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Is “friction” responsible for the reduction of fusion rates far below the Coulomb barrier?

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Abstract

Observed rates of the fusion of interacting heavy ions well below the Coulomb barrier are considerably lower than estimates obtained from penetration factors. An interpretation of this discrepancy has been in terms of tunnelling in semiclassical models, with the observed depletion being taken as evidence of a “friction” under the barrier. An extension of that approach is to consider tunnelling in fully quantal models. We consider tunnelling in one-dimensional models to investigate possible sources for such a friction. Under certain conditions, we find that tunnelling may be enhanced or diminished by up to 50%, which finds analogy with observation, without the invocation of a friction under the barrier.

Fusion reactions near the Coulomb barrier play a large part in nucleosynthesis in the Big Bang and stellar environments. Theoretical understanding is necessary given that most of these reactions, required as input in nucleosynthesis models, may not be measured in the laboratory due to the very small cross sections involved.

For reactions far below the Coulomb barrier (see, for example, [1,2]), measured fusion cross sections are considerably lower compared to their estimates from penetration factors. Normally, the conjecture is that an energy loss has occurred under the Coulomb barrier. Intuitively, that loss may be understood as a “friction” [3], accounting for coupling to other reaction channels. An alternative postulate (see [1], for example) is that the nucleus-nucleus optical potential involved in fusion processes may require a much larger diffuseness than that for elastic scattering. But that approach may be problematic given that the coupling of the nonelastic and elastic channels in the nucleus-nucleus interaction should be specified self-consistently. The role of breakup in the depletion of fusion has also been investigated [4], wherein fusion involving weakly bound nuclei may be diminished by up to 35%. Herein, we investigate the tunneling hypothesis and the notion of a “friction”.

The invocation of a friction is a result of the use of semi-classical models. It is an alternative to the purely quantal nature of tunneling. The kinetic energy under a barrier should be negative and time under the barrier must be made imaginary, or at least complex, to compensate for the classical anomaly. That is essential if a position and velocity are to be used as measures of the propagation of the fusing ions under the barrier. In such an analytic continuation of classical physics to complex trajectories and complex time, can one then contemplate a random Langevin force to describe this friction? For a simpler understanding of the (quantal) real time processes, a fully quantal model of tunneling is necessary.

Herein we shall not follow the approach of Caldeira and Leggett [3] (see also [5,6]) in which the tunneling degree of freedom is coupled to a bath of harmonic oscillators. From that approach, a conclusion was drawn that a loss of transmission occurs. But recent studies [7–9] show that for some chaotic potentials, barrier penetration in fact is enhanced. Thus we seek a more pedagogical approach recognizing that, if Langevin processes exist to account for friction, the effective potential experienced by the tunneling particle will not be smooth. Thus we wish to study tunneling through rough potentials *in real time*.

Herein, to facilitate such an investigation, we construct models where wave packets are prepared far from the barrier. These will be broad packets having few (if any) components with energy higher than the barrier. Such packets are boosted toward the barrier and we use the time-dependent Schrödinger equation (TDSE) as the equation of motion. *A priori*, we shall use two (non-equivalent) approaches, namely

- (i) space fluctuations of a time independent barrier, and
- (ii) time fluctuations of a spatially smooth barrier.

The potentials of case (i) may induce enough incoherence in the wave propagation to trigger some localization [10] so diminishing the transmission. Either case may represent couplings to other channels.

Our one-dimensional model assumes spatially even barriers of the type

$$V(x, t) = v(t) \exp(-2\omega x^2) \quad (1)$$

for which the TDSE is

$$i\hbar \frac{\partial \Psi}{\partial t} = \left\{ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V(x, t) \right\} \Psi. \quad (2)$$

Arbitrarily we have chosen $\omega = 0.5$ and, for our reference model, $v(t) = 1$.

