REACTION BARRIER TRANSPARENCY FOR COLD FUSION WITH DEUTERIUM AND HYDROGEN

Yeong E. Kim,
Jin-Hee Yoon
Department of Physics, Purdue University
West Lafayette, IN 47907

Alexander L. Zubarev
Racah Institute of Physics, Hebrew University
Jerusalem 91904, Israel

Mario Rabinowitz
Electric Power Research Institute
Palo Alto, CA 94303

Abstract

An improved parametric representation of Coulomb barrier penetration is presented. These detailed calculations are improvements upon the conventionally used Gamow tunneling coefficient. This analysis yields a reaction barrier transparency (RBT) which may have singular ramifications for cold fusion, as well as significant consequences in a wide variety of fusion settings.

1. Introduction

Recently, Kim and Zubarev[1] developed a general and realistic barrier transmission model which can accommodate simultaneously both non-resonance and Coulomb barrier transmission resonance contributions. The derivations for both cases will be presented. The resonance analysis culminates in a reaction barrier transparency (RBT) which is due to the interaction of the transmitted and reflected waves yielding constructive interference in a narrow energy regime. Although RBT may have significant consequences for a wide variety of fusion problems, we will explore cold fusion applications here.

2. Conventional Parameterization

The conventional protocal for determining low-energy (< 20 keV) fusion cross-sections $\sigma(E)$ is to extrapolate experimental values of $\sigma(E)$ measured at high energies using the parameterization[2]

$$\sigma(E) = \frac{S(E)}{E}\, T_G(E) \tag{1}$$

where $T_G(\mathrm{E}) = \exp[-(E_G/E)^{1/2}]$, $E_G = (2\pi\alpha Z_1 Z_2)^2 \mu c^2/2$ with the reduced mass $\mu = m_1 m_2/(m_1 + m_2)$ and E is the center-of-mass (CM) kinetic energy. The transmission

coefficient ("Gamow" factor) $T_G(E)$ results from the approximation $E << B$ (Coulomb barrier height). This technique is used for nuclei in non-resonance reactions such as in standard solar model, and magnetic and inertial confinement calculations.

In order to generalize the conventional Gamow transmission coefficient, we introduce for the fusing system the following potential which consists of an interior square-well nuclear potential and an exterior Coulomb repulsive potential,

$$V(r) = \begin{cases} -V_0 , & r < R \\ Z_1 Z_2 e^2 / r , & r \geq R \end{cases} . \tag{2}$$

For the potential barrier given by eq. (2), an approximate S-wave ($\ell = 0$) solution for $T(E)$ can be calculated in the Wentzel-Kramers-Brillouin (WKB) approximation as[3]

$$\begin{aligned} T_R^{\mathrm{WKB}}(E) &= \exp\left\{-2\left(\frac{2\mu}{\hbar^2}\right)^{1/2} \int_R^{r_a} \left(\frac{Z_1 Z_2 e^2}{r} - E\right)^{1/2} dr\right\} \\ &= \exp\left(-\left(\frac{E_G}{E}\right)^{1/2}\left(\frac{2}{\pi}\right)\left\{\cos^{-1}\left[\left(\frac{E}{B}\right)^{1/2}\right] - \left(\frac{E}{B}\right)^{1/2}\left(1 - \frac{E}{B}\right)^{1/2}\right\}\right) \end{aligned} \tag{3}$$

where B is the Coulomb barrier height, $B = Z_1 Z_2 e^2 / R$ and r_a is the classical turning point, $Z_1 Z_2 e^2 / r_a = E$. Note that $T_R^{WKB}(E)$ is defined only for $E \leq B$ and that $T_R^{WKB}(E) = 1$. The traditional Gamow transmission coefficient used in eq. (1) can be obtained from eq. (3) with $R = 0$ (or equivalently $E << B$):

$$\begin{aligned} T_G(E) &= T_R^{\mathrm{WKB}}(E) = \exp\left\{-2\left(\frac{2\mu}{\hbar^2}\right)^{1/2} \int_0^{r_a} \left(\frac{Z_1 Z_2 e^2}{r} - E\right)^{1/2} dr\right\} \\ &= \exp\left[-\left(\frac{E_G}{E}\right)^{1/2}\right] . \end{aligned} \tag{4}$$

