)v_{ij}\sigma(\vec{v}_{ij}) \end{aligned} \tag{20}$$

where V_r is the system volume.

After transforming the ith and jth particle coordinates into the relative and center of mass (CM) coordinates, and integrating the CM coordinates, eq. (20) reduces to ($r = |\vec{r}_i - \vec{r}_j|$)

$$R_f^{new} = \frac{n_i n_j}{(1+\delta_{ij})V_r}\int d^3r \int d^3v \; g(r)f(\vec{v})v_0\sigma(v_0) \tag{21}$$

using the assumption that the pair number density $n(\vec{r}_i)n(\vec{r}_j)$ is related to the radial distribution function $g(r)$ by $n(\vec{r}_i)n(\vec{r}_j) = n_i n_j g(r)$ with n_i and n_j representing the average number densities. $g(r)$ is defined as the number of particles, on the average, in the volume $4\pi r^2 dr$ centered about a given particle divided by the number that would be in the same volume if the system behaved as an ideal gas [23]. $g(r)$ can be calculated from a molecular dynamics simulation [23].

Since $\sigma(v_0)$ is experimentally measured with v_0 representing the asymptotic relative speed v_0 in the potential free region ($V(r) = 0$), we must use $v_0\sigma(v_0)$ instead of $v\sigma(v)$ in eq. (21), where v_0 and v are related by the total pair energy (E_0) conservation, $E_0 = \mu v_0^2/2 = \mu v^2/2 + V(r)$ with the reduced mass μ.

For a collisionless ideal gas ($V(r) = 0$), we have $v_0 = v$ and $g(r) = 1$, and hence R_f^{new}, eq. (21), reduces to the conventional fusion rate formula: $R_f^{new} \to R_f^{conv}$, where

$$R_f^{conv} = \frac{n_i n_j}{1+\delta_{ij}}\int d^3v \; f(\vec{v})v\sigma(v) \; . \tag{23}$$

R_f^{new} becomes substantially different from R_f^{conv} at lower temperatures.

6. Uncertainties for the Electron Screening Effect

We investigate non-adiabatic effects in the quantum mechanical description of the electron screening effect for nuclear reaction rates. At low energies, the fusion reaction cross-sections of charged nuclei can be also written as

$$\sigma(E) = G(E)|\psi_E(0)|^2/v \tag{24}$$

where $G(E)$ is the so-called astrophysical factor, which embodies the nuclear aspects of the process, E and v are the collision (kinetic) energy and the relative nuclear velocity, respectively, $\psi_E(0)$ is the wave function at the origin, and $|\psi_E(0)|^2 = (2\pi\alpha c/v)\exp(-2\pi\alpha c/v)$. At low energies, the behavior of $\sigma(E)$ is dominated by Coulomb repulsion between the nuclei. In cold fusion and laboratory beam experiments the ion is incident on a target consisting mostly of neutral atoms or molecules, and hence incident ions can recombine, partially or totally, with the electrons they encounter while moving through the target. As a consequence, the final nuclear collision, which leads to nuclear fusion, occurs while the nuclei are surrounded by one or several electrons. These electrons become more deeply bound in the Coulomb field of the unified nuclei, and transfer kinetic energy to the internuclear degree of freedom. Therefore, the cross-section measured in the laboratory beam experiments are not equal to the cross-section for bare nuclei. Recent results for $\sigma(E)$ from laboratory beam experiments for nuclear reactions involving light nuclei at low energies (> 3 keV) show that the extracted $S(E)$ increases toward lower energies instead of being a constant extrapolated from higher energy data, indicating the importance of the electron screening. However, recent theoretical calculations [13, 14] of the electron screening effect based on the adiabatic Born-Oppenheimer approximation (the united atom model with the screening energy, 15.7 $Z^{7/3}$ eV) yield limiting values which are much smaller (by $\sim 1/2$) than those extracted from the experimental data for reactions ^{3}He$(d,p)^4$He [9,10], ^{6}Li$(p,\alpha)^3$He, ^{6}Li$(d,\alpha)^4$He, and ^{7}Li$(p,\alpha)^4$He [11]. This discrepancy between the experimental data and the conventional theoretical estimate for the electron screening effect is not understood at present.

We will now examine the united atom approximation for low-energy $d + de$ reaction. For this case we need to calculate

$$|\psi_E(0)|^2 = \int |\psi_E(\vec{r},\vec{\rho})|^2 d\vec{\rho}|_{r=0} \, . \tag{25}$$

For the total $d + de$ energy $\epsilon = E - |E_{1s}| = (E - 13.6 \text{ eV})$ where $\vec{r} = \vec{r}_{d_1} - \vec{r}_{d_2}, \vec{\rho} = \vec{r}_e - (\vec{r}_{d_1} + \vec{r}_{d_2})/2$, we assume that $\psi(\vec{r},\vec{\rho})$ in eq. (26) is the solution of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu}\Delta_r - \frac{\hbar^2}{2m_e}\Delta\rho + \frac{e^2}{r} + V(\vec{r},\vec{\rho})\right)\psi = \epsilon\psi \, , \tag{26}$$

where

$$V(\vec{r},\vec{\rho}) = -\left(\frac{e^2}{\left|\vec{\rho} - \frac{\vec{r}}{2}\right|} + \frac{e^2}{\left|\vec{\rho} + \frac{\vec{r}}{2}\right|}\right) \tag{27}$$

and μ is the reduced mass of deuteron, $\mu = M_d/2$, with the deuteron rest mass M_d.