The problem could be intractable as there are four conflicting considerations, namely:

- (1) Gaussian wave packets, or quasi-Gaussian ones, are required to maintain an analogy of classical particles with maximally well-defined positions and velocities as far as is possible. But
- (2) under the barrier the wave will certainly not be Gaussian and at best one might observe probability bumps. Then
- (3) wave packets must be broad enough to avoid excessive zero-point energies, but
- (4) the same packets, or their bumps if any, should be narrower than the width of the barrier if the particles are to be localized within the barrier.

These problems will be addressed as necessary below.

Given the precise determination of the energies of projectiles in experiment, realistic wave packets must be initiated significantly broader than the barrier. Our even barrier [Eq. (1)] is centered at the origin with a width of order 1. For the one-dimensional problem, we choose an initial wave packet of the form

$$\Psi_I(x, 0) = \pi^{-1/4} \exp\{-ax^2 - bx - c\}, \quad (3)$$

where the initial parameters are $a_0 = 1/(2\lambda_0^2)$, $b_0 = 3/\lambda_0 - iK$, and $c_0 = (\ln \lambda_0)/2 + 9/2$, with $\lambda_0 = 5$ being the initial width of the packet. The momentum of the packet is given by K and the subscript indicates that the packet moves from the left (negative values of x). With these choices the initial packet also has the form

$$\Psi_I(x, 0) = \frac{\pi^{-1/4}}{\sqrt{5}} \exp \left[-\frac{(x+15)^2}{50} + iKx \right]. \quad (4)$$

Typically, $0.3 \leq K \leq 1.3$ whence the kinetic energy ($K^2/2$) is well below the height of the barrier. With initial momentum $K \sim 1$ and similar orders of

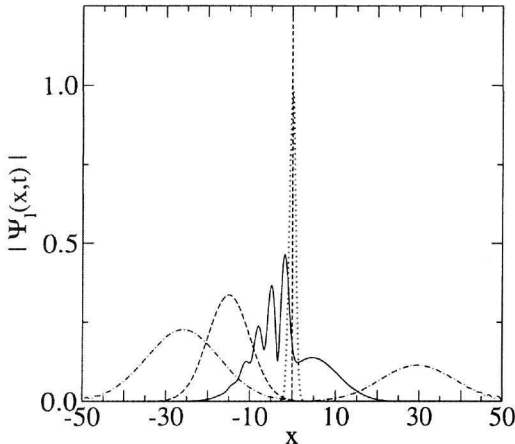


Fig. 1. Modulus of the wave packet $|\Psi_l(x, t)|$ at times $t = 0$ (dashed line), 18 (solid line), and 40 (dot-dashed line). The potential is portrayed by the dotted line.

magnitude for all parameters, the packet will collide with the barrier typically at times $\sim 10/K$, the penetration reaching its peak at $\sim 15/K$, and full transmission and reflection should be complete by $\sim 30/K$.

Taking the Hamiltonian as $H = -\partial^2/(2\partial x^2) + e^{-x^2}$, the modulus $|\Psi_l(x, t)|$ of the wave packet is shown in Fig. 1 at times $t = 0, 18$, and 40, for the momentum $K = 1.06$. The potential is frozen in time with $v(t) = 1$. The energy is 0.571834 which includes the zero point kinetic energy (0.01) and a small contribution from the potential energy (0.000034); the latter due to the overlap of the tails of the potential and initial wave packet. The energy of the colliding packet is slightly above half the barrier height.

The difference between the negative and positive sides of the packet at $t = 18$ is most telling. The modulus for negative values of x shows clearly the interference between the incoming and reflected waves while that on the positive- x side exhibits a good fraction of the transmitted packet. At $t = 40$ we clearly observe two distinct *Gaussian* packets corresponding to the reflected and transmitted waves. The shapes of the reflected and transmitted waves have been effectively restored to the original Gaussian shape, with no memory of the interaction with the potential.