3. Kim-Zubarev Parameterization

$T_G(E)$, eq. (4), represents the probability of bringing two particles to zero separation distance. This implies that the Coulomb barrier $Z_1 Z_2 e^2 / r$ also exists inside the nuclear surface of radius R, which is unphysical and unrealistic. In order to accommodate more realistic transmission coefficients. Kim and Zubarev[1,4] have recently introduced a more general parameterization for $\sigma(E)$ based on the P-matrix parameterization of the fusion reaction S-matrix.

To obtain improved and more general transmission coefficients, we use partial wave solutions of the Schrodinger equation. For the potential described by eq. (2), a general solution of the radial Schrodinger equation for the exterior wave function in the exterior region ($r \geq R$) is given by[5]

$$u_\ell^{ext}(r) = u_\ell^{(-)}(r) - \eta_l u_\ell^{(+)}(r) \tag{5}$$

where

$$u_\ell^{(+)}(r) = e^{-i\delta_\ell^c}[G_\ell(r) + i\ F_\ell(r)]\ . \tag{6}$$

δ_ℓ^c is the Coulomb phase shift and $u_\ell^{(-)}$ is the complex conjugate of $u_\ell^{(+)}$. F_ℓ and G_ℓ are the regular and irregular Coulomb wave functions normalized asymptotically $(r \to \infty)$ as

$$\begin{aligned} F_\ell(r) &\approx \sin[kr - \ell\pi/2 - \gamma\ell n(2kr) + \delta_\ell^c] \\ G_\ell(r) &\approx \cos[kr - \ell\pi/2 - \gamma\ell n(2kr) + \delta_\ell^c] \end{aligned} \tag{7}$$

where γ is the Sommerfeld parameter, $\gamma = Z_1 Z_2 e^2 / \hbar\upsilon$ and k is related to E by $E = \hbar^2 k^2 / 2\mu$.

In terms of the partial wave S-matrix, η_l, in eq. (5), the fusion reaction total cross-section $\sigma_r(E)$ is given by[5]

$$\sigma_r(E) = \frac{\pi}{k^2}\sum_l (2l+1)(1 - |\eta_l|^2)\ . \tag{8}$$

To accommodate the statistical factor and to compensate the two-body approximation involved in deriving eq. (8), we introduce the partial wave S-factor, $S_l(E)$, which is expected to be nearly energy-independent or weakly energy-dependent, and rewrite

$$\sigma_r(E) \approx \sigma(E) = \frac{1}{E}\sum_{l=0}^{\infty} S_l(E) T_l(E) = \sum_l \sigma_l(E) \tag{9}$$

where $S_l(E)$ is the l-th partial wave S-factor and

$$\sigma_l(E) = \frac{S_l(E)}{E} T_l(E) \tag{10}$$

with

$$T_l(E) = 1 - |\eta_l|^2\ . \tag{11}$$

In order to determine the partial wave S-matrix η_l in eq. (5), we introduce the P-matrix as the logarithmic derivative of the interior wave function $u_l^{\text{int}}(r)$ at $r = R$:

$$P_l^{int} = R\left.\frac{du_l^{int}/dr}{u_l^{int}}\right|_{r=R} = \Re P_l^{int} + i\Im P_l^{int} \tag{12}$$

where $\Re P_l^{\text{int}}$ and $\Im P_l^{\text{int}} < 0$ are the real and imaginary parts of P_l^{int}, respectively. For the exterior wave function, the P-matrix at $r = R$ is defined as

$$P_l^{ext} = R\,\frac{du_l^{ext}/dr}{u_l^{ext}}\bigg|_{r=R} = R\,\frac{du_l^{(-)}/dr - \eta_l du_l^{(+)}/dr}{u_l^{(-)} - \eta_l u_l^{(+)}}\bigg|_{r=R} \tag{13}$$