Let us introduce an operator $\hat{H}$,

$$\hat{H} = -\frac{\hbar^2}{2m_e}\Delta\rho - \frac{2e^2}{\rho} \tag{28}$$

and the eigenfunction $\psi_n(\vec{\rho})$ satisfying

$$\hat{H}\psi_n(\vec{\rho}) = E_n\psi_n(\vec{\rho}) \ . \tag{29}$$

We expand the solution of eq. (26) in terms of $\psi_n(\vec{\rho})$ as

$$\psi(\vec{r},\vec{\rho}) = \sum F_n(\vec{r})\psi_n(\vec{\rho}) \tag{30}$$

where $F_n(\vec{r})$ satisfy

$$-\frac{\hbar^2}{2\mu}\Delta_r F_n(\vec{r}) + \frac{e^2}{r}F_n(\vec{r}) + \sum V_{nm}F_m = (\epsilon - E_n)F_n(\vec{r}) \ . \tag{31}$$

For the case of $L = 0$, $\ell_r = \ell_\rho = 0$, we have

$$-\frac{\hbar^2}{2\mu}\frac{d^2F_n}{dr^2} + \frac{e^2}{r}F_n + \sum_m \tilde{V}_{nm}F_m = (\epsilon - E_n)F_n \tag{32}$$

where

$$\tilde{V}_{nm} = \left\langle \psi_n | \tilde{V} | \psi_m \right\rangle \ , \qquad \tilde{V}(r,\rho) = 2e^2\begin{cases} 0 \ , & \rho \geq r/2 \\ \dfrac{1}{\rho} - \dfrac{2}{r} \ , & r/2 \geq \rho \end{cases} \ . \tag{33}$$

If we restrict to the case of $n = 1$ and $m = \epsilon$ (continuum state) and neglect $V_{\epsilon n \neq 1}$ and $V_{\epsilon\epsilon'}$, eq. (32) reduces to

$$-\frac{\hbar^2}{2\mu}\frac{d^2F_1}{dr^2} + \tilde{V}_{11}F_1 + \int \tilde{V}_{1\varepsilon}F_\varepsilon d\varepsilon + \sum_{n\neq 1}\tilde{V}_{1n}F_n = (\epsilon - E_1)F_1 \tag{34a}$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2F_\varepsilon}{dr^2} + \tilde{V}_{\varepsilon 1}F_1 + \frac{e^2}{r}F_\varepsilon = (\epsilon - \varepsilon)F_\varepsilon \ . \tag{34b}$$

In terms of solutions, F_1 and F_ε, of eq. (34), the probability integral in eq. (25) can be written as (see Appendix A)

$$|\psi_E(0)|^2 = \int |\psi_E(\vec{r},\vec{\rho})|^2 d\vec{\rho}|_{r=0} \approx \left|\frac{F_1(r)}{r}\right|^2_{r=0} + \int \left|\frac{F_\varepsilon(r)}{r}\right|^2 d\varepsilon\bigg|_{r=0} \tag{35}$$

where $|F_1(r)/r|^2_{r=0}$ corresponds to the conventional united atom approximation

$$|\psi_E^{U.A.}(0)|^2 = \left|\frac{F_1(r)}{r}\right|^2_{r=0} \tag{36}$$

while the other term $\int |F_\varepsilon(r)/r|^2 d\varepsilon|_{r=0}$ corresponds to the non–adiabatic correction term. For the low–energy case of $E \lesssim 10$ eV, our estimates of eqs. (35) and (36) using solutions F_1 and F_ε, of eq. (34) yield the ratio (see Appendix A)

$$\frac{|\psi_E(0)|^2}{|\psi_E^{U.A.}(0)|^2} \gtrsim 10 \tag{37}$$

which indicates the importance of the non–adiabatic contribution for the electron screening effect. We are extending our calculation of the ratio, eq. (58) to higher energies, $E \lesssim 10$ keV.

7. Non-Square Integrability for the Electron Screening Effect

In this section, we show that there is a very serious difficulty associated with the conventional formula for nuclear fusion rate in the presence of electron degrees of freedom due to non-square integrability of the probability integral $|\psi_E(0)|^2$ in eq. (24), which has been ignored in previous theoretical calculations. The probability integral in eq. (24) is written as $|\psi_E(0)|^2 = (2\pi\alpha c/v)\exp(-2\pi\alpha c/v)$ representing the probability of bringing two charged nuclei to zero separation distance in the absence of electrons. We will consider ${}^3\mathrm{H}(d,n){}^4\mathrm{He}$ reaction for simplicity and use the three-body $d + e+$ ^{3}H (det) initial state. The probability integral $|\psi_E(0)|^2$ in eq. (24) for this case is

$$|\psi_E(0)|^2 = \int |\psi_E(\vec{r},\vec{\rho})|^2 d^3\rho|_{r=0} \tag{38}$$

where $\psi_E(\vec{r},\vec{\rho})$ is the det wave function with $\vec{r} = \vec{r}_d - \vec{r}_t$ and $\vec{\rho} = \vec{r}_e - (m_d\vec{r}_d + m_t\vec{r}_t)/(m_d + m_t)$. We demonstrate that the integral in eq. (38) is not square-integrable over ρ, when $\psi_E(\vec{r},\vec{\rho})$ is the exact solution of the three-body rearrangement scattering problem involving more than three bodies (five bodies, d, e^-, t, ^{4}He, and n for ${}^3\mathrm{H}(d,n){}^4\mathrm{He}$ reaction) and more than one channel in the final state.