We display in Figs. 2 to 5, the transmitted norm of the wave Ψ_l . The transmitted norm is defined as a function of time as

$$T(t) = \int_5^\infty |\Psi_l(x, t)|^2 dx. \quad (5)$$

The lower bound in the integral, $x = 5$, is chosen to be far enough away from the barrier to ensure no contamination of the transmitted wave by the barrier. We are also interested in the asymptotic value of the transmitted

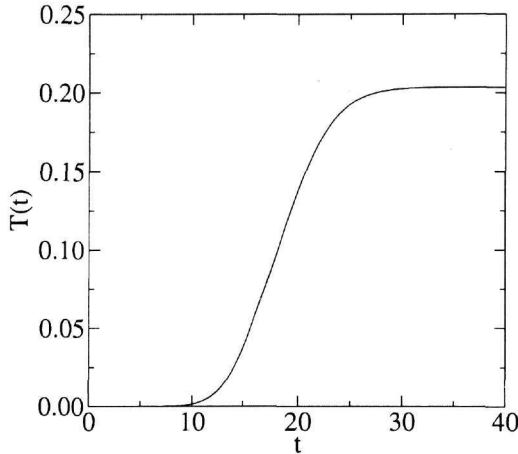


Fig. 2. Transmitted norm $T(t)$ for the case $K = 1.06$ and for the reference potential. norm, $T(\infty)$. This observable is also important for comparisons of different potentials. Fig. 2 shows the case for the reference potential, $V(x) = e^{-x^2}$, with $K = 1.06$. The asymptotic value for this case is $T(\infty) = 0.203$ confirming the earlier observation of 20% transmission for the wave with $K = 1.06$.

Given the same starting wave packet as in Eq. (3), transmission through a barrier $V_1(x)$ will be less than that through barrier $V_2(x)$ if $V_1(x) > V_2(x)$, $\forall x$. Details of the shape of the incident packet may change this result. But we assume packets to be close to eigenstates, for which theorems bounding growth and curvatures of waves in relation to the potential hold. To investigate deviations from this estimate, we compare results for potentials where $V_1(x) > V_2(x)$ for some x , and $V_1(x) < V_2(x)$ for other values.

This is achieved by using the following modulation to our base potential,

$$W(x) = \sigma e^{-2\omega x^2} \left[\sin(11x) \sin(13\sqrt{2}x) \cos(2\pi x) \cos\left(\frac{5x}{\sqrt{2}}\right) + \tau \sin(3\sqrt{\pi}x) \sin(7x) \right], \quad (6)$$

where σ is the strength of the modulation and τ , which is weakly dependent on σ , is used to cancel the semi-classical effect introduced by $W(x)$ (discussed below). To achieve a fair comparison to our base potential, we rely on the action integral

$$\mathcal{A} = \int_{x_l}^{x_r} dx \sqrt{2[E - V(x) - W(x)]}, \quad (7)$$

where E is the energy of the packet and x_l and x_r are the left and right turning points respectively. Of course this assumes that there are only two such turning points. We compare potentials for which \mathcal{A} is invariant. Note that this criterion

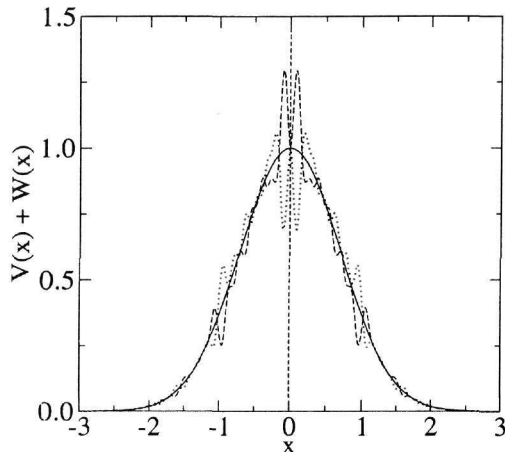


Fig. 3. The potentials used for solving the TDSE. The base potential ($W(x) = 0$) is given by the solid line, while the potentials for $\sigma = 0.5$ (ears up) and $\sigma = -0.5$ (ears down) are given by the dashed and dotted lines respectively.

