Jensen inequalities for tunneling probabilities in complex systems

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The Jensen theorem is used to derive inequalities for semiclassical tunneling probabilities for systems involving several degrees of freedom. These Jensen inequalities are used to discuss several aspects of sub-barrier heavy-ion fusion reactions. The inequality hinges on general convexity properties of the tunneling coefficient calculated with the classical action in the classically forbidden region.

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I. INTRODUCTION

In complex quantum systems with several active degrees of freedom, one usually finds a strong deviation of the tunneling probability from the prediction of the simple one-dimensional barrier penetration model. Experiments on the fusion of nuclei at sub-barrier energies have clearly shown a very large enhancement of the tunneling probability when compared to simple one-dimensional barrier model calculations. In several important theoretical papers [1–5] addressing the tunneling problem in systems coupled to a reservoir attempts were made to obtain semiquantitative, albeit important estimates of the effects of the reservoir's degrees of freedom on the tunneling dynamics of the subsystem of interest. More detailed numerical calculations based on the coupled-channels description of, e.g., sub-barrier fusion, attempt to give a quantitative description within a restricted dimension of the reservoir (the number of channels strongly coupled to the entrance channel) [6–9].

Furthermore, a very low energy fusion of light nuclei such as $^2\mathrm{H} + {}^2\mathrm{H}$ has been of interest over the last two decades in the context of the so-called cold fusion. In this endeavor the effect of the environment is important. Recent work on the fusion of such light nuclei has indicated that in metals electron screening is enhanced, reducing the fusion barrier and accordingly enhancing fusion probability. Of course such light ion reactions are of great importance in astrophysics [10] and the understanding of the effect of the environment on them has been under intensive experimental [11–13] and theoretical [14–17] scrutiny. It would be a useful compliment to the above discussion to find general inequalities that involve the tunneling probability for a subsystem of the many-degrees-of-freedom system when compared to the subsystem alone (with the coupling to the reservoir being averaged). This is the aim of the present work. We rely on a general theorem in analysis referred to as the Jensen theorem.

The paper is organized as follows. In Sec. II, we introduce Jensen's inequality and show that what is known as Peierls theorem is an example of such an inequality. We use the scattering of heavy ions to illustrate this. In Sec. III we discuss the tunneling in systems with many degrees of freedom. The coupling is treated in the sudden limit. The uniform approximation (also known as Kemble's formula) of the tunneling probability is then introduced and its evaluation below and above the barrier is discussed. In Sec. IV the Jensen's inequality is applied to tunneling. The coupling Hamiltonian is taken to be a function of the reservoir's variables, while the radial separation is fixed at the barrier position. In Sec. V numerical examples are presented for heavy ion fusion. Both heavy systems and very light systems are considered. In the latter, we found that the application of Jensen's inequality is impractical. Finally, in Sec. VI several concluding remarks are given. In Appendix A we give supplementary details about how the uniform approximation formula of the tunneling probability is evaluated above the barrier, while in Appendix B, supplementary details of the applicability of Jensen's inequality at deep sub-barrier energies are given.

II. THE JENSEN INEQUALITY AND PEIERLS THEOREM

The Jensen inequality [18] ensures that if $F(f(\zeta))$ is a functional of a function $f(\zeta)$, then $\langle F(f(\zeta))\rangle_\zeta \geqslant F(\langle f(\zeta)\rangle_\zeta)$ if and only if F is a convex functional of f within the interval in which the average $\langle\ \rangle_\zeta$ is being calculated. One possible way of explicitly stating the Jensen inequality is the following:

$$\frac{\int_a^b d\zeta\,\phi(\zeta)F(f(\zeta))}{\int_a^b d\zeta\,\phi(\zeta)} \geqslant F\left[\frac{\int_a^b d\zeta\,\phi(\zeta)f(\zeta)}{\int_a^b d\zeta\,\phi(\zeta)}\right], \qquad (1)$$

if and only if $F(f)$ is a convex functional of f within the interval $[a,b]$, and $\phi(\zeta)$ is any positive integrable function. If the convexity turns out to be a concavity, the inequality is reversed.

One immediate consequence of the Jensen inequality is Peierls theorem, which was used by Peierls [20] to prove that the canonical partition function, $Z(\beta)$, defined by $Z(\beta) = Tr[\exp(-\beta H)]$, is greater than or equal to $\exp[-\beta \mathrm{Tr} H]$.

Using Peierls theorem, Johnson and Goebel (JG) derived an inequality involving the reflection above the barrier in order to assess the effect of breakup on the elastic scattering of halo nuclei [19]. That inequality clarified why the reaction cross section calculated within the Glauber model is appreciably smaller than that calculated using the optical limit of the model, a point first emphasized in [21], thus resulting in larger radii of halo nuclei. In the following we show that the result of JG [19] and that of [21] can be considered as a consequence of the Jensen inequality.

In their above cited work, JG considered the elastic S-matrix element for the lth partial wave

$$S_l(E,\zeta) = \exp[2i\delta_l(E,\zeta)] = \exp[f] \quad (2)$$

where the phase shift δ_l, in the JWKB approximation is given by

$$\delta_l(E,\zeta) = \lim_{r\to\infty}\left\{\int_{r_0}^{r} dr' k_l(r',\zeta) - \int_{r_0^{(0)}}^{r} dr' k_l^{(0)}(r')\right\}. \quad (3)$$

Above, $k_l(r,\zeta)$ is the local wave number given by $k_l(r,\zeta) = \sqrt{\frac{2\mu}{\hbar^2}[E - V_l(r) - F_l(r)G(\zeta)]}$, where $F_l(r)G(\zeta)$ is the contribution for the effective potential which is due to the coupling to the reservoir, which was considered to be separable. The free particle local wave number is denoted by $k_l^{(0)}(r)$, r_0 is the classical turning point defined by $k_l(r_0,\zeta) = 0$, and $r_0^{(0)}$ is the corresponding one for the free local wave number. The asymptotic wave number is denoted by $k = k_l^{(0)}(r=\infty)$ and the mass by μ.