If $\psi_E(\vec{r},\vec{\rho})$ in eq. (38) is replaced by an approximate adiabatic representation as customarily done in previous conventional theoretical estimates, then the probability integral in eq. (38) may be square-integrable. However, the square-integrability of eq. (38) with use of an approximate solution for $\psi_E(\vec{r},\vec{\rho})$ is meaningless, if eq. (38) is proven to be not square-integrable when the exact solution for $\psi_E(\vec{r},\vec{\rho})$ is used.

For ${}^3\mathrm{H}(d,n){}^4\mathrm{He}$ reaction, $d+(e^-,t) \longrightarrow (e^-,{}^4\mathrm{He})+n+Q$ and $d+(e^-,t) \longrightarrow e^- + {}^4\mathrm{He} + n + Q$, Schrödinger equation and Hamiltonian can be written as

$$\left(\tilde{E} - \tilde{H}\right)|\tilde{\psi}\rangle = 0\ , \quad \tilde{E} = \begin{pmatrix} E & 0 \\ 0 & E+Q \end{pmatrix}, \quad \tilde{H} = \begin{pmatrix} H_{det} & V_{det,e^4\mathrm{He}n} \\ V_{e^4\mathrm{He}n,det} & H_{e^4\mathrm{He}n} \end{pmatrix} \tag{39}$$

with $H_{det} = T_r + T_\rho + V_{de} + V_{et} + V_{dt}$ and $H_{e^4\mathrm{He}n} = T_{r'} + T_{\rho'} + V_{e^4\mathrm{He}} + V_{^4\mathrm{He}n}$. $T's$ are kinetic energy operators, $\vec{r} = \vec{r}_d - \vec{r}_t$, $\vec{r}\,' = \vec{r}_n - \vec{r}_{^4\mathrm{He}}$, $\vec{\rho} = \vec{r}_e - (m_d\vec{r}_d + m_t\vec{r}_t)/(m_d + m_t)$, and $\vec{\rho}\,' = \vec{r}_e - (m_n\vec{r}_n + m_{^4\mathrm{He}}\vec{r}_{^4\mathrm{He}})/(m_n + m_{^4\mathrm{He}})$. H_{det} and $H_{e^4\mathrm{He}n}$ are the channel Hamiltonians for the det and $e^4\mathrm{He}n$ channels, respectively. For $\vec{\rho} \longrightarrow \infty$ and $r < b$ (b is the nuclear interaction range), eq. (39) can be written as

$$\begin{aligned}&\left[E + \frac{\hbar^2}{2\mu}\frac{d^2}{d\rho^2} + \frac{\hbar^2}{2M}\frac{d^2}{dr^2} + \frac{2}{r} - V_{dt}(r)\right]\psi_{det}(r,\rho) = \\ &r\rho \int d\Omega_{\vec{r}} d\Omega_{\vec{\rho}} V_{det,e^4\mathrm{He}n}(\vec{r},\vec{r}\,')\psi_{e^4\mathrm{He}n}(\vec{r}\,',\vec{\rho})d\vec{r}\,'\ .\end{aligned} \tag{40}$$

From behavior of the asymptotic solution $\psi_{det}(0,\rho \longrightarrow \infty)$ of eq. (40), we show the non-square-integrability of eq. (38) in the following.

We can show (see Appendix B)

$$\psi_{det}(0,\vec{\rho}) \approx \sum_n C_n \frac{d^{2n}}{d\rho^{2n}} y(\rho) \tag{41}$$

where $y(\rho) = \rho \int d\Omega_{\vec{\rho}} \psi_{e^4\mathrm{He}n}(0,\vec{\rho})$ and C_n are constants. Therefore, if $\psi_{e^4\mathrm{He}n}(0,\vec{\rho})$ is not square-integrable, then $\psi_{det}(0,\vec{r})$ is also not square-integrable due to eq. (40). To show $\psi_{e^4\mathrm{He}n}(0,\vec{\rho})$ is not square-integrable, we use the following approximation, $\psi_{e^4\mathrm{He}n}(0,\vec{\rho}) \approx e^{i\vec{k}_\epsilon \vec{r}} \phi_{\vec{k}}(\vec{\rho})$, where $\phi_{\vec{k}}(\vec{\rho})$ is the $(e, {}^4\mathrm{He})$ Coulomb function for positive energy $\hbar^2 k^2/2m_e$, $k_\epsilon = m_e v_\epsilon$, and v_ϵ is the recoil velocity of ^{4}He as calculated from the momentum conservation. We have

$$\lim_{\rho\to\infty} y(\rho) \sim \frac{1}{kk_\epsilon \rho} \sum_{\ell m} (-1)^\ell e^{i\delta_\ell^c} \times$$

$$\times \sin\left(k\rho - \frac{\ell\pi}{2} - \eta \ell n 2k\rho + \delta_\ell^c\right) \sin\left(k_\epsilon r - \frac{\ell\pi}{2}\right) Y_{\ell m}(\hat{k}_\epsilon) Y^*_{\ell m}(\hat{k}) \ .$$

