Simple model for accurate calculation of Coulomb-barrier penetration factors in molecular fusion rates

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We have developed a simple model that yields an approximate analytical expression for the Coulomb-barrier penetration factor in terms of the reduced mass M of the nucleon pair, the mass m of the particle that binds together the nuclei, the inner turning point r_i for the state under consideration, and the variation in the electronic or muonic contribution $E_e(r)$ to the total energy between $r=0$ and r_i. In the case of muon-catalyzed $d+t\rightarrow\alpha+n$ fusion, our model yields fusion rates within 25% of those obtained from much more elaborate calculations. The remarkable accuracy of our simple model results from the fact that it is highly accurate for small r, the region that we demonstrate makes the predominant contribution to Coulomb-barrier penetration factors. Furthermore, we use this observation to explain the old puzzle of why the adiabatic approximation yields such accurate fusion rates.

The claims of having achieved "cold fusion" in the electrolysis of D_2O using palladium or titanium cathodes[1,2] precipitated a large number of theoretical studies of d-d fusion rates, both for gaseous D_2 (Refs. 3 and 4) and for deuterium in metals.[5] The overwhelming consensus of these theoretical studies, as well as the vast majority of experimental studies,[6] is that "cold fusion" in the electrolysis of D_2O is unlikely to exist.

In our own work soon after the announcements,[1,2] we developed a simple analytical model to calculate fusion rates for high-lying vibrational states of D_2, which agree remarkably well with much more elaborate theoretical calculations.[3] Although interest in electrolytic "cold fusion" is on the wane, there is continuing interest in the very real subject of muon-catalyzed fusion,[7] in which fusion proceeds through various states of the $(dd\mu)^+$ and $(dt\mu)^+$ molecular ions. Hence we believe it is worthwhile to present our model, which allows the "back-of-the-envelope" calculation of muonic fusion rates within 25%. Such a simple yet reliable method is of considerable importance in the ongoing studies[8] of fusion from resonant states of the $(dt\mu)^+$ molecular ion. Achieving convergence of the fusion rate in a three-body calculation on such diffuse states requires the use of quite large bases in the variational calculation of the resonant wave function, and if the basis is insufficiently flexible, the calculated fusion rates can be wrong by many orders of magnitude. In contrast, the analytical results from our simple model are much more reliable, in the sense that they are likely to be accurate within 25%. This is about as accurate a calculation as one can hope to do because of uncertainties in the details of the nucleon-nucleon interaction at distances of 1–10 fm, and the nonseparability of nuclear force effects.

Our analysis is built upon the fundamental article of Jackson[9] on muon-catalyzed fusion. We have also profited from the article by Zeldovich and Gershtein[10] on this topic. The idea of studying a simple analytical model was inspired by a relatively recent article by van Siclen and Jones[11] on fusion rates for D_2 and D_2^+. In the course of reading this article, we realized that the replacement of their rather crude approximation to the internuclear potential with a more realistic yet still tractable approximation would lead to vastly improved estimates of fusion rates.

All our analysis is carried out within the adiabatic approximation, which even in the case of muon-catalyzed fusion, where $m/M\simeq\frac{1}{9}$, yields very accurate fusion rates.[3] Following Jackson, the fusion rate can be written as

$$\Lambda_f = A|\psi(0)|^2 , \tag{1}$$

with

$$\psi(0)=\left[\frac{m}{a_0}\right]^{3/2}\frac{1}{\sqrt{4\pi}}\lim_{r\rightarrow 0}\frac{u(r)}{r} , \tag{2}$$

where m is the mass of the negatively charged particle in units of the electron mass m_e, a_0 is the Bohr radius, A is the nuclear reaction constant, and $u(r)$ is the radial wave function ($\hbar=1$ is assumed here and elsewhere). Within the WKB approximation, as modified by Langer to account for the "hard wall" at $r=0$,

$$u_{\mathrm{WKB}}(r)=\begin{cases} N|Q(r)|^{-1/2}\exp\left[-\int_r^{r_i'}|Q(r')|dr'\right] & \text{for } r<r_i' , \\ 2N[Q(r)]^{-1/2}\cos\left[\int_{r_i'}^{r}Q(r')dr'-\frac{\pi}{4}\right] & \text{for } r_i'<r<r_o' , \end{cases} \tag{3}$$