At high energies, one may expand the local wave number in powers of $\frac{V_l(r)+F_l(r)G(\zeta)}{E}$ and retain the leading term. This constitutes the eikonal approximation considered by JG [19]. This approximation gives, for the phase shift,

$$\delta_{\text{eikonal}}(E,b,\zeta) = -\frac{\mu}{\hbar^2 k}\int_b^\infty r dr \frac{V_l(r) + F_l(r)G(\zeta)}{\sqrt{r^2-b^2}}, \quad (4)$$

where the impact parameter $b = \frac{l+1/2}{k}$. We consider, as JG, the case where the potential, and accordingly the form factor, is purely absorptive ($V_l(r) = -iW_l(r)$ and $F_l(r) = \frac{V_l(r)}{dr}$). Then the phase shift δ_{eikonal} becomes pure imaginary and f real. From the Jensen inequality and from the fact that $\delta_{\text{eikonal}}(E,b,\zeta)$ is a linear function of $G(\zeta)$ we obtain the following inequality:

$$\overline{S_l(E,\zeta)} \geqslant \exp[-2|\overline{\delta_{\text{eikonal}}(E,b,\zeta)}|] \quad (5)$$

which is the result obtained in the work of JG.

The above inequality only holds for imaginary phase shifts. Clearly the actual heavy-ion scattering at intermediate energies involves complex phase shifts, and this fact points to an inherent limitation of the work of JG. This limitation is removed if we go to very low energies and consider fusion which is dominated by quantum tunneling (with real action integral).

III. TUNNELING IN SYSTEMS WITH MANY DEGREES OF FREEDOM AND FUSION REACTIONS

In order to apply the Jensen inequality to tunneling and fusion reactions, we recall first the expression for tunneling probability provided by the coupled-channel treatment in the case of a coupling to an oscillator reservoir with zero frequency (sudden approximation), which can be cast as a simple average [22]:

$$\langle T_l(E)\rangle_\zeta \equiv \int d\zeta\, |\phi_0(\zeta)|^2 T_l[E, V_l(r) + H_{\text{int}}(r,\zeta)], \quad (6)$$

where $T_l[E, V_l(r) + H_{\text{int}}(r,\zeta)]$ is the transmission probability evaluated at energy E with an effective potential $V_l(r) + H_{\text{int}}(r,\zeta)$, in which $H_{\text{int}}(r,\zeta)$ is the potential term due to the coupling to the reservoir. The wave function $\phi_0(\zeta)$ denotes the ground state wave function related to the reservoir coupling. Of course wave functions for excited states of the considered reservoir coupling can be used instead. The above equation refers to the limit in which the intrinsic energies are small compared to the coupling interaction, so that the reservoir Hamiltonian is set equal to zero. For simplicity, we consider in the following the coupling Hamiltonian to be operative only at $r = R_l$, where R_l is the position of the angular momentum-dependent barrier. Thus, $H_{\text{int}}(r,\zeta) = H_{\text{int}}(R_l,\zeta)$. Although this is a very rough approximation, it is a first step in the direction of assessing the effects of the contribution of the coupled potential on the transmission coefficient.

Using the Kemble [23] form of the transmission probability below the barrier, which guarantees a $1/2$ transmission at the top of a symmetrical barrier [24], and takes into account multiple reflections inside the barrier to all order if the uniform approximation is used in a path integral formulation of tunneling [25], $T_l[E, V_l(r) + H_{\text{int}}(R_l,\zeta)]$ is found to be

$$T_l[E, V_l(r) + H_{\text{int}}(R_l,\zeta)] = \frac{1}{1+\exp\{g_l[E, V_l(r) + H_{\text{int}}(R_l,\zeta)]\}}, \quad (7)$$

with $g_l[E, V_l(r) + H_{\text{int}}(R_l,\zeta)]$ being twice the action integral S_l, and is given by

$$g_l[E, V_l(r) + H_{\text{int}}(R_l,\zeta)] = \sqrt{\frac{8\mu}{\hbar^2}}\int_{r_1(l,\zeta)}^{r_2(l,\zeta)} dr \sqrt{V_l(r) + H_{\text{int}}(R_l,\zeta) - E}, \quad (8)$$

where $r_1(l,\zeta)$ and $r_2(l,\zeta)$ are the real classical turning points which are the roots of $V_l(r) + H_{\text{int}}(R_l,\zeta) = E$.

For the transmission probability above the barrier, a detailed discussion was given, e.g., in [26] which shows that $T_l[E, V_l(r) + H_{\text{int}}(R_l,\zeta)]$ can be written in exactly the same form as for sub-barrier energies, if due attention is given to the localization of the turning points and the branch cut in the imaginary r plane arising from the square root. In Appendix A, we give the full details of the arguments used by [26].

It is important to comment about the way the turning points move around in the complex r plane as the energy is changed gradually from below to above the barrier. Below the barrier, there are two real turning points, the outer one r_2 and the inner one r_1. As the energy is increased these turning points, which are actually branch points, come closer and closer and eventually they "collide" as E reaches the top of the barrier, and move out into the complex plane, becoming complex conjugate of each other for E above the barrier. This is shown in Figure 4 of [26]. The inner turning point moves to the upper half plane, while the outer turning point moves to the lower half plane. The calculation of the tunneling action which in our notation is $g/2$, is performed introducing the branch cuts which render such action real both below and above the barrier.