We introduce the P-matrix for $u_l^{(+)}$ as

$$P_l^{(+)} = R\,\frac{du_l^{(+)}/dr}{u_l^{(+)}}\bigg|_{r=R} = \Delta_l + is_l \tag{14}$$

where Δ_l and s_l are the real and imaginary parts of $p_l^{(+)}$, respectively. By matching the logarithmic derivatives at $r = R$, i.e., $P_l^{\text{int}} = P_l^{ext}$, we obtain[1,4]

$$T_l(E) = 1 - |\eta_l|^2 = \frac{-4s_l \Im P_l^{int}}{(\Delta_l - \Re P_l^{int})^2 + (s_l - \Im P_l^{int})^2} \tag{15}$$

where

$$\Delta_l = \Re P_l^{(+)} = R\,\frac{G_l G_l' + F_l F_L'}{G_l^2 + F_l^2}\bigg|_{r=R}, \tag{16}$$

and

$$s_l = \Im P_l^{(+)} = R\,\frac{G_l F_l' - F_l G_L'}{G_l^2 + F_l^2}\bigg|_{r=R}. \tag{17}$$

In the Kim-Zubarev parameterization of $T_l(E)$, $\Im P_l^{\text{int}}$ and $\Re P_l^{\text{int}}$ are to be parameterized directly or in terms of a potential model wave function for the interior region ($r < R$).

4. Reaction Barrier Transparency

We note that the reaction barrier transparency (RBT), $T_l(E) \approx 1$, can occur when $\Delta_l = \Re P_l^{\text{int}}$ and $s_l = -\Im P_l^{\text{int}}$. For simplicity, our discussion in this paper will be limited to the S-wave case, $l = 0$, in the following. Generalization to the $l \neq 0$ cases is straight forward.[4]

For the potential given by eq. (2), a general solution for the interior ($r \leq R$) wave function is

$$u^{int}(r) = e^{-iKr} + c\, e^{+iKr} \tag{18}$$

where $\hbar^2 K^2 / 2\mu = V_0 + E$ with $E = \hbar^2 K^2 / 2\mu$. We introduce two real parameters τ_0 and ϕ_0 and write $c = \tau_0 e^{i\phi_0} (\tau_0 < 1)$.

If the lowest partial wave ($l = 0$) contribution is expected to be dominant for low energies (≤ 20 keV), then the total cross-section $\sigma(E)$ is given by

$$\sigma(E) \approx \sigma_0(E) = \frac{S_0^{KZ}(E)}{E} T_0^{KZ}(E) \tag{19}$$

$$T_0^{KZ}(E) = \frac{-4s_0 \Im P_0^{int}}{(\Delta_0 - \Re P_0^{int})^2 + (s_0 - \Im P_0^{int})^2} = \frac{4s_0 \bar{K}_1 R}{(\Delta_0 - \bar{K}_2 R)^2 + (s_0 + \bar{K}_1 R)^2} \tag{20}$$

where

$$s_0 = R[(G_0 F_0' - F_0 G_0')/(G_0^2 + F_0^2)]_{r=R} = [kR/(G_0^2 + F_0^2)]_{r=R} \tag{21}$$

$$\Delta_0 = R[(G_0 G_0' + F_0 F_0')/(G_0^2 + F_0^2)]_{r=R} \tag{22}$$

$$\bar{K}_1(E, \tau_0, \phi_0) = -\Im P_0^{int} = \frac{K(1 - \tau_0^2)}{1 + 2\tau_0 \cos(2KR + \phi_0) + \tau_0^2} \tag{23}$$

and

$$\bar{K}_2(E, \tau_0, \phi_0) = \Re P_0^{int} = \frac{-2K\tau_0 \sin(2KR + \phi_0)}{1 + 2\tau_0 \cos(2KR + \phi_0) + \tau_0^2} \ . \tag{24}$$

and $T_0^{KZ}(E) = 1 - |\eta_0|^2$ is given by

$T_0^{KZ}(E)$, eq. (20), is described by four parameters, V_0, R, τ_0 and ϕ_0. $T_0^{KZ}(E)$ contains both non-resonance and resonance contributions, and also the interference term between them. The four parameters can be determined from the cross-section containing both a resonance part (resonance energy and width) and a non-resonance background.