where r_i' and r_o' are the inner and outer zeros of

$$Q^2(r)=-\frac{1}{4r^2}+2M[E-V(r)] , \tag{4}$$

and the normalization constant N for a bound state is given by

$$N=\left[2\int_{r_i'}^{r_o'}[Q(r)]^{-1}dr\right]^{-1/2} . \tag{5}$$

[For a simple harmonic oscillator, $N=(M\omega/2\pi)^{1/2}$, where for the electronic or muonic ground state of isotopically substituted H_2 the dependence of ω on the nucleon-nucleon reduced mass is given by $\omega=0.603(m/M)^{1/2}$, and for H_2^+ it is given by $\omega=0.302(m/M)^{1/2}$.] Furthermore, Jackson[9] showed that

$$\lim_{r\to 0}\frac{u_{\mathrm{WKB}}(r)}{r}=N\exp(-\lambda/2) , \tag{6}$$

where

$$\lambda=\lambda(0)=\int_0^{r_i'}\left[2|Q(r)|-\frac{1}{r}\right]dr+\ln\left[\frac{r_i'}{2ma_0}\right] . \tag{7}$$

Thus within the WKB-Langer approximation the fusion rate for a bound state is given by

$$\Lambda_f=A\left[\frac{m}{a_0}\right]^3\frac{N^2}{4\pi}\exp(-\lambda) . \tag{8}$$

The use of this expression is appropriate in a case where fusion proceeds primarily through a few well-separated discrete states (e.g., conventional muon-catalyzed d-t fusion occurs mainly from the $J=0$, $v=0$ state and the $J=0$, $v=1$ state). If the fusion proceeds primarily from a manifold of degenerate or nearly degenerate states, one should multiply the right-hand side of Eq. (8) by the density of $J=0$ states $d\mathcal{N}/dE$. In the WKB-Langer approximation, the quantization condition is

$$\mathcal{N}(E)+\tfrac{1}{2}=\frac{1}{\pi}\int_{r_i'}^{r_o'}Q(r)dr , \tag{9}$$

so that

$$\frac{d\mathcal{N}}{dE}=\frac{1}{\pi}\int_{r_i'}^{r_o'}\frac{dQ}{dE}dr+\frac{Q(r_o')}{\pi}\frac{dr_o'}{dE}-\frac{Q(r_i')}{\pi}\frac{dr_i'}{dE} . \tag{10}$$

Since $Q(r_o')=0=Q(r_i')$, and $dQ/dE=M/Q$, it follows that

$$\frac{d\mathcal{N}}{dE}=\frac{M}{\pi}\int_{r_i}^{r_o'}[Q(r)]^{-1}dr=\frac{M}{2\pi}\frac{1}{N^2} , \tag{11}$$

which contains an N^{-2} that cancels the N^2 in Eq. (8). Thus, if fusion occurs from a manifold of closely separated bound states, the fusion rate per unit energy $d\Lambda_f/dE$ is given by

$$\frac{d\Lambda_f}{dE}=A\left[\frac{m}{a_0}\right]^3\frac{1}{4\pi}\frac{M}{2\pi}\exp(-\lambda) . \tag{12}$$

This formula also applies to fusion from continuum (scattering) states, as can be shown by first putting the system in a box and then taking the walls to infinity. [In this case, $Q(r_o')\neq 0$, but $dr_o'/dE=0$; therefore, the surface terms in Eq. (10) still vanish.]

Since in our work we shall be concerned with values of M that are at least an order of magnitude larger than the mass m of the negatively charged particles that bind together the nuclei, in the calculation of the barrier penetration exponent λ it makes no significant difference if we replace the inner turning point r_i' of $Q^2(r)$ with the classical inner turning point r_i, for which $V(r_i)-E=0$. Similarly, in the calculation of the normalization constant N, it makes no significant difference if we replace the turning points r_i' and r_o' of $Q(r)$ with the classical turning points r_i and r_o of $k(r)=\{2M[E-V(r)]\}^{1/2}$, provided that in the integral $Q(r)$ is replaced with $k(r)$. Indeed, it has been argued that the most accurate results can be obtained by the seemingly inconsistent procedure of including the Langer correction in the calculation of the barrier penetration factor, but dropping it in the evaluation of properties, such as the energy and the normalization constant, which are determined by integration over the classically allowed region.[12]