Guided by Brink and Takigawa [26], Kemble [23], and Miller and Good [24], we adapted the following practical prescription used in the numerical calculation. The expression for the tunneling probability is formally similar to that used below the barrier,

$$T_l[E, V_l(r) + H_{\rm int}(R_l,\zeta)] = \frac{1}{1+\exp\{g_l[E, V_l(r) + H_{\rm int}(r,\zeta)]\}}, \tag{9}$$

with $g_l[E, V_l(r) + H_{\rm int}(R_l,\zeta)]$ given by

$$g_l[E, V_l(r) + H_{\rm int}(R_l,\zeta)] = \sqrt{\frac{8\mu}{\hbar^2}}\int_{z_1(l,\zeta)}^{z_2(l,\zeta)} dr\sqrt{(V_l(r) + H_{\rm int}(R_l,\zeta) - E)}, \tag{10}$$

where $z_1(l,\zeta)$ and $z_2(l,\zeta)$ are the complex conjugate roots ($z_1 = z_2*$) of the equation $V_l(r) + H_{\rm int}(R_l,\zeta) - E = 0$, assuming a parabolic form for the potential, as done by [23]. As emphasized by [26], z_1 is located in the upper half plane, which makes z_2 to be in the lower half plane (see Appendix A). In the actual evaluation of g_l, the above turning points are used, but the potential $V_l(r)$ inside the square root in the integral g_l is treated exactly. Clearly, a consistent way to perform the calculation is to follow [26] by first locating the exact complex turning points and then choosing the integration path along the branch cut that guarantees a real g_l. This procedure is demonstrated in Appendix A for the analytically doable parabolic approximation which shows that g_l (above the barrier) $= g_l$(below the barrier) $= \frac{2\pi}{\hbar\omega_l}[V_l(R_l) - E]$. The conclusion that g_l (above the barrier) $= g_l$ (below the barrier), if the correct integration route and turning points in the complex r plane are employed, is a general property of well-behaved interactions.

IV. JENSEN'S INEQUALITY AND TUNNELING

Bringing the Jensen inequality into the context of tunneling and fusion probability, one can state that

$$\langle T_l(E)\rangle_\zeta \geqslant T_l[E, V_l(r) + \langle H_{\rm int}(R_l,\zeta)\rangle_\zeta], \tag{11}$$

if and only if $T_l[E, V_l(r) + H_{\rm int}(R_l,\zeta)]$ is a convex functional of $H_{\rm int}(R_l,\zeta)$. In the equation above, $\langle H_{\rm int}(R_l,\zeta)\rangle_\zeta$ is defined as $\langle H_{\rm int}(R_l,\zeta)\rangle_\zeta \equiv \int_a^b d\zeta|\phi_0(\zeta)|^2 H_{\rm int}(R_l,\zeta)$ and $|\phi_0(\zeta)|^2$ is the square modulus of the normalized ground-state wave function related to the reservoir. The same definition holds for the average $\langle T_l(E)\rangle_\zeta$. Hence, it is necessary to determine whether the transmission probability is a convex or a concave function of $H_{\rm int}(R_l,\zeta)$ [where $H_{\rm int}(R_l,\zeta)$ is regarded as a simple variable] in order to make a comparison of the type of inequality (11). The interval $[a, b]$ stands for all possible values that the coordinate related to the oscillator reservoir, ζ, may assume.

Let us introduce the quantity $w(\zeta) = E - H_{\rm int}(R_l,\zeta)$, which will be used in our calculations in order to make the physical comprehension clearer, that is, $w(\zeta)$ will stand for the effective energy. Because $w(\zeta)$ is a linear function of $H_{\rm int}(R_l,\zeta)$, the sign of the second derivative of the tunneling probability T_l, with respect to $w(\zeta)$ determines if T_l is a convex functional of the function $H_{\rm int}(R_l,\zeta)$ or a concave one. For the region bellow the barrier, such second derivative would be, according to Eqs. (7) and (8),

$$\frac{\partial^2 T_l}{\partial w^2} = \frac{\exp[h_l(w)]}{(1+\exp[h_l(w)])^3}\left\{(\exp[h_l(w)]-1)(f_l(w))^2 + (\exp[h_l(w)]+1)\left(\frac{\partial f_l(w)}{\partial w}\right)\right\}, \tag{12}$$

in which $h_l(w) = \sqrt{\frac{8\mu}{\hbar^2}}\int_{r_1(l,w)}^{r_2(l,w)} dr\sqrt{V_l(r) - w}$ and $f_l(w) = \sqrt{\frac{2\mu}{\hbar^2}}\int_{r_1(l,w)}^{r_2(l,w)}\frac{dr}{\sqrt{V_l(r)-w}}$.

For heavy ions at near-barrier energies, the effective tunneling potential $V_l(r)$ is usually approximated by a an inverted parabola, which enables us to follow the Hill-Wheeler procedure [27], in order to obtain a closed form for the Kemble tunneling probability. For such heavy ions, the extra degree of freedom, namely the coordinate ζ, would correspond to the displacement due to vibrational modes, and the coupled reservoir would be represented by an oscillator in this case. Therefore, for such cases,

$$V_l(r) = V_{HWl}(r) \equiv V_l(R_l) - \tfrac{1}{2}\mu\omega_l^2(r - R_l)^2. \tag{13}$$

Hence

$$h_l(w) = \sqrt{\frac{8\mu}{\hbar^2}}\int_{r_1(l,w)}^{r_2(l,w)} dr\sqrt{V_l(R_l) - \frac{1}{2}\mu\omega_l^2(r-R_l)^2 - w} = \frac{2\pi}{\hbar\omega_l}[V_l(R_l) - w] \tag{14}$$

and

$$f_l(w) = \sqrt{\frac{2\mu}{\hbar^2}}\int_{r_1(l,w)}^{r_2(l,w)}\frac{dr}{\sqrt{V_l(R_l) - \frac{1}{2}\mu\omega_l^2(r-R_l)^2 - w}} = \frac{2\pi}{\hbar\omega_l} \Rightarrow \frac{\partial f_l(w)}{\partial w} = 0. \tag{15}$$

The above result combined with Eq. (12) yields

$$\frac{\partial^2 T_l}{\partial w^2} = \frac{\exp[h_l(w)]}{(1+\exp[h_l(w)])^3}(\exp[h_l(w)]-1)(f_l(w))^2 > 0 \tag{16}$$

and finally,

$$\langle T_l[w(\zeta), V_{HWl}(r)]\rangle_\zeta \geqslant T_l[\langle w(\zeta)\rangle_\zeta, V_{HWl}(r)]$$

or, since $\langle w(\zeta)\rangle_\zeta = E - \langle H_{\rm int}(R_l,\zeta)\rangle_\zeta$,

$$\langle T_l[E, V_{HWl}(r) + H_{\rm int}(R_l,\zeta)]\rangle_\zeta \geqslant T_l[E, V_{HWl}(r) + \langle H_{\rm int}(R_l,\zeta)\rangle_\zeta] \tag{17}$$

for all l-partial wave functions and different values of μ. Thus within the parabolic approximation for the potential, all systems show enhanced tunneling.