Because any $d^{2n}y(\rho)/d\rho^{2n}$ is a linear superposition, only two functions $g_1(r)$ and $g_2(r)$ are needed

$$\frac{d^{2n}y(\rho)}{dr^{2n}} = \alpha^{(n)} g_1(\rho) + \beta^{(n)} g_2(\rho) \tag{42}$$

where

$$g_1(\rho) = \frac{1}{\rho} \sum_{\ell m} (-1)^\ell e^{i\delta_\ell^c} \sin\left(k\rho - \frac{\ell\pi}{2} - \eta \ell n 2k\rho + \delta_\ell^c\right) \sin\left(k_\epsilon \rho - \frac{\ell\pi}{2}\right) Y_{\ell m}(\hat{k}_\epsilon) Y^*_{\ell m}(\hat{k})$$

and

$$g_2(\rho) = \frac{1}{\rho} \sum_{\ell m} (-1)^\ell e^{i\delta_\ell^c} \cos\left(k\rho - \frac{\ell\pi}{2} - \eta \ell n 2k\rho + \delta_\ell^c\right) \cos\left(k_\epsilon \rho - \frac{\ell\pi}{2}\right) Y_{\ell m}(\hat{k}_\epsilon) Y^*_{\ell m}(\hat{k}) \ . \tag{43}$$

For $\rho \to \infty$, we obtain the final result $\psi_{det}(0,\rho) = \alpha g_1(\rho) + \beta g_2(\rho)$ which leads to the non-square-integrability of eq. (38).

Since the conventional definition $\sigma(E)$ given by eq. (24) has difficulties associated with non-square integrability of eq. (38), we introduce an alternative formulation. For the previous example of $^3\mathrm{H}(d,n)^4\mathrm{He}$, we need to solve eqs. (39) under the boundary condition in $e^4\mathrm{He}n$ channel [1],

$$\psi_{e^4\mathrm{He}n} \sim \sum_\beta T^{(\beta)} \phi_\beta(\vec{r}_{e^4\mathrm{He}}) U^+\left(\vec{K}_\beta, \vec{R}\right) \tag{44}$$

for $R \to \infty$ where $r_{e^4\mathrm{He}}(R)$ is the relative distance between e and ^{4}He (e^4He and n). U^+ is the outgoing wave between $(e, {}^4\mathrm{He})$ and n, with a momentum K_β, and β indicates the quantum numbers of $(e, {}^4\mathrm{He})$ atomic states including continuum states. $T^{(\beta)}$ is given by

$$T^{(\beta)} = \left\langle e^{-i\vec{K}_\beta \vec{R}}, \phi_\beta(\vec{r}_{e^4\mathrm{He}}) | V_{e^4\mathrm{He}n,det} | \psi_{det} \right\rangle + \left\langle e^{-i\vec{K}_\beta \vec{R}}, \phi_\beta(\vec{r}_{e^4\mathrm{He}}) | V_{^4\mathrm{He}n} | \psi_{e^4\mathrm{He}n} \right\rangle \ . \tag{45}$$

Since it is very difficult to calculate $T^{(\beta)}$ given by (45), we use some approximations.

(i) The coupling interaction $V_{e^4\mathrm{He}n,det}$ may be replaced by $V_{^4\mathrm{He}n,dt}$ (bare nuclei) since electrons are not expected to affect the nuclear rearrangement process significantly. For example, we can use some sets of the interaction $\left\{V_{dt}, V_{^4\mathrm{He}n}, V_{dt,^4\mathrm{He}n}\right\}$, which reproduce the experimental data.

(ii) From (45), we see that $\psi_{e^4\mathrm{He}n}$ is needed only for $r' \lesssim b$ (where b is the range of $^4\mathrm{He} - n$ interaction). For this internal region of r', $\psi_{e^4\mathrm{He}n}$ may be expanded in terms of some basis functions.

With these approximations, we can define σ as

$$\sigma \sim \sum_\beta |T^{(\beta)}|^2 \tag{46}$$

We are using this alternative formulation for investigating the electron screening effect.

8. Three-Body Fusion Reactions

Recently, energetic protons ($\lesssim$ 17 MeV) and α particles ($\lesssim$ 6.5 MeV) have been observed in experiments in which deuterated Ti target is bombarded with 150 keV deuteron beam [5]. The observed proton and α-particle energy spectrum cannot be explained with existing two-body fusion reactions but is consistent with a three-body fusion reaction, $d + d + d \to p + n + {}^4\mathrm{He}$ [5]. The observed rate $R^{(3)}$ is $\sim 10^{-6}R^{(2)}$ where $R^{(2)}$ is the observed fusion rate for $D(d,p)T$ with 150 keV deuteron beam, i.e., $R^{(3)}/R^{(2)} \approx 10^{-5}$. However, the conventional theoretical estimate for $R^{(3)}/R^{(2)}$ is $\sim 10^{-17}$ [5] or much less, and hence the observed value of 10^{-6} for $R^{(3)}/R^{(2)}$ is anomalous. In this section, we describe the 3d fusion cross-section $\sigma^{(3)}(E)$ and rate $R^{(3)}(E)$ based on the optical theorem and a solution of three-body Schrödinger equation.

The scattering problem for three particles ($3 \to 3$) has been investigated in the context of the formal scattering theory [25-29]. The hyperspherical harmonics (h.h.) expansion method was first introduced in 1935 by Zernike and Brinkman [30] but has not been used until 1960 for the few-body bound-state problem [31-33]. More recently, it has been used for the ($3 \to 3$) scattering problem [34-39].