is better suited to the comparison of smooth potentials only; we use it for want of a better criterion applicable as well to rough potentials. Fig. 3 shows three such potentials for $E = 0.571834$. The base potential $V(x)$ is portrayed by the solid line. The modulations introduced by Eq. (6) correspond to the case $\sigma = 0.5$, $\tau = -0.111$ (dashed line, “ears up”) and $\sigma = -0.5$, $\tau = -0.132$ (dotted line, “ears down”). The slight difference in the value of τ comes from the condition of satisfying the action specified in Eq. (7). If one requires that the average modulations vanish, i.e. $\mathcal{W} = \int_{-\infty}^{\infty} W(x)dx = 0$, then $\tau = -0.118$; a value not too different from the two values given. In fact, for $\tau = -0.111$, $\mathcal{W} = 8 \times 10^{-4}$, while for $\tau = -0.132$, $\mathcal{W} = 2 \times 10^{-3}$. Thus the modulations we have introduced do not change the action and the associated changes in the average of the potential are negligible.

In Fig. 4, we display the transmitted norm $T(t)$ for the three potentials described and for an incident wave packet with $K = 1.06$. Transmission is hardly affected by the changes to the reference potential. For the “ears up” potential $T(40) = 0.202$ while for the “ears down” it is 0.204. These are to be compared with the value of 0.203 found using the reference potential. These changes, of the order of a percent, are small in comparison to the associated variations of the potentials from the reference; the modulations of which are as much as 30%. That is especially so in the region of the “ears”.

Results have been obtained also for the same potentials but with lower incident momenta. For $K = 0.6$, hence $E = 0.190034$, the condition of fair comparison [Eq. (7)] of potentials with modulations defined by Eq. (6) requires $\tau = 0.050$ for $\sigma = 0.5$ and $\tau = -0.084$ for $\sigma = -0.5$. These parameters give also the “ears up” and “ears down” potentials respectively with fluctuations on refer-

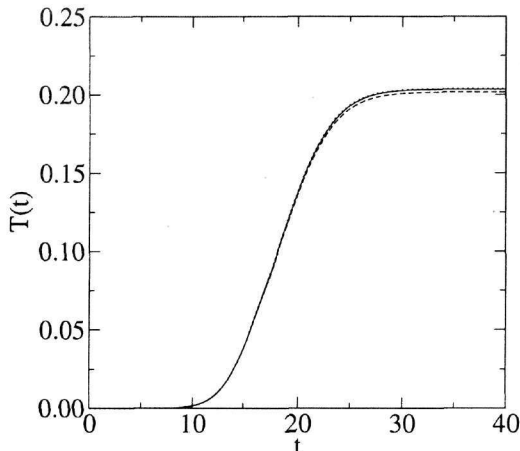


Fig. 4. Transmitted norms for a wave packet with $K = 1.06$ incident on the three potentials. The curves correspond to the results obtained for the reference (solid line), “ears up” (dashed line), and “ears down” (dotted line) potentials.

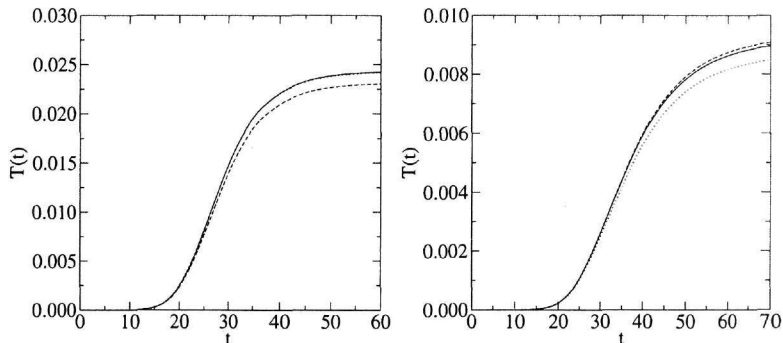


Fig. 5. As for Fig. 4 but for $K = 0.6$ (left) and $K = 0.42$ (right).

ence $\sim \pm 30\%$ in the ears. The results for the transmitted norm in this case are displayed in Fig. 5. For the “ears-up” potentials at this energy, the transmission now appears depleted as the value of $T(\infty)$ in this case is 0.0226. But there is little change for the “ears-down” case from the asymptotic transmitted norm obtained for the reference potential, 0.0239.