Calculating the second derivative of the transmission probability represented by Eqs. (9) and (10) and following the same procedure described above, one finds that

$$\langle T_l[E, V_{HWl}(r) + H_{\rm int}(R_l,\zeta)]\rangle_\zeta \leqslant T_l[E, V_{HWl}(r) + \langle H_{\rm int}(R_l,\zeta)\rangle_\zeta] \tag{18}$$

for energies above the potential barrier. It means that within the parabolic approximation for the potential, all systems show hindered transmission above the barrier.

The inequalities (17) and (18), attained solely by the application of the Jensen inequality to an analytical form of the transmission coefficient in which we consider a linear coupling to the reservoir, have a direct correspondence to an empirically well-known result obtained through numerical calculations for different models, namely that the linear coupling to an oscillator enhances the tunneling probability at energies below the potential barrier in the absence of coupling, while hinders the transmission probability at energies above the barrier. In fact, the inequalities (17) and (18) lead exactly to such rule in the special case that $\langle H_{\rm int}(R_l,\zeta)\rangle_\zeta = 0$.

We now assess the application of the Jensen inequality for the case of low energies. By "*low*" energies, we mean small values of the function $w(\zeta)$. Here the coupling to the reservoir could stand for coupling to the electronic degrees of freedom. The parabolic approximation for the potential barrier is not suitable for this case, and we shall use a general ion-ion effective interaction, which has the form

$$V_l(r) \equiv V_N(r) + \frac{Z_1 Z_2 e^2}{r} + \frac{\hbar^2 l(l+1)}{2\mu r^2}, \tag{19}$$

where $V_N(r)$ is the nuclear attractive potential. Although not being parabolic, the above potential barrier can be regarded as locally parabolic for regions close to the top of the barrier. For that reason, we still make use here of the Eq. (7) in order to evaluate the tunneling probability. As shown in the Appendix B, whatever specific analytic form the short-range nuclear interaction, $V_N(r)$, may take, a potential barrier resulting from $V_l(r)$ of Eq. (19) always leads to the following important Jensen inequality for very small values of w and/or E:

$$\begin{aligned}\langle T_l[E, V_l(r) + H_{\rm int}(R_l,\zeta)]\rangle_\zeta \\ \geqslant T_l[E, V_l(r) + \langle H_{\rm int}(R_l,\zeta)\rangle_\zeta],\end{aligned} \tag{20}$$

where $V_l(r)$ is defined by Eq. (19).

This very general result implies that whatever attractive nuclear potential model one may use, the plot of the curve of the transmission probability versus $w(\zeta)$, where $w(\zeta) = E - H_{\rm int}(R_l,\zeta)$, is always convex for small values of w, leading to enhanced tunneling.

So far we have concentrated our attention on the lth transmission coefficient. The experimental data, on the other hand, are represented by the fusion cross section defined by

$$\sigma_F(E) = \frac{\pi\hbar^2}{2\mu E}\sum_{l=0}^{\infty}(2l+1)T_l(E) = \sum_{l=0}^{\infty}\sigma_l(E). \tag{21}$$

From Eq. (21), we see that the dependence of $\sigma_F(E)$ on the coupling $H_{\rm int}(R_l,\zeta)$ lies only on the terms $T_l(E)$. Then, if it is possible to state that, for instance, $T_l(E)$ is a convex functional of $H_{\rm int}(R_l,\zeta)$ for all values of the quantum number l, then one can also state that $\sigma_F(E)$ is a convex functional of $H_{\rm int}(R_l,\zeta)$. The above lends support to the general idea that there is an enhancement of the fusion cross section when coupling to the degrees of freedom of the reservoir are taken into account, namely,

$$\langle \sigma_F(w(\zeta))\rangle_\zeta \geqslant \sigma_F(\langle w(\zeta)\rangle_\zeta) \tag{22}$$

for the fusion process occurring via tunneling through a potential barrier.

This is easily seen at deep sub-barrier energies, where in fact the transmission coefficient or tunneling probability can be approximated by an exponential, since the action in the uniform approximation for the transmission coefficient is small:

$$\begin{aligned}\sigma_F(E) &= \frac{\pi\hbar^2}{2\mu E}T_0(E) \\ &= \frac{\pi\hbar^2}{2\mu E}\exp[-g_0(E, V(r) + H_{\rm int}(R_l,\zeta))].\end{aligned} \tag{23}$$

As shown in Appendix B, the above function is convex in $H_{\rm int}(R_l,\zeta)$ for $w(\zeta)\to 0$, and thus its average over ζ is greater than that calculated with $\langle H_{\rm int}(R_l,\zeta)\rangle_\zeta$. Thus, we can state

$$\begin{aligned}\langle \exp[-g_0(E, V(r) + H_{\rm int}(R_l,\zeta))]\rangle_\zeta \\ \geqslant \exp[-g_0(E, V(r) + \langle H_{\rm int}(R_l,\zeta)\rangle_\zeta)]\end{aligned} \tag{24}$$

which represents the very low energy tunneling version of the JG inequality of elastic scattering eikonal S-matrix element of halo nuclei.

It is by now well known that a large enhancement in σ_F over the no-coupling limit has been observed for most heavy-ion fusion systems at sub-barrier energies [30]. Recently, it has been reported that at deep sub-barrier energies, this enhancement is reduced [31] [unfortunately, this effect has been widely called "hindrance," which should not be confused with what we mean by hindrance in this paper, namely, a concave behavior of $T_l(w(\zeta))$ as a function of $H_{\rm int}(R_l,\zeta)$].