We note that $T_0^{KZ}(E) \approx 1$ when RBT condition, $\Delta_0 = \overline{K}_2 R$ and $s_0 \approx \overline{K}_1 R$, is satisfied in eq. (20). The resonance energy E_r (for $T_0^{KZ}(E_r) \approx 1$) and width Γ are determined by the parameters τ_0 and ϕ_0 for fixed values of V_0 and R. The resonance behavior of $T_0^{KZ}(E)$, generated from fitting $\sigma(E)$ with particular values of parameters, is a reaction barrier transparency (RBT) due to an interplay of Coulomb barrier and nuclear interaction, and is to be distinguished from conventional resonances such as narrow neutron ($\Delta_0 = 0$) capture resonances, which are primarily due to the nuclear interaction. The resonances present in $\sigma(E)$, which are shown by some related experiments to be of a non-RBT type, are to be treated by conventional methods. Very broad resonance behaviors for cross-sections observed in many nuclear reactions[6] such as for reactions ^{2}H(D,p)^{3}He, ^{2}H(D,n)^{3}He, ^{3}He(D,p)^{4}He, and ^{3}H(D,n)^{4}He may correspond to RBT resonances and may yield different low-energy extrapolations from those obtained by the use of the conventional transmission coefficient, $T_G(E)$, since the low-energy tail of the RBT resonance is expected to be different from that of the conventional case.

For the case of a non-resonance cross-section, $\tau_0 = 0$, and $T_0^{KZ}(E)$, eq. (20), reduces to the result given by Blatt and Weisskopf[5],

$$T_{BW}(E) = \frac{4s_0 KR}{\Delta_0^2 + (s_0 + KR)^2} \ . \tag{25}$$

It should be noted that $T_{BW}(E)$, eq. (25), does not have a resonance structure while $T_0^{KZ}(E)$ does.

In the previous parameterizations of $\sigma(E)$ the resonance part of $\sigma(E)$ is parameterized with the Breit-Wigner resonance formula to be subtracted from the experimental data[2,3] or included in $S(E)$ in eq. (1).[6] The non-resonance formula, eq. (1), is then used to fit the resultant "data." Our more general formula for $T_0^{KZ}(E)$, eq. (20), with eq. (19), will allow us to parameterize the experimental data exhibiting the RBT resonance behavior by the same formula, eq. (19), thus avoiding separate use of the Breit-Wigner formula for subtracting the resonance contribution from $\sigma(E)$. Furthermore, the interference term between the resonance and non-resonance contributions is automatically included in eqs. (19) and (20). The formulation described by eqs. (9), (15), (19), and (20) is a generalization of eq. (1) and thus can provide a more realistic and general parameterization method for low-energy nuclear fusion cross-sections needed for the solar neutrino and astrophysical calculations, magnetic and inertial confinement fusion calculations, and low-energy (cold) fusion rate calculations.

5. Fusion Rate Estimates with Narrow RBT

Since $\cos(2KR+\phi_0)$ (in eqs. (23) and (24)) and $\sin(2KR+\phi_0)$ (in eq. (23)) satisfies $\cos^2(2KR+\phi_0)+\sin^2(2KR+\phi_0)=1$, τ_0 can be expressed in terms of K, $\bar{K}_1$ and $\bar{K}_2$ as

$$\tau_0^2 = \frac{(K-\bar{K}_1)^2+\bar{K}_2^{\,2}}{(K+\bar{K}_1)^2+\bar{K}_2^{\,2}} \tag{26}$$

For the case of $\bar{K}_2 R = \Delta_0$ and $\bar{K}_1 R = Ns_0$ (RBT condition) where $N > 0$ is a real constant, we obtain using eq. (26)

$$\tau_0^2 = \frac{(KR-Ns_0)^2+\Delta_0^2}{(KR+Ns_0)^2+\Delta_0^2} \tag{27}$$

and

$$1-\tau_0^2 = \frac{4Ns_0KR}{(KR+Ns_0)^2+\Delta_0^2} \tag{28}$$

After determining τ_0 from eq. (27), ϕ_0 can be determined from

$$\sin(2KR+\phi_0) = \frac{1-\tau_0^2}{2\tau_0}\left(\frac{-\Delta_0}{Ns_0}\right) \tag{29}$$

From eq. (20), the maximum value of $t_0^{KZ}(E)$ is then given by

$$T_0^{max}(E) = \frac{4Ns_0^2}{(1+N)^2 s_0^2} = \frac{4N}{(1+N)^2} \tag{30}$$

which yields $T_0^{\max}(E)=1$ for $N = 1$ and $T_0^{\max}(E)<1$ otherwise.