In the expression *supra*, the range of the nuclear force has been taken to be infinitesimally small. In fact, the effect of the small but nonzero range r_N of the nuclear force on the barrier penetration factor λ is quite small. Since for very small r

$$2|Q(r)|-\frac{1}{r}\simeq r4M[V(r)-E]\simeq 4M , \tag{13}$$

the effect of the nonzero range of the nuclear force on λ is

$$\lambda(r_N)-\lambda(0)\simeq -4Mr_N . \tag{14}$$

With $r_N\simeq 5$ fm $\simeq 10^{-4}$ electronic a.u. and M on the order of $(1\text{–}2)\times 10^3$ (in units of m_e), the nonzero nuclear size effect on λ typically does not exceed 1, which increases the barrier penetration probability by less than a factor of 3. This effect can, of course, be included simply by the addition of the correction (14) to our final results.

Our next task is to find a reasonably accurate approximation to $V(r)$ which permits the analytic evaluation of the λ integral in Eq. (7). For small r, $V(r)$ of course

behaves like $1/r$, the Coulomb repulsion energy for the pair of hydrogen isotopes, plus the electronic or muonic energy, which is due to the motion of the electron or muon in the field of two hydrogen nuclei and whatever other atoms and molecules may be present. If for short distances the variation in the electronic or muonic energy can be assumed relatively small, then we can approximate $V(r)-E$ by

$$V_0(r)-E=\frac{1}{r}-\frac{1}{r_i} , \tag{15}$$

which vanishes, of course, at the classical inner turning point r_i. Then

$$|Q(r)|\simeq\frac{1}{r}\left[\frac{1}{4}+2Mr_i\left[\frac{r}{r_i}-\frac{r^2}{r_i^2}\right]\right]^{1/2} , \tag{16}$$

and in this approximation the λ integral in Eq. (7) can now be evaluated in closed form. For $Mr_i\gg 1$, we obtain

$$\lambda=\pi\sqrt{2Mr_i}-2-\ln(4M/m)+O(1/(Mr_i)) , \tag{17}$$

so that in this simple approximation the barrier penetration factor is proportional to

$$e^{-\lambda}\simeq 4\frac{M}{m}\exp[-(\pi\sqrt{2Mr_i}-2)] . \tag{18}$$

The zero-order approximation (17) is capable of improvement. Since

$$V(r)=\frac{1}{r}+E_e(r) , \tag{19}$$

where $E_e(r)$ is the electronic or muonic energy in the Born-Oppenheimer approximation,

$$V(r)=\frac{1}{r}+E_e(r_i)+E_e(r)-E_e(r_i) . \tag{20}$$

Hence

$$V(r)-E=\frac{1}{r}-\frac{1}{r_i}+\Delta E_e(r) , \tag{21}$$

where $\Delta E_e(r)=E_e(r)-E_e(r_i)$ can be treated perturbatively in Eq. (7). Thus to first order,

$$\begin{aligned}|Q(r)|&=\left[\frac{1}{4r^2}+2M[V(r)-E]\right]^{1/2}\\&=\left[\frac{1}{4r^2}+2M[V_0(r)-E]+2M\Delta E_e(r)\right]^{1/2}\\&\simeq\left[\frac{1}{4r^2}+2M[V_0(r)-E]\right]^{1/2}\\&\quad+M\Delta E_e(r)\left[\frac{1}{4r^2}+2M[V_0(r)-E]\right]^{-1/2} .\end{aligned} \tag{22}$$

By examining the first term in a Taylor-series expansion of (21) about $r=r_i$,

$$\begin{aligned}V(r)-E&=\frac{1}{r}-\frac{1}{r_i}+E_e(r)-E_e(r_i)\\&\simeq-\frac{r-r_i}{r_i^2}+(r-r_i)E_e'(r_i) ,\end{aligned} \tag{23}$$