V. NUMERICAL EXAMPLES

From the results depicted by Eqs. (17) and (18) and by Eq. (20), one is compelled to infer that, in general, the tunneling probability T_l would tend to be a convex functional of the function $w(\zeta)$, when $w(\zeta)$ assumes values which are smaller than the potential barrier height, and a concave functional of $w(\zeta)$ for higher values of this function. In order to assess the validity of the analytical results we obtained so far, we plot the transmission probability as a function of w, as it can be seen in Fig. 1, for the systems (a) ^{64}Ni + ^{64}Ni and (b) ^{16}O + ^{150}Sm, both for $l = 0$. There, the tunneling probability was defined by Eqs. (7) and (8) and by Eqs. (9) and (10), respectively, for values of w below and above the top of the barrier. The potential barrier used was the ion-ion effective interaction represented by Eq. (19), where the nuclear interaction was taken to be the Woods-Saxon potential:

$$V_N(r) = \frac{-V_0}{1 + \exp\left(\frac{r-R_0}{a_p}\right)} \tag{25}$$

in which the diffuseness a_p was 0.65 fm, the effective nuclear radius of the system was taken to be $R_0 = 1.31(\sqrt[3]{A_1} + \sqrt[3]{A_2}) - 1.68$ fm, where A_1 and A_2 are the mass numbers of the nuclei involved in the fusion reaction, and the potential strength V_0 was adjusted to make the potential above to coincide with the numerical value provided by the São Paulo potential on the effective nuclear surface [28,29].

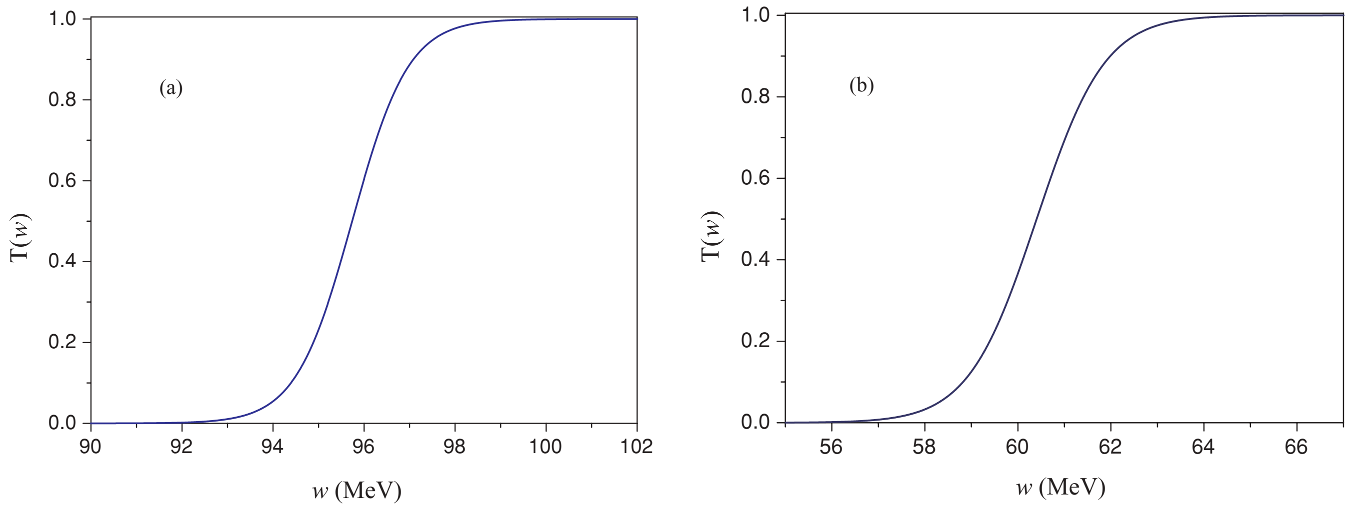

FIG. 1. (Color online) Tunneling probability versus the function $w(\zeta)$ for $l = 0$, for the systems (a) ^{64}Ni + ^{64}Ni and (b) ^{16}O + ^{150}Sm. The curves show a convex dependence of the tunneling probability functional on the function $w(\zeta)$ in the classically forbidden region $0 \leqslant T(w) \leqslant 0, 5$, while in the classically allowed region the curves become concave. Since the concavity changes, the Jensen inequality is reversed when one goes from below to above the barrier region, and as a consequence the enhancement seen in the former region becomes a hindrance in the latter.

This general property of convexity of the unaveraged tunneling probability for $T_l(w) \leqslant 0.5$ implies an enhanced tunneling or fusion, as experimental data seem to clearly indicate [30].

However, plots of the tunneling probability as a function of $w(\zeta)$ for very light ions (such as hydrogen and helium isotopes) display a different behavior concerning the concavity of the curves, as shown in Fig. 2 for the systems (a) ^{2}H + ^{2}H and (b) ^{3}H + ^{3}H, both graphics for $l = 0$. These graphics were obtained using the same method as in Fig. 1, i.e., the transmission probability was defined by Eqs. (7) and (8) and by Eqs. (9) and (10), respectively, for values of w below and above the top of the barrier. The potential barrier used was also given by Eq. (19), where the nuclear interaction had Woods-Saxon form. For such light ions, the curve of T_l versus $w(\zeta)$ presents three inflection points instead of only one, becoming concave before w reaches the value correspondent to the top of the potential barrier. This result is in contradiction with the general analytical result represented by Eq. (17), where the parabolic potential was used to approximate the real potential barrier. That happens possibly because for light ions such approximation for the potential barrier is not suitable, as it appears that a more accurate approximation that would take into account the highly asymmetrical character of the potential curve would be required. A third degree polynomial would be a better fit for this purpose, but the analytical treatment becomes extraordinarily more complicated. In addition, the asymmetrical character of the barrier limits even the validity of the analytical form for the tunneling probability represented by Eqs. (7) and (8).