A different picture occurs for the case $K = 0.42$, or $E = 0.098234$. This is displayed in the right of Fig. 5 for the same potentials used previously. For the lowest momentum considered, there is a slight enhancement in the transmission from the “ears-up” potential and a significant depletion with the “ears-down” potential. This is the reverse situation to that with $K = 0.6$.

It is noteworthy that, with any of these modifications to the reference potential, the effect on the transmission is minimal; changes being at most of the order of 10%. This is not sufficient to explain the observed depletion of fusion

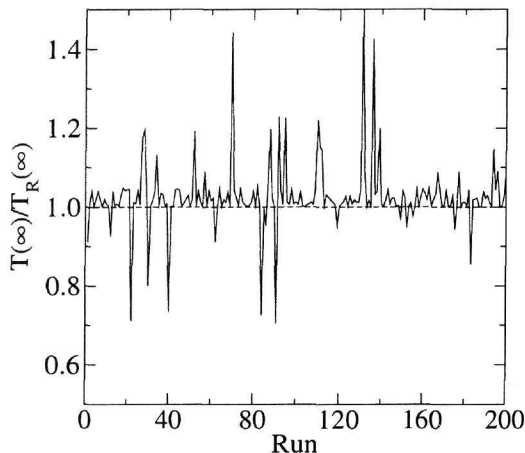


Fig. 6. Ratio of $T(\infty)$ against the reference value ($T_R(\infty) = 0.0239$) for the runs made using the random pair of $\{\Omega_c, \Omega_s\}$ specified in Eq. (8). For these calculations, $K = 0.6$. The line is a guide to the eye.

rates below the Coulomb barrier.

As the spatial fluctuations are unlikely to be the source of the large loss of fusion that is observed experimentally, we turn our attention to time-dependent fluctuations on the base potential. We assume those fluctuations are of the form

$$v(t) = 1 + \gamma \cos(\Omega_c t) \sin(\Omega_s t). \quad (8)$$

We take $\gamma = 0.2$ while Ω_c and Ω_s are chosen at random with uniform distributions varying between 0 and 5 for Ω_c and between -5 and 5 for Ω_s . These parameters are then sampled allowing for a good simulation of the chaotic character of $(v(t) - 1)$.

We start again with our initial wave packet, Eq. (4). The fine structures in the packet experience the weakly correlated components of the oscillating fluctuations and so we need not be concerned about any time periodicity in $V(x, t)$. The sampling space is one of 200 to 500 potentials (independent choices for Ω_c and Ω_s) and we use the asymptotic value of the transmitted norm $T(\infty)$ as the measure of effect of the time-dependent potentials in comparison to that from the reference potential for which $v(t) = 1$. The latter we designate as $T_R(\infty)$.

Displayed in Fig. 6 is the ratio of $T(\infty)/T_R(\infty)$, obtained from 200 runs for a packet with initial momentum $K = 0.6$. The reference value for this case is $T_R(\infty) = 0.0239$. For most of the pairs sampled, the transmission is close to the reference potential. But there are a few instances where the tunneling is greatly enhanced as well as others where it is greatly reduced. Variations of as much as 50% occur. The distribution of values of $T(\infty)$ for $K = 0.6$ is