one can see that as long as r_i is not too close to the equilibrium separation $r_{\rm eq}$ [at which point the two terms in (23) would become equal, and hence the perturbation $\Delta E_e(r)$ would become comparable to the unperturbed potential $V_0(r)-E$], the first-order approximation (22) will be reasonably accurate even close to r_i, and its accuracy improves for smaller r. Since in the electronic case fusion from highly excited vibrational states is orders of magnitude more probable than from low-lying states,[3] and in the muonic case even the ground vibrational state of $(dt\mu)^+$ lies nearly halfway up the well, with $r_i=1.363$ a.u. and $r_{\rm eq}=1.997$ a.u., for the relevant states the assumption that r_i is well away from $r_{\rm eq}$ is justified. If $\Delta E_e(r)$ is represented by a polynomial in r, the integral of the last term in Eq. (22) can again be done in closed form. In the case of a linear approximation,

$$\begin{aligned}\Delta E_e(r)&\simeq[E_e(0)-E_e(r_i)](1-r/r_i)\\&=\Delta E_e(1-r/r_i) ,\end{aligned} \tag{24}$$

we obtain

$$\begin{aligned}\lambda=&(\pi\sqrt{2Mr_i}-2)(1+\tfrac{1}{8}\Delta E_e r_i)\\&-\ln(4M/m)+O(1/(Mr_i)) ,\end{aligned} \tag{25}$$

so that in this first-order approximation,

$$e^{-\lambda}\simeq 4\frac{M}{m}\exp[-(\pi\sqrt{2Mr_i}-2)](1+\tfrac{1}{8}\Delta E_e r_i)] . \tag{26}$$

We therefore see that the effect of the linear approximation to the decrease in the electronic energy is to reduce the constant in the exponential by a factor of $\frac{1}{8}\Delta E_e r_i$. Systematic higher-order approximations can, of course, be carried out. But even the simple approximation (25) is already very useful. If the linear approximation (24) to $E_e(r)$ is rather accurate, as it is for the ground electronic or muonic state of H_2 for r_i between 0.2 and 1.0 a.u./m, or for the ground electronic or muonic state of H_2^+ for r_i less than 1.5 a.u./m, then Eq. (25) is capable of giving quite good results. For example, in the electronic case, for the $J=0$, $v=20$ excited vibrational state of D_2, for which $M=1835$, $E=-1.0006$ a.u., and $r_i=0.77652a_0$, we find that

$$\begin{aligned}\Delta E_e&=E_e(0)-E_e(r_i)\\&=-2.9037-(E-1/r_i)=-0.6153 .\end{aligned} \tag{27}$$

From Eq. (25) we obtain the approximation

$$\lambda\simeq 146.9 , \tag{28}$$

which agrees quite nicely with the more accurate value of

$$\lambda=145.06 , \tag{29}$$

obtained by integration using the full Born-Oppenheimer

potential[3] in Eq. (7). This yields a fusion rate smaller by a factor of about $e^{1.9} \simeq 6.7$ than the adiabatic fusion rate of about 3×10^{-56} sec^{-1}.[3]

For muonic molecular ions, the much smaller value of $Mr_i = (M/m) m r_i$ leads to even more accurate results. For the muonic molecular ion $(dt\mu)^+$, we have employed the Born-Oppenheimer approximation with the diagonal adiabatic correction term, which includes effects through $O(m/M)$. The muon mass is $206.77 m_e$, the deuteron mass is $3670.5 m_e$, and the triton mass is $5496.9 m_e$, which yield a d-t reduced mass $M = 2200.9 m_e$ and a d-t total mass of $9167.4 m_e$. Our colleague, K. Szalewicz, has obtained for the $J=0$, $v=0$ state and the $J=0$, $v=1$ state the fusion parameters listed in Table I. With

$$E_e(0) = \left[-\frac{m_d + m_t}{m_\mu + m_d + m_t} \right] 2.0 \text{ muonic a.u.} ,$$
$$= (-0.978)2.0 \text{ muonic a.u.} ,$$
$$= -1.956 \text{ muonic a.u.} , \quad (30)$$

for the $v=0$ state we find that

$$\Delta E_e = E_e(0) - E_e(r_i) ,$$
$$= -1.956 - (E - 1/r_i) ,$$
$$= -0.680 \text{ muonic a.u.} , \quad (31)$$

and for the $v=1$ state we find that

$$\Delta E_e = -0.598 \text{ muonic a.u.} \quad (32)$$

The use of these values of ΔE_e and the appropriate values of r_i and M/m in Eq. (26) yields the estimates