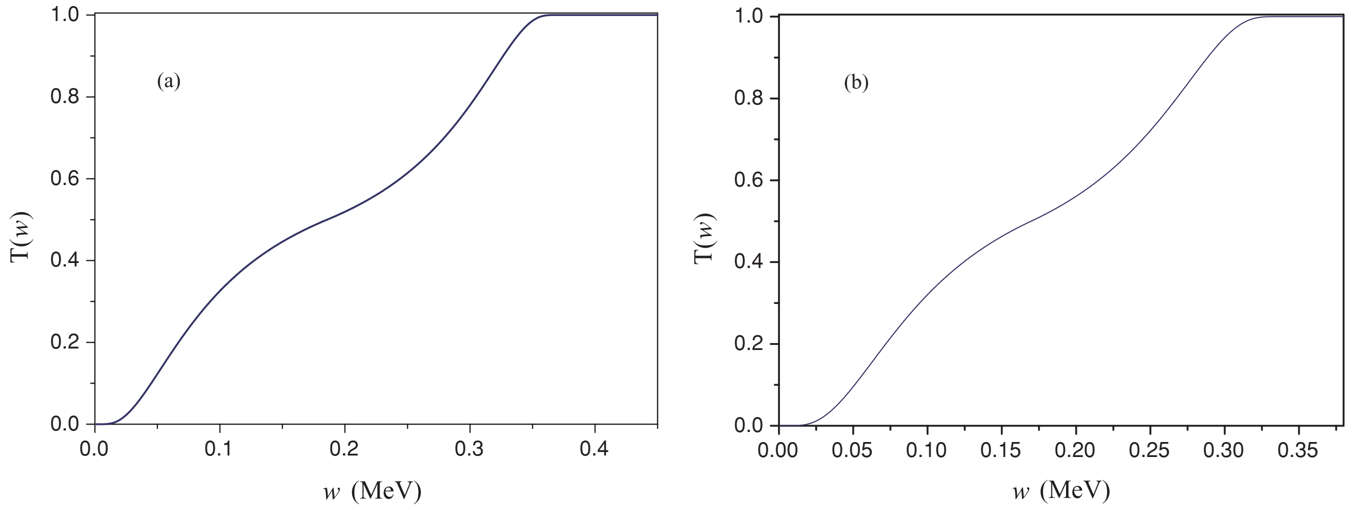

FIG. 2. (Color online) Tunneling probability versus the function $w(\zeta)$ for $l = 0$, for the systems (a) ^{2}H + ^{2}H and (b) ^{3}H + ^{3}H. Both curves show more than one inflection points, when compared to the heavy ion systems of Fig. 1, which may be due to the highly asymmetrical potential barrier in such very light systems. The Jensen inequality reverses several times, making it of lesser practical use in such systems.

VI. CONCLUSIONS

In conclusion we have considered some general properties of the tunneling probability for systems coupled to a reservoir. Using the Jensen inequality, we have shown that within the Kemble/uniform approximation theory of the tunneling probability, the average tunneling probability is in general larger than that calculated when the reservoir degrees of freedom are averaged out at the outset. On the other hand, the average transmission probability at energies above the barrier is in general smaller than that calculated when the reservoir degrees of freedom are averaged out at the outset. This has an immediate consequence on sub-barrier fusion of heavy ions, where data seem to indicate an enhanced tunneling owing to the coupling to the reservoir (coupled channels effects). In addition, we have shown that the results obtained by JG [19] can be generalized by using the Jensen inequality. The underlying mathematical dependence of the tunneling probability as a function of the reservoir coupling, namely the tunneling probability is in general a convex functional of the coupling hamiltonian in the classically forbidden region, and a concave functional of the coupling in the classically permitted region allows the Jensen inequality to be applied to this research field in order to compare two different forms of reaction probabilities, both of physical interest. The inequalities obtained in this work lend support to the idea that the one-dimensional barrier penetration model leads to inherent deviations from the expected values for the transmission coefficient, even if its parameters are adjusted in the best possible way in order to represent the physical phenomenon.

Our results for very light ion fusion shown in Fig. 2 do not allow the use of the Jensen inequality, applied to the Kemble/uniform approximation tunneling probability, since several reversals of the inequality occur as the "energy" changes. Thus the peculiar behavior presented by the curves of tunneling probability for light ions indicates that for such systems a more accurate treatment of semiclassical tunneling through an asymmetrical potential barriers is called for [24] in order to determine whether one has enhancement or hindrance owing to the presence of the environment.

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APPENDIX A

We discuss here how to evaluate the action integral in the formula of the tunneling probability in the uniform approximation by considering the branch cuts for the square root in a consistent way.

We follow the paper by Brink and Takigawa [26], which we call paper I in the following, and use this letter (I) to label the turning points and the way to choose the branch cuts arising from the square root inside the action integral S.

The tunneling probability in the uniform approximation/Kemble is given by

$$T = \frac{1}{1+\exp[g]}, \tag{A1}$$

$$g \equiv 2S = 2\int_{r_1}^{r_2} \sqrt{\frac{2m}{\hbar^2}(V(r)-E)}dr, \tag{A2}$$

where the r_1 is the inner turning point and r_2 the outer turning point, respectively.

Our concern is how to evaluate the action integral $g/2$ in a consistent way when the energy E varies from below to above the potential barrier.

For illustration, let us consider a parabolic potential barrier,

$$V(r) = V_0 - \tfrac{1}{2}m\Omega^2(r-R_0)^2. \tag{A3}$$

In this case, the action integral becomes

$$g = 2\frac{m\Omega}{\hbar}\int_{r_1}^{r_2}\sqrt{(r_2-r)(r-r_1)}dr, \tag{A4}$$

$$r_2 = R_0 + \sqrt{\frac{2(V_0-E)}{m\Omega^2}} = R_0 + \Delta r, \tag{A5}$$

$$r_1 = R_0 - \Delta r. \tag{A6}$$

The phase of the argument of the square root in Eq. (A4) should be chosen to be consistent with the choice of the branch cuts so as to give the correct result for $E < V_0$, a case whose result is well known. As we see later, this consideration leads to

$$g = 2\frac{m\Omega}{\hbar}e^{-\frac{\pi}{2}i}\int_{r_1}^{r_2}\sqrt{(r-r_1)(r-r_2)}dr. \tag{A7}$$

1. The case when $E \leqslant V_0$

Let us first consider the tunneling probability under the barrier, i.e., the case when $E \leqslant V_0$.

If the potential is real, as is in our case here in this paper, two turning points lie on the real axis of the complex r plane.