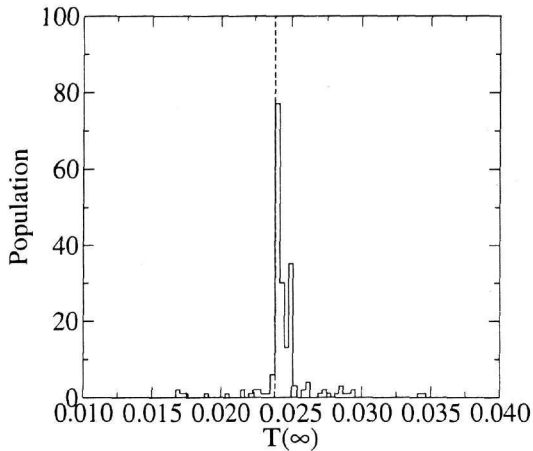


Fig. 7. Distribution of values of $T(\infty)$ for the runs shown in Fig. 6, for which $K = 0.6$. The reference value $T_R(\infty) = 0.0239$ is indicated by the dashed line.

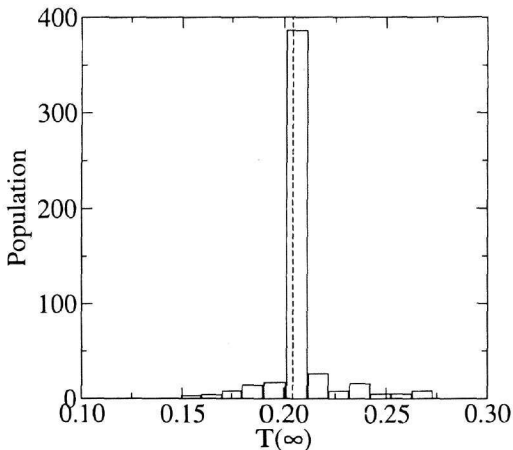


Fig. 8. As for Fig. 7 but for $K = 1.06$ and using a sample of 500 potentials. The value of $T_R(\infty)$ for the reference potential is 0.2039.

displayed in Fig. 7. As indicated in Fig. 6, the introduction of time fluctuating potentials increases slightly the value of $T(\infty)$ on average indicating that the transmission is enhanced, if only a little. That is a general feature we find for many conditions and one such is shown in Fig. 8. Therein the histogram for runs with $K = 1.06$ (sample size of 500) are displayed. The slight increase of $T(\infty)$ on average is evident again.

We have considered various cases of tunneling in a fully quantal approach, changing the base potential in our model by adding either space-dependent or time-dependent fluctuations to see if there is any enhancement in the transmission of the packet beyond the barrier. For the cases of the space-dependent

fluctuations, the induced changes were made such that the action was invariant so allowing for a fair comparison of the results obtained with those of the base (reference) potential. The effects of those changes seem to be momentum dependent. For a high incident momentum, corresponding to $K = 1.06$, there is very little change in the transmission of the wave through the barrier. For much lower momenta, particularly the case for $K = 0.42$, there is change, with the “ears up” potential producing a reduction in the transmission. The same occurs at this momentum for an effectively random change in the modulating potential. But the size of the changes in the transmission are not very large, typically $\sim 10\%$ and given that we can produce both enhancement and depletion by such (relatively large) changes in the barrier, we conclude that the cause of the large ($\sim 50\%$) loss of fusion observed experimentally is unlikely to be solely, or even largely, caused by changes in the transmission due to space fluctuations in the barrier.

By perturbing the barrier with time-dependent oscillations, we have been able to produce a small systematic increase in the transmission. Yet with our sample over a large number of potentials and at various incident momenta we were only able to find small numbers of cases where the transmission was either greatly enhanced or greatly diminished. The enhancement may correspond to a situation where fusion is also enhanced and vice-versa. However, the number of such cases is relatively few, and the average of all lead to small enhancements in transmission for all momenta.

In all cases, there is one overriding consideration: there is no evidence for a “friction”, or decoherence, related to a Langevin process with complex time. By considering the full quantal TDSE no such effects with classical analogues, or those involving complex time, are needed to produce changes to the observed transmission. But those changes are not significant enough to indicate that the source of the depletion of fusion rates in heavy-ion reactions at extreme sub-Coulomb barrier energies comes from changes in tunneling.

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