For the 3d fusion reaction, we consider two-channel case,

$$d + d + d \longrightarrow \begin{cases} d + d + d \\ p + n + {}^4\mathrm{He} \quad (Q = 21.62 \text{ MeV}) . \end{cases} \tag{47}$$

Three–body Schrödinger equation in the elastic channel is (we suppress the spin and isospin degrees of freedom for simplicity)

$$-\frac{\hbar^2}{2m}\left(\nabla_{\vec{x}}^2 + \nabla_{\vec{y}}^2\right)\Psi(\vec{x},\vec{y}) + V\Psi(\vec{x},\vec{y}) = E\Psi(\vec{x},\vec{y}) \tag{48}$$

where $\vec{x} = \sqrt{\frac{1}{2}}(\vec{r}_2 - \vec{r}_3)$, $\vec{y} = \sqrt{\frac{2}{3}}\left[\frac{1}{2}(\vec{r}_2 + \vec{r}_3) - \vec{r}_1\right]$, $V = V^C + V^S = \left(V_{12}^C + V_{23}^C + V_{13}^C\right) + \left(V_{12}^S + V_{23}^S + V_{13}^S\right)$ with $V^S = V_{Re}^S - iV_{Im}^S$. We introduce the hyperspherical harmonics expansion for $\Psi(\vec{x}, \vec{y})$ as

$$\Psi(\vec{x}, \vec{y}) = \sum_{K\ell_x\ell_y} \Psi_K^{\ell_x\ell_y LM}(\rho)\Phi_K^{\ell_x\ell_y LM}(\Omega) \ , \tag{49}$$

where $\rho^2 = x^2 + y^2$ (hyperradius), and

$$\Phi_K^{\ell_x\ell_y LM}(\Omega) = \sum_{m_x m_y} \langle LM|\ell_x m_n \ell_y m_y\rangle \bar{\Phi}_K^{\ell_x\ell_y m_x m_y}(\Omega)$$

with $\bar{\Phi}_K^{\ell_x\ell_y m_x m_y}(\Omega) \propto Y_{\ell_x m_x}(\hat{x})Y_{\ell_y m_y}(\hat{y})$. If we write $\Psi_K^{\ell_x\ell_y LM}(\rho) = U_K^{\ell_x\ell_y LM}(\rho)/\rho^{5/2}$, eq. (48) reduces to

$$\frac{d^2U_k^{\ell_x\ell_y LM}(\rho)}{d\rho^2} + \left[\frac{2mE}{\hbar^2} - \frac{(K+3/2)(K+5/2)}{\rho^2}\right]U_K^{\ell_x\ell_x LM}(\rho) = \frac{2m}{\hbar^2}V_{KK'}^{\ell_x\ell_y,\ell'_x\ell'_y}U_{K'}^{\ell'_x\ell'_y,LM}(\rho) \tag{50}$$

where

$$V_{KK'}^{\ell_x\ell_y,\ell'_x\ell'_y} = \langle\Phi^{\ell_x\ell_y LM}|V|\Phi^{\ell'_x\ell'_y LM}\rangle \ . \tag{51}$$

For $K = 0(\ell_x = 0, \ell_y = 0, L = 0)$ case (known as "true" [28] or "democratic" state [35]), eq. (50) reduces to

$$\frac{d^2U}{d\rho^2} + \left(k^2 - \frac{15/4}{\rho^2}\right)U = \frac{2m}{\hbar^2}\tilde{V}U \ , \tag{52}$$

where $\tilde{V} = \tilde{V}^C + \tilde{V}^S$ with $\tilde{V} = V_{00}^{00,00}$. For $\tilde{V} = \tilde{V}^C$(i.e. $\tilde{V}^S = 0$), the solution of eq. (52) is

$$U^C(\rho) = C(k\rho)^{5/2}e^{-ik\rho}M\left(\frac{5}{2} - i\eta, 5, 2ik\rho\right), \tag{53}$$

where M is the Whittaker function and $C = 2^{3/2}e^{-\pi\eta/2}|\Gamma\left(\frac{5}{2} + i\eta\right)|/\Gamma(5)$.

In terms of T-matrix, the $K = 0$ elastic 3d nuclear scattering amplitude, $f_{3B}^{(el)}$, can be written as

$$f_{3B}^{(el)} = -\frac{2m}{\hbar^2 k^{7/2}}\langle U^C|T|U^C\rangle \ . \tag{54}$$

Using the optical theorem [39], $\sigma_r = \sqrt{2\pi}\left(\pi^2/k^{5/2}\right)Im\left(f_{3B}^{(el)}\right)$, and eq. (54), we obtain the following expression for the 3d fusion cross-section,

$$\sigma^{(3)}(E) = \sigma_r \approx \frac{2m}{\hbar^2 k^6}\pi^2\sqrt{2\pi}\int_0^\infty U^C(\rho)W(\rho,\rho')U^C(\rho')d\rho d\rho' \tag{55}$$

where $W(\rho,\rho') = -Im\langle U^C|T|U^C\rangle$. If we parameterize $W(\rho,\rho') = -Im\langle U^C|T|U^C\rangle = \lambda g(\rho)g(\rho')$ with $g(\rho) = e^{-\beta\rho}\rho^{3/2}$, we obtain

$$\sigma^{(3)}(E) \approx \lambda\frac{2m}{\hbar^2 k_3}\pi^2\sqrt{2\pi}C^2\frac{(4!)^2}{(\beta^2 + k_3^2)^5}e^{4\phi\eta_3} \tag{56}$$

where

$$|C|^2 = \frac{1}{36}\left(\frac{9}{4}+\eta_3^2\right)\left(\frac{1}{4}+\eta_3^2\right)\frac{\pi e^{-2\pi\eta_3}}{1+e^{-2\pi\eta_3}} . \tag{57}$$

Other quantities in eqs. (56) and (57) are $\phi = \tan^{-1}(k_3/\beta)$, $k_3 = (2mE/\hbar^2)^{1/2}$, $\eta_3 = 1/(2k_3 R_B^{(3)})$, $R_B^{(3)} = \hbar^2/(2mZ_{eff}e^2)$, $Z_{eff} = 16/(\pi\sqrt{2}) \approx 3.6$, and $\lambda = V_0/a^4$.