The action integral is taken along the real r axis

$$r = r_1 + \rho, \quad dr = d\rho. \tag{A8}$$

As stated before, we introduce the branch cuts following paper I, i.e., the upward branch cut stemming from the inner turning point $r_1(-\frac{3}{2}\pi < \arg(r-r_1) < \frac{1}{2}\pi)$, and the downward branch cut from the outer turning point $r_2(-\frac{1}{2}\pi < \arg(r-r_2) < \frac{3}{2}\pi)$ (see Fig. 2 in I). The magnitude and the phase of $r-r_2$ and $r-r_1$ along the integration path are then given by

$$r - r_2 = (2\Delta r - \rho)e^{i\pi}, \tag{A9}$$

$$r - r_1 = \rho e^{i0}. \tag{A10}$$

Therefore,

$$g = 2\frac{m\Omega}{\hbar}e^{-\frac{\pi}{2}i}e^{i\pi/2}\int_0^{2\Delta r}\sqrt{(2\Delta r-\rho)\rho}d\rho \quad \text{(A11)}$$

$$= 2\pi\frac{V_0-E}{\hbar\Omega}. \quad \text{(A12)}$$

The tunneling probability is thus given by

$$P = \frac{1}{1+e^{\frac{2\pi(V_0-E)}{\hbar\Omega}}}. \quad \text{(A13)}$$

This agrees with the well-known result. It is commonly referred to as the Hill-Wheeler formula. This also shows that the phase choice Eq. (A7) is correct.

2. The case when $E \geqslant V_0$

The turning points move into the complex r plane, i.e., become complex numbers, at energies above the potential barrier. We could say that as the energy is increased from below the barrier to above the barrier, the turning points move toward each other on the real axis till they reach R_0 at $E = V_0$ at which point they "collide" and "scatter" into the complex r plane. As can be seen in Fig. 4 in I, the inner turning point, r_1, moves to upper half plane, while the outer turning point, r_2, moves to the lower half plane.

Therefore, corresponding to Eqs. (A5) and (A6), we have, for the outer and the inner turning points,

$$r_2 = R_0 + e^{-\frac{\pi}{2}i}\sqrt{\frac{2(E-V_0)}{m\Omega^2}} = R_0 + e^{-\frac{\pi}{2}i}\Delta' r, \quad \text{(A14)}$$

$$r_1 = R_0 + e^{\frac{\pi}{2}i}\sqrt{\frac{2(E-V_0)}{m\Omega^2}} = R_0 + e^{\frac{\pi}{2}i}\Delta' r. \quad \text{(A15)}$$

The integration is taken vertically along the imaginary r axis, which we denote as

$$r = R_0 + iy, \quad dr = idy. \quad \text{(A16)}$$

Along the integration path, our choice of the branch cuts lead to

$$r - r_2 = e^{\frac{\pi}{2}i}(y-(-\Delta' r)) = e^{\frac{\pi}{2}i}(y+\Delta' r), \quad \text{(A17)}$$

$$r - r_1 = e^{-\frac{\pi}{2}i}(\Delta' r - y). \quad \text{(A18)}$$

Therefore, the action integral becomes

$$g = 2\frac{m\Omega}{\hbar}e^{-\frac{\pi}{2}i}i\int_{\Delta' r}^{-\Delta' r} dy e^{\frac{\pi}{4}i}\sqrt{y+\Delta' r}e^{-\frac{\pi}{4}i}\sqrt{\Delta' r - y} \quad \text{(A19)}$$

$$= -2\frac{m\Omega}{\hbar}\int_{-\Delta' r}^{\Delta' r}\sqrt{(y+\Delta' r)(\Delta' r - y)}dy \quad \text{(A20)}$$

$$= -\frac{2\pi(E-V_0)}{\hbar\Omega}. \quad \text{(A21)}$$

This is the desired result. Formally, it is the same as Eq. (A12) for energies below the potential barrier.

For the general case of a potential such as the one used here, the arguments above still holds, namely the Kemble/uniform approximation formula for the tunneling probability $T = \frac{1}{1+\exp[g]}$ with g being twice the action integral in the classically forbidden region (the barrier region), holds both below and above the barrier, if due attention is given to the location of the branch points and the integration path. Clearly adding the coupling interaction does not alter this general conclusion.

APPENDIX B

In this appendix we apply the Jensen inequality for the tunneling probability for very small w and/or E, Eq. (17).

From Eq. (12), it follows that for small values of $w(\zeta)$, one has

$$\frac{\partial^2 T_l}{\partial w^2} \approx \frac{\exp[2h_l(w)]}{(1+\exp[h_l(w)])^3}\left\{(f_l(w))^2 + \left(\frac{\partial f_l(w)}{\partial w}\right)\right\}, \quad \text{(B1)}$$

where $f_l(w)$ and $h_l(w)$ are defined as in Eq. (12). From the equation above, we see that the sign of $\frac{\partial^2 T_l}{\partial w^2}$ will depend exclusively on the term $\{(f_l(w))^2 + (\frac{\partial f_l(w)}{\partial w})\}$. We will show that such term, considering the potential barrier for fusion reaction with which we are dealing [Eq. (19)], is always positive when $w(\zeta)$ tends to zero. In order to do this, we first assume the contrary, namely we suppose that $\{(f_l(w))^2 + (\frac{\partial f_l(w)}{\partial w})\}_{w\to 0} \leqslant 0$. Then,

$$\lim_{w\to 0}\left\{-\frac{d}{dw}\left(\frac{1}{f_l(w)}\right)\right\} \leqslant -1 \Rightarrow 1 \geqslant \lim_{w\to 0}\{w f_l(w)\}$$

$$\Rightarrow 1 \geqslant \lim_{w\to 0}\left\{\sqrt{\frac{2\mu}{\hbar^2}}w\int_{r_1(l,w)}^{r_2(l,w)}\frac{dr}{\sqrt{V_l(r)-w}}\right\}.$$