$$e^{-\lambda} \simeq 4(10.64)\exp(-13.19)$$
$$\simeq 7.96 \times 10^{-5} \quad (33)$$

for the $v=0$ state, and

$$e^{-\lambda} \simeq 4(10.64)\exp(-12.41)$$
$$\simeq 1.74 \times 10^{-4} \quad (34)$$

for the $v=1$ state. Use in Eq. (8) of these values of $e^{-\lambda}$, the normalization constants N^2 from Table I, and $A = 1.2 \times 10^{-14}$ cm^3 sec^{-1} for the intrinsic $d + t \rightarrow \alpha + n$ fusion rate constant[13] yields values of the fusion rate Λ_f shown in Table II, along with the more accurate fusion rates obtained by (i) the evaluation of the λ integral in the WKB-Langer approximation with the full Born-Oppenheimer plus adiabatic correction potential, (ii) the numerical solution of the Schrödinger equation using the full Born-Oppenheimer plus adiabatic correction potential, and (iii) the solution of the three-body Schrödinger equation in a large basis-set calculation. One sees that even for the least favorable case of the ground state, our approximate result is within 25% of that obtained by method (i), and fortuitously happens to agree even better with the progressively more exact values obtained by methods (ii) and (iii). For the $v=1$ excited state, the agreement is somewhat better.

TABLE I. Molecular parameters for the $J=0$, $v=0$ state and the $J=0$, $v=1$ state of the $(dt\mu)^+$ molecular ion. The energy E was obtained by accurately solving the Schrödinger equation for the Born-Oppenheimer plus adiabatic correction potential.

v	E (muonic a.u.)	r_i (muonic a.u.)	N^2
0	−0.542 630	1.363	0.122 225
1	−0.491 391	1.154	0.052 182 6

TABLE II. Fusion rates in sec^{-1} for the $J=0$, $v=0$ state and the $J=0$, $v=1$ state of $(dt\mu)^+$, as calculated using our Eqs. (30)–(34) and compared with fusion rates obtained by (i) evaluation of the WKB-Langer λ integral in Eq. (7) using the Born-Oppenheimer plus adiabatic correction potential, (ii) accurate numerical solution of the Schrödinger equation using the Born-Oppenheimer plus adiabatic correction potential, and (iii) solution of the three-body Schrödinger equation in a large basis.

v	This work	(i)	(ii)	(iii)
0	0.55×10^{12}	0.70×10^{12}	0.66×10^{12}	0.63×10^{12}
1	0.52×10^{12}	0.65×10^{12}	0.57×10^{12}	0.53×10^{12}

Such astoundingly accurate results from such a simple "back-of-the-envelope" calculation might well seem to call for an explanation. The key is that the dominant contribution to the λ integral in Eq. (7) comes from values of r between 0 and a few tenths of an a.u., where the actual $V(r) - E$ is extremely well represented by our approximation

$$\frac{1}{r} - \frac{1}{r_i} + \left[1 - \frac{r}{r_i} \right] \Delta E_e , \quad (35)$$

which also correctly tends to 0 as $r \rightarrow r_i$. This approximation is relatively less accurate for r between a few tenths of an a.u. and r_i, but over this region the integrand is rather small. Thus the region where our approximation is relatively less accurate contributes relatively little to the λ integral.

The above analysis should serve to correct the argument, which widely circulated in the aftermath of the "cold fusion" announcements,[1,2] that barrier penetration integrals are primarily determined not by the small-r but by the large-r behavior of the integrand. According to this argument, in the WKB approximation (which really should be modified by the Langer correction),

$$\lambda_{\text{WKB}} = 2\sqrt{2M} \int_0^{r_i} [V(r) - E] dr , \quad (36)$$

so with $V(r) - E \simeq 1/r$,

$$\lambda_{\text{WKB}} \simeq 2\sqrt{2M} \int_0^{r_i} \frac{dr}{r^{1/2}} , \quad (37)$$

and $\int dr\, r^{-1/2}$ is convergent as $r \rightarrow 0$, but divergent for large r. The last statement is true but not relevant, since as $r \rightarrow r_i$ the integrand in (36) tends not to $1/r_i^{1/2}$ but to 0, which greatly reduces the contribution to the integral from the region where r is a few tenths of an a.u. less than r_i. Using our zeroth-order approximation (15) in Eq. (36), we obtain

$$\lambda_{\rm WKB} \simeq 2\sqrt{2M}\int_0^{r_i}\left[\frac{1}{r}-\frac{1}{r_i}\right]^{1/2} dr = \pi\sqrt{2Mr_i}\ . \qquad (38)$$