Assuming that $T_0^{KZ}(E)$, eq. (20), has a Breit-Wigner resonance form with a width Γ at a resonance energy $E = E_r$, the width Γ at low energies can be written as[4] $\Gamma \approx \left(s_0(E_r) + \overline{K}_1 R\right) \times 10^7$ eV. Since $s_0(E_r) \approx 0.3 T_G(E_r)$ and $\overline{K}_1 R = N s_0(E_r)$, we obtain for $N >> 1$

$$\Gamma \approx (0.3 \times 10^7 \text{eV})\ N\ T_G(E_r) \tag{31}$$

and

$$T_0^{KZ}(E_r)\Gamma = (1.2 \times 10^7 \text{eV})\ T_G(E_r) \tag{32}$$

using $T_0^{KZ}(E) \approx 4/N$ from eq. (30). Since $T_G(E_r)$ is very small near ambient temperature, $kT = E_r = 0.025\,\text{eV}$, Γ is also very narrow; $\Gamma = 10^{-10}$ eV and $\Gamma = 100^{-100}$ eV for $T_0^{KZ}(E_r) \approx 10^{17} T_G(E_r)$ and $T_0^{KZ}(E_r) \approx 10^{107} T_G(E_r)$, respectively. Precise values of Γ for different fusion reactions can only be determined by experiments at present.

For the fusion cross-section $\sigma(E) \approx S(0) T_0^{KZ}(E)/E\, S(E) \approx S(0) = 53$ keV-barns for $D(D,p)T$ and $D(D,n)^3$He, the fusion rate can be estimated as

$$\begin{aligned} < \sigma v >_{new} &= \int \sigma(v) v f(v)\ d^3 v \\ &= \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \frac{1}{(kT)^{3/2}} \int_0^\infty \sigma(E) E e^{-E/kT} dE \\ &= \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \frac{S(0)}{(kT)^{3/2}} \int_0^\infty T_0^{KZ}(E) e^{-E/kT} dE \\ &\approx \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \frac{S(0)}{(kT)^{3/2}} T_0^{KZ}(E_r) e^{-E_r/kT} \int_{E_r - \frac{\Gamma}{2}}^{E_r + \frac{\Gamma}{2}} dE \end{aligned} \tag{33}$$

or

$$\begin{aligned} < \sigma v >_{new} &\approx \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \frac{S(0)}{(kT)^{3/2}} T_0^{KZ}(E_r) e^{-E_r/kT}\ \Gamma \\ &= \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \frac{S(0)}{(kT)^{3/2}} e^{-E_r/kT}\ T_G(E_r)\ (1.2 \times 10^7\ \text{eV}) \end{aligned} \tag{34}$$

Since the conventional estimate is given by

$$< \sigma v >_{conv} = \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \frac{S(0)}{(kT)^{3/2}} \int_0^\infty T_G(E) e^{-E/kT} dE\ , \tag{35}$$

we can conclude $\langle \sigma \upsilon \rangle_{new} \approx \langle \sigma \upsilon \rangle_{conv}$ for the equilibrium Maxwell-Boltzmann distribution $f(\upsilon)$ at ambient temperature of $kT \approx 0.025$ eV. However, non-equilibrium energy sweeping through the narrow RBT may result in a greatly enhanced fusion rate[7] as in cold fusion experiments. Recent observations[8-11] of anomalous neutron bursts during thermal cycling with deuterated high T_C superconducting materials may be attributable to energy sweeping involving a non-equilibrium state during the superconducting phase transition.