Now, let us make

$$\lim_{w\to 0}\left\{\int_{r_1(l,w)}^{r_2(l,w)}\frac{dr}{\sqrt{V_l(r)-w}}\right\} = \lim_{w\to 0}\left\{\int_{r_1(l,w)}^{r^*}\frac{dr}{\sqrt{V_l(r)-w}}\right\} + \lim_{w\to 0}\left\{\int_{r^*}^{r_2(l,w)}\frac{dr}{\sqrt{V_l(r)-w}}\right\}$$

in which $r_1(l,w) < r^* < r_2(l,w)$. Here r^* is chosen to be greater than the distance at which the attractive nuclear potential becomes negligible. Hence, for $w \to 0$, we have

$$1 \geqslant \lim_{w\to 0}\left\{\sqrt{\frac{2\mu}{\hbar^2}}wI_1\right\} + \lim_{w\to 0}\left\{\sqrt{\frac{2\mu}{\hbar^2}}wI_2\right\}, \quad \text{(B2)}$$

where $I_1 \equiv \int_{r_1(l,w)}^{r^*}\frac{dr}{\sqrt{V_l(r)-w}}$ and $I_2 \equiv \int_{r^*}^{r_2(l,w)}\frac{dr}{\sqrt{V_l(r)-w}}$. Clearly I_1 is bounded for all values of $w \to 0$, and therefore $\lim_{w\to 0}\{\sqrt{\frac{2\mu}{\hbar^2}}wI_1\} = 0$. That leave us with the inequality

$$1 \geqslant \lim_{w\to 0}\left\{\sqrt{\frac{2\mu}{\hbar^2}}wI_2\right\}. \quad \text{(B3)}$$

We now turn to the question whether wI_2 is bounded for $w \to 0$. Performing a change of variables, namely $y = V_l(r) - w$, one gets for I_2

$$I_2 = \int_{V(r^*)-w}^{0}\frac{dy}{\sqrt{y}}\frac{dV_l^{-1}(y+w)}{dy}.$$

Since the point r^* is taken to be much greater than the effective nucleus radius, the contribution for the total potential $V_l(r)$ of the attractive Woods-Saxon potential can be neglected within the interval $(r^*, r_2(l, w))$. Therefore, in the calculations for I_2, we approximate

$$V_l(r) \approx \frac{C_1}{r} + \frac{C_{2l}}{r^2} \tag{B4}$$

in which $C_1 = Z_1 Z_2 e^2$ and $C_{2l} = \frac{\hbar^2 l(l+1)}{2\mu}$. Clearly C_1 and C_{2l} are non-negative. Here we first assume that $l \neq 0$, and therefore C_{2l} is strictly positive. From Eq. (B4), we have

$$r = \frac{C_1 + \sqrt{C_1^2 + 4(y+w)C_{2l}}}{2(y+w)}$$

and accordingly

$$I_2 = \int_{\frac{C_1}{r^*}+\frac{C_{2l}}{r^{*2}}-w}^{0} dy \left[\frac{C_{2l}}{(y+w)\sqrt{y(C_1^2 + 4(y+w)C_{2l})}} - \frac{C_1 + \sqrt{C_1^2 + 4(y+w)C_{2l}}}{2\sqrt{y}(y+w)^2} \right].$$

It is not difficult to prove that $\frac{\partial I_2}{\partial C_1} > 0$. A direct consequence of this fact is that $\lim_{C_1 \to 0}\{I_2(C_1)\} \leqslant I_2(C_1)$, since C_1 is positive. Hence

$$\frac{\sqrt{C_{2l}}}{w}\sqrt{1 - \frac{w(r^*)^2}{C_{2l}}} \leqslant I_2 \Rightarrow \sqrt{C_{2l}} \leqslant \lim_{w\to 0}\{wI_2(w)\}.$$

Combining the last result with the inequality (B3) we find

$$1 \geqslant \sqrt{\frac{2\mu}{\hbar^2}} \lim_{w\to 0}\{wI_2(w)\} \geqslant \sqrt{\frac{2\mu}{\hbar^2}C_{2l}}$$

which implies the absurd result that $\sqrt{l(l+1)} \leqslant 1$ since $C_{2l} = \frac{\hbar^2 l(l+1)}{2\mu}$. By assumption, $l \neq 0$, and hence the minimum value for the term $\sqrt{l(l+1)}$ is $\sqrt{2}$. That leads us to a contradiction, and therefore our initial assumption, $\{(f_l(w))^2 + (\frac{\partial f_l(w)}{\partial w})\}_{w\to 0} \leqslant 0$ cannot be true. Let us examine now the case where $l = 0$, which means that the effective potential $V_l(r)$ used in I_2 will be just the Coulomb potential:

$$V_0(r) \approx \frac{C_1}{r}.$$

With the above potential, the integral I_2 becomes, for $w \to 0$,

$$I_2 = \frac{r^*}{\sqrt{w}}\sqrt{\frac{C_1}{wr^*} - 1} + \frac{2C_1}{w^{\frac{3}{2}}} \arctan \times \left\{ \exp\left[\operatorname{arccosh}\left(\sqrt{\frac{C_1}{wr^*}} \right) \right] \right\} - \frac{\pi C_1}{2w^{\frac{3}{2}}}. \tag{B5}$$

Multiplying both sides of Eq. (B5) by w and taking the limit $w \to 0$, we find that $\lim_{w\to 0}\{wI_2(w)\} = \infty$, and therefore the inequality (B3) can neither be satisfied for the case of the partial wave with $l = 0$, nor the case $l \neq 0$. This proves that the assumption we made at the beginning of this section, namely $\{(f_l(w))^2 + (\frac{\partial f_l(w)}{\partial w})\}_{w\to 0} \leqslant 0$, is false. Therefore, recalling Eq. (B1), we have that for small values of $w(\zeta)$, $\frac{\partial^2 T_l}{\partial w^2} > 0$, which implies, for $w \to 0$, that

$$\langle T_l[E, V_l(r) + H_{\text{int}}(R_l, \zeta)]\rangle_\zeta \geqslant T_l[E, V_l(r) + \langle H_{\text{int}}(R_l, \zeta)\rangle_\zeta], \tag{B6}$$

where $V_l(r)$ is defined by Eq. (19).

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