We note that $\sigma^{(3)}(E)$ in eq. (56) has a dimensionality of the 5th power of length $[L^5]$ since $f_{3B}^{(el)}$ has a dimensionality $[L^{5/2}]$ expected from the solution, $\Psi(\rho) = e^{i\vec{k}\cdot\vec{\rho}} + f_{3B}^{(el)} e^{ik\rho}/\rho^{5/2}$, while two-body fusion cross-section $\sigma^{(2)}(E)$ has a dimensionality of $[L^2]$. For comparison, we use eq. (11) for the 2d cross-section

$$\sigma^{(2)}(E) \approx \frac{S^{(2)}(E)}{E} e^{-2\pi\eta_2} . \tag{58}$$

Since Kasagi et al. [5] observed energetic protons and α particles indicative of $d+d+d \to p+n+{}^4$He reaction only when deuteron concentration in the TiD_x target reaches $x > 1.2$, we can assume that some fraction f of deuterons in the TiD_x are mobile when x becomes greater than 1.2 with mobile deuteron number density $fn_D = fn_{Ti}/2 \approx f(3\times 10^{22})/\text{cm}^3$. For these mobile deuterons fn_D, the number of deuteron pairs we can form with mobile deuterons per unit volume is $(fn_D)^2/2 + f(1-f)n_D^2/2 = fn_D^2/2$. The incident deuteron can now interact with one of these deuteron pairs and can form a "true" or "democratic" three-body state, leading to $d+d+d \to p+n+{}^4$He fusion with the cross-section described by $\sigma^{(3)}(E)$, eq. (56). The 3d fusion probability $P^{(3)}$ is then given by

$$P^{(3)}(E_d) = fn_D^2 \int_0^{E_d} \frac{\sigma^{(3)}(E_{cm}^{(3)})}{|dE/dx|} dE \tag{59}$$

compared with the 2d fusion probability $P^{(2)}$ given by [40]

$$P^{(2)}(E_d) = n_D \int_0^{E_d} \frac{\sigma^{(2)}(E_{cm}^{(2)})}{|dE/dx|} dE \tag{60}$$

where dE/dx is the stopping power for d in the target T_iD_x, and E_d is the laboratory kinetic energy of the incident deuteron.

To make an order of magnitude estimate for the ratio $\left(P^{(3)}/P^{(2)}\right)$, we approximate the ratio as

$$R = \frac{P^{(3)}(E_d)}{P^{(2)}(E_d)} \approx fn_D \frac{\sigma^{(3)}(E_{cm}^{(3)})}{\sigma^{(2)}(E_{cm}^{(2)})} \tag{61}$$

where $E_{cm}^{(3)} = (2/3)E_d$ and $E_{cm}^{(2)} = E_d/2$. In eq. (56), λ (or V_0 and a for $\lambda = V_0/a^4$) and β are parameters to be determined from theory and/or experiment. In the following, we assume $V_0 \approx 10$ MeV, $a = 2\ fm$, and $\beta = 0.065\ fm^{-1} (\beta^{-1} = 15 fm)$. For the 2$d$ fusion cross-section $\sigma^{(2)}(E)$, we use eq. (58) with $S^{(2)}(E) \approx S_0 \approx 50$

keV–b. For $f = 0.1$, we obtain the following results for R. R (in units of 10^{-6}) = 0.40, 0.42, 0.42, 0.40, 0.38, and 0.36 for E_d = 100, 110, 120, 130, 140, and 150 keV, respectively, which is comparable with the results of $R_{\text{exp}} \approx (1-3) \times 10^{-6}$ within an order of magnitude.

It is known that the asymptotic behavior of the real part of the effective potential is $1/\rho^3$ [41]. However this long-range asymptotic dependence does not apply to the imaginary part. Therefore, the use of a small value of $\beta^{-1} = 15\ fm$ is reasonable.

The quantum number K is closely related to the impact parameter. In terms of classical orbits, a large value of K implies that three particles cannot come close together. For $K = 0$, all three particles seem to converge to or diverge from a scattering center [42]. Therefore the $K = 0$ "true" (or "democratic") three-body state is important for the three-body fusion reaction.

If the experimental data of Kasagi et al. [5] is conclusively determined to be due to $d + d + d \rightarrow p + n + {}^4$He fusion by future p–^{4}He coincidence measurements by Kasagi et al. and independently by other groups, the experimental result and its theoretical understanding based on "true" (or "democratic") three-body state may have very important implications for nucleosynthesis and stellar evolutions, since there are possibilities that other three-body fusion reactions may be involved in astrophysical problems, such as pycnonuclear triple-alpha fusion [43-45].