To illustrate how much the small-r region and how little the large-r region contribute to this integral, we show in Table III the values of the normalized integral

$$\frac{1}{\pi\sqrt{2Mr_i}}2\sqrt{2M}\int_0^{r}\left[\frac{1}{r'}-\frac{1}{r_i}\right]^{1/2} dr'$$
$$= \frac{2}{\pi}\left\{\arcsin\left[\frac{r}{r_i}\right]^{1/2} + \left[\frac{r}{r_i}\left[1-\frac{r}{r_i}\right]\right]^{1/2}\right\} \qquad (39)$$

for some representative values of r/r_i. One sees the remarkable fact that the tiny region near the nuclear coalescence where $0 \le r/r_i \le 0.01$ contributes more to the integral than the wide region below the turning point where $0.60 \le r/r_i \le 1.00$. The inclusion of the linear approximation (24) to the change in $E_e(r)$ would further reduce the integrand and hence the relative contribution from the region near the turning point r_i. Since M/m is of the order of 10 or larger, the inclusion of the Langer correction would leave unchanged the qualitative features of this analysis.

The predominant contribution of the small-r region to the λ integral and hence to the fusion rate provides an understanding of why even for a relatively large value of m/M such as $\frac{1}{10}$ the adiabatic approximation yields such accurate fusion rates. Nonadiabatic effects are relatively largest when all three interparticle distances are comparable, and relatively smallest when one interparticle distance is much less than the other two. Hence the fusion rate, which is primarily determined by the behavior of the wave function for very small internuclear distances, is very well approximated by the adiabatic fusion rate, with discrepancies of only a few percent for the (00) and (01) states of $(dt\mu)^+$. In contrast, the sticking fractions for these states are primarily determined by the behavior of the $(dt\mu)^+$ wave function where the two nuclei have coalesced and the muon is also quite close to them,[14] so that the nonadiabatic effects alter these sticking fractions by about 20%.

In summary, we have developed a simple approximation, capable of systematic improvement, to the internuclear potential, which permits the accurate evaluation of Coulomb-barrier penetration probabilities and hence of fusion rates in muon-catalyzed fusion. Even in the least favorable case of the $J=0$, $v=0$ ground state of $(dt\mu)^+$, it yields a fusion rate within 25% of more exact values, and its accuracy improves for states of higher energy. We expect that it will be useful in a wide variety of circumstances, including the calculation of fusion rates for resonant states of $(dt\mu)^+$. We have shown that the remarkable accuracy of our approximation is a consequence of the under-appreciated fact that the predominant contribution to a Coulomb-barrier penetration integral comes from the small-r region. Moreover, we have used this fact to answer the long-standing question of why the adiabatic approximation to fusion rates is so accurate in muon-catalyzed fusion, where the Born-Oppenheimer parameter $\kappa=(m/M)^{1/4}\simeq\frac{1}{2}$ is certainly not small.

TABLE III. The contributions to the λ integral in the WKB approximation for $0 \le r \le r_i$.

r/r_i	$\int_0^r\left[\frac{1}{r'}-\frac{1}{r_i}\right]^{1/2}dr' \Big/ \int_0^{r_i}\left[\frac{1}{r'}-\frac{1}{r_i}\right]^{1/2}dr'$
0.00	0.000
0.01	0.127
0.05	0.282
0.10	0.396
0.20	0.550
0.30	0.661
0.40	0.748
0.50	0.818
0.60	0.876
0.70	0.922
0.80	0.959
0.90	0.986
1.00	1.000

Note added in proof. The fusion rates for the $3/2^+$ state of $dt\mu$ recently calculated by K. Szalewicz *et al.*, Phys. Rev. A **42**, 3768 (1990), differ from those in our Table II because of a factor of $\frac{3}{2}$ for spin symmetry and a slightly different nuclear reaction constant A. Since these factors are multiplicative, they of course do not effect any of our relative comparisons.

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