6. RBT Mechanism for Other Fusion Reactions

In view of our new result $T_0^{KZ}(E)$, eq. (20) or $T_l\ (E)$, eq. (15), it is appropriate to ask whether some fusing systems can support an RBT at low energies near the fusion threshold. This can only be answered at present by experiments. It should be emphasized that RBT cold fusion is possible not only with deuterium but also with hydrogen since $T_0^{KZ}(E)$, eq. (20), is applicable to both cases as long as the RBT exist in fusing systems involving deuterium or hydrogen, such as in nuclear fusion reactions with the entrance channels, *D* + *D*, *D* + *Li*, *D* + *Pd*, *H* + *D*, *H* + *K*, etc.

Given the RBT mechanism for cold fusion the question remains why fusion products are observed in cold fusion experiments at a much lower level than commensurate with the observed excess heat. This question can only be addressed separately for each fusion reaction since the exit channels are different for each reaction. The anomalous excess heat and tritium production reported in many electrolysis or similar experiments may not be due to *D* - *D* fusion, but may include nuclear fusion with hydrogen and/or impurity nuclei which are always present. This scenario and others such as ${}^{6}Li(d,p)^{7}Li$, ${}^{7}Li(d,{}^{4}He)^{5}He$, etc. may explain the results of excess heat, tritium and neutron production observed in heavy water(with *Li*) electrolysis experiments. Scenarios for other cases involving both deuterium and hydrogen may be possible and need to be investigated.

7. Summary and Conclusion

Our progressively more generalized parametric representation of Coulomb barrier tunneling yields significant improvements upon the conventionally used Gamow tunneling coefficient. This analysis yields RBT which is due to the interaction of the transmitted and reflected quantum waves yielding constructive interference in a narrow energy regime. RBT appears to have important ramifications for cold fusion.

References

1. Y. E. Kim and A. L. Zubarev, “Coulomb Barrier Transmission Resonance for Astrophysical Problems”, Purdue Nuclear Theory Group Report PNTG-93-8 (August 1993), to be published in Modern Physics Letters B.
2. W. A. Fowler, G. R. Caughlan, and B. A. Zimmermann, “Thermonuclear Reaction Rates”, Annual Review of Astronomy and Astrophysics, 5, 525 (1967).
3. Y. E. Kim, M. Rabinowitz, J.-H. Yoon, and R. A. Rice, International Journal of Theoretical Physics, **32**, 301 (1993).
4. Y. E. Kim and A. L. Zubarev, “P-Matrix Parameterization of S-Matrix for Fusion Reaction Cross-Section”, Purdue Nuclear Theory Group Report PNTG-94-8 (1994), to be published.
5. J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics*, Wiley, New York (1952), Chapter VIII.
6. G. S. Chulick, Y. E. Kim, R. A. Rice, and M. Rabinowitz, “Extended Parameterization of Nuclear-Reaction Cross Section for Few-Nucleon Nuclei”, Nuclear Physics, **A551,** 255 (1993).

7. Y. E. Kim, “Time-Delayed Apparent Excess Heat Generation in Electrolysis Fusion Experiments”, Mod. Phys. Lett. 6, 1053 (1991).
8. F. Celani et al., “Search for Neutron Emission from Deuterated High Temperature Superconductors in a Very Low Background Environment”, Proc. of the Second International Conference on Cold Fusion, Como, Italy, June 6-July 4, 1991 (Italian Physical Society Conference Proceedings, Vol. 33), p. 113.
9. F. Celani et al., “Measurements in the Gran Sasso Laboratory: Evidence for Nuclear Effects in Electrolysis with *Pd/Ti* and in Different Tests with Deuterated High Temperature Superconductors”, AIP Conf. Proc. No. 228 (1991), p. 62.
10. G. Lipson et al., “Possible Cold Nuclear Fusion in Deuterated Ceramic $YBa_2Cu_3O_{7-x}$“, Sov. Phys. Dokl. 36, 849 (1991).
11. G. Lipson et al., “Neutron Generation in $YBa_2Cu_3O_{7-\delta}D_y$ High Temperature Superconductors Stimulated by a Superconducting Phase Transition”, Sov. Phys. Dokl. 38, 119 (1993).