9. Summary and Conclusions

We have examined uncertainties due to many approximations made in the conventional theoretical formulations of low-energy nuclear fusion reactions, and presented new improved formulations which avoid some of these approximations. Some of the new formulations lead to unexpected results. One striking result is a possibility that a near cancellation of the Gamow factor (or "Coulomb barrier transparency" (CBT)) can not be ruled out completely at present. Another surprising result is that the large value of the 3d fusion rate recently observed in the laboratory beam experiment [5] may be justified theoretically in terms of a solution of the quantum mechanical three-body problem. Since there are still a great deal of uncertainty and absence of reliable reproducibility at a desirable level of $\sim 100\%$ for reported anomalous effects [3], it is at present premature to make definitive tests and comparisons of the predictions of our new improved formulations with the experimental data [3].

Appendix A

Let us rewrite eq. (34b) in an integral form

$$\left.\frac{F_\epsilon(r)}{r}\right|_{r\to 0} = \frac{2\mu}{\hbar^2}\Gamma(1+\eta_\epsilon)\frac{X(r)}{2k_\epsilon r}\int_r^\infty Y(r)V_{\epsilon 1}(r)\frac{F_1(r)}{r}r\,dr \qquad (A1)$$

where η_ϵ is the Sommerfeld parameter for $(d+d)$

$$\eta_\epsilon = \frac{1}{2k_\epsilon R_B}\ , \quad k_\epsilon = 2\mu\,\frac{\epsilon - E_{1S} - E}{\hbar^2} \qquad (A2)$$

R_B is the Bohr radius $R_B = 14.4123 fm$ for $(d+d)$, and $X(R)$ and $Y(r)$ are the Whittaker functions

$$X(r) = e^{-k_\epsilon r}(2k_\epsilon r)M(1+\eta_\epsilon, 2, 2k_\epsilon r)$$

and

$$Y(r) = e^{-k_\epsilon r}(2k_\epsilon r)U(1+\eta_\epsilon, 2, 2k_\epsilon r)\ . \tag{A3}$$

We assume $F_1(r)$ to be the regular Coulomb function with energy $E + E_{scr}$ where E_{scr} is the screening energy. We will integrate (A1) from $r = 0$ to $r = \rho_B$, where $\rho_B = 0.529 \cdot 10^{-8}$cm. If $k_\epsilon^2 \rho_B R_B << 1$ and $k_E^2 \rho_B R_B << 1$ for $k_\epsilon^2 = (2\mu/\hbar^2)(\varepsilon - E_{1S} - E)$ and $k_E^2 = 2\mu(E + E_{scr})/\hbar^2$, we can use the following approximation [46]

$$\frac{X(r)}{2k_\epsilon r} \approx L_1(r) + \frac{(k_\epsilon r)^2}{6} L_2(r) \tag{A4}$$

$$\Gamma(1+\eta_\epsilon)Y(r) = H_1(r) - \frac{1}{3}k_\epsilon^2 r R_B H_2(r) \tag{A5}$$

$$\frac{F_1(r)}{r} = C\left[L_1(r) - \frac{(k_E r)^2}{6} L_2(r)\right] \tag{A6}$$

where

$$|C|^2 = \frac{2\pi\eta_E}{e^{2\pi\eta_E} - 1}\ , \quad \eta_E = \frac{1}{2k_E R_B}\ , \tag{A7}$$

$$L_n(r) = n!\left(\frac{r}{R_B}\right)^{n/2} I_n\left(2\left(\frac{r}{R_B}\right)^{1/2}\right) \tag{A8}$$

and

$$H_n(r) = \frac{2}{(n-1)!}\left(\frac{r}{R_B}\right)^{-n/2} K_n\left(2\left(\frac{r}{R_B}\right)^{1/2}\right) \tag{A9}$$

Using eqs. (A4)–(A9),

$$\psi_\epsilon(\rho) \approx \frac{1}{\hbar}\frac{\sqrt{2m_e}}{(\rho_{B/2})^{1/2}}\sqrt{\frac{\rho_B}{2\rho}} J_1\left(\sqrt{\frac{16\rho}{\rho_B}}\right) \quad (\text{for } \epsilon \approx 0) \tag{A10}$$

and

$$\psi_{1S}(\rho) = 2\left(\frac{\rho_B}{2}\right)^{-3/2} e^{-2\rho/\rho_B} \tag{A11}$$

we can calculate $V_{\epsilon 1}(r)$ in eq. (A1) which we can integrate over ϵ from $\epsilon = 0$ to $\epsilon' = 10$ eV to obtain $F_\epsilon(r)/r|_{r\to 0}$ from eq. (A1). (Eqs. (A4) – (A10) are valid for $\epsilon < 10$ eV.) Our numerical estimate yields

$$\int_0^{\epsilon'} \left|\frac{F_\epsilon(r)}{r}\right|^2_{r\to 0} d\epsilon \approx 6.4|C^2|\ . \tag{A12}$$

Using eq. (A12) and the following relation for $\epsilon' \approx 10$ eV

$$\int_0^{\epsilon'} \left|\frac{F_\epsilon(r)}{r}\right|^2_{r=0} d\epsilon < \int_0^{\infty} \left|\frac{F_\epsilon(r)}{r}\right|^2_{r=0} d\epsilon$$

we obtain eq. (37) for the very low–energy case of $k_\epsilon^2 \rho_B R_B << 1$ and $k_E^2 \rho_B R_B << 1$.

Appendix B

Consider a set of functions $\varphi_n(r)$ satisfying

$$\int_0^b \varphi_n^*(r)\varphi_m(r)dr = \delta_{nm} \quad \text{and} \quad \int_0^b \varphi_n^*(r)\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V(r)\right)\varphi_m(r)dr = E_n\delta_{nm} \tag{B1}$$

where E_n are positive numbers.

We can represent the solution of the equation (64) in a form

$$\psi_{det}(r,\rho) = \sum_n \psi_n(\rho)\varphi_n(r) \ . \tag{B2}$$

Using (40) and (B1) we obtain

$$\left(k_n^2 + \frac{d^2}{d\rho^2} + -\frac{2\mu}{\hbar^2}\cdot\frac{2}{\rho}\right)\psi_n(\rho) \approx \gamma_n y(\rho) \ , \quad B \le \rho \le \infty \tag{B3}$$

where B is a sufficiently large distance in the asymptotic region and

$$\gamma_n = \frac{2\mu}{\hbar^2}\int_0^b \varphi_n(r) r V_{det,e^4\mathrm{He}n}(\vec{r},\vec{r}\,') \cdot d\Omega_{\vec{r}} d\vec{r}\,'$$

with $k_n^2 = 2\mu(E - E_n)/\hbar^2$. Let us introduce a Green's function satisfying

$$\left(k_n^2 + \frac{d^2}{d\rho^2} + \frac{2\mu}{\hbar^2}\frac{2}{\rho}\right)G(\rho,\rho') = \delta(\rho - \rho') \ . \tag{B4}$$

The solution of (B4) is given by

$$G(\rho,\rho') = \lambda_n \begin{cases} (f_1(\rho) + \delta_n f_2(\rho))f_2(\rho'), \rho \le \rho' \\ f_1(\rho)(f_1(\rho') + \delta_n f_2(\rho')), \rho' \le \rho \end{cases} \tag{B5}$$

where λ_n is defined in terms of $f_1(\rho) = G_0(\rho) + iF_0(\rho)$ and $f_2(\rho) = G_0(\rho) - iF_0(\rho)$ as $(F_0(\rho)(G_0(r))$ is the regular (irregular) Coulomb function)

$$\lambda_n[f_1'(\rho)(f_1(\rho) + \delta_n f_2(\rho)) - f_1(\rho)(f_1'(2) + \delta_n f_2'(\rho))] = 1 \tag{B6}$$

and δ_n is determined by boundary conditions at $\rho = B$. The solution $\psi_n(\rho)$ of eq. (B3) can now be written as

$$\psi_n(\rho) = \lambda_n\gamma_n\Big[f_1(\rho)\int_B^r (f_1(\rho') + \delta_n f_2(\rho'))y(\rho')d\rho' + (f_1(\rho) + \delta_n f_2(\rho))\int_r^\infty f_1(\rho')y(\rho')d\rho'\Big] \tag{B7}$$

For $r \geq B$ with a large value of B, we can obtain asymptotical expressions for $f_1(\rho)$ and $f_2(\rho)$ as $f_1(\rho) = e^{i(k_n\rho - S_n \ell n 2k_n\rho + \eta_n)}$ and $f_2(\rho) = e^{-i(k_n\rho - S_n\ell n 2k_n\rho+\eta_n)}$ where $Imk_n > 0$, $S_n = 2e^2/\hbar v_n$, $v_n = \hbar k_n/\mu$, $e^{2i\eta_n} = \Gamma(1+iS_n)/\Gamma(1-iS_n)$.

For large values of ρ and B, we can rewrite (B7) as

$$\psi_n(\rho) \approx \delta_n\lambda_n\gamma_n\Big[f_1(\rho)\int_B^\rho f_2(\rho')y(\rho')d\rho' + f_2(\rho')\int_\rho^\infty f_1(\rho')y(\rho')d\rho'\Big] \tag{B8}$$

Using $f_1(\rho) \approx \frac{1}{ik_n}f_1'(\rho)$ and $f_2(\rho) \approx -\frac{1}{ik_n}f_2'(\rho)$, we obtain

$$\begin{aligned} &f_1(\rho)\int_B^\rho f_2(\rho')y(\rho')d\rho' + f_2(\rho)\int_\rho^\infty f_1(\rho')y(\rho')d\rho' \\ &\approx -\frac{2}{ik_n}y(\rho) + \frac{1}{k_n^2}\Big(f_1(\rho)\int_B^\rho f_2(\rho')y''(\rho')d\rho' + f_2(\rho)\int_\rho^\infty f_1(\rho')y''(\rho')d\rho'\Big) \end{aligned} \tag{B9}$$

for $\rho \to \infty$. Eq. (B9) leads to the following generalization,

$$\begin{aligned} &f_1(\rho)\int_B^\rho f_2(\rho')y^{(N)}(\rho')d\rho' + f_2(\rho)\int_\rho^\infty f_1(\rho')y^{(N)}(\rho')d\rho' \\ &\approx -\frac{2}{ik_n}y^{(N)}(\rho) + \frac{1}{k_n^2}\Big(f_1(\rho)\int_B^\rho f_2(\rho')y^{(N+2)}(\rho')d\rho' + f_2(\rho)\int_\rho^\infty f_1(\rho')y^{(N+2)}(\rho')d\rho'\Big) \end{aligned} \tag{B10}$$

From (B2), (B8), (B9), and (B10), we obtain eq. (41).

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