Semiclassical theory of quantum tunneling in multidimensional systems

N. Takigawa* and G. F. Bertsch
National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy
Michigan State University, East Lansing, Michigan 48824
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A semiclassical method is applied to the problem of quantum tunneling in the presence of internal oscillator degrees of freedom. Comparison with coupled channel calculations verifies the accuracy of the semiclassical method. Providing the coupling has a physically reasonable form factor, the coupling produces an enhancement in the tunneling rate. The enhancement becomes larger when the tunneling degree of freedom couples with a harmonic oscillator with lower frequency. The semiclassical method is found to be quite useful in situations where the coupled channel method becomes numerically difficult.

The effect on quantum tunneling of the internal degrees of freedom has been much discussed recently[1–12] in connection with the large enhancement of subbarrier fusion cross sections found in heavy ion collisions.[10–19] An interesting question in this respect is the relative roles of high- and low-frequency collective excitations of the individual nuclei. The problem is quite difficult to study by the numerical coupled channel methods, when many degrees of freedom are involved simultaneously and one deals with energies much below the barrier. We shall examine the problem using the influence functional formalism of Feynman's path integral method. This method conveniently clarifies the importance of the potential renormalization, and the decisive role of the functional form of the coupling to the internal motion. We compare the results of the path integral method with those of coupled channel calculations to verify the accuracy of the path integral method.

The problem studied is the quantum tunneling of a system, in which the collective tunneling degree of freedom linearly couples to a harmonic oscillator. The corresponding Hamiltonian is postulated as

$$H=\frac{\hat{p}^2}{2\mu}+U(\hat{r})+\hbar\omega(a^\dagger a+\tfrac{1}{2})+\sigma\cdot f(\hat{r})\cdot(a^\dagger+a) \ , \quad (1)$$

where $\hat{r}$ and $\hat{p}$ are the coordinate and the conjugate momentum of the collective tunneling motion. Physically, the coupling coefficient σ is the amplitude of the zero point oscillation of the harmonic oscillator. The function f is a form factor with the dimension of a force, to be specified later.

We focus only on the collective motion, and consider an inclusive tunneling probability $P_{\rm in}$. It is associated with the matrix elements of the Green's function as follows:[20,21]

$$P_{\rm in}=\sum_\beta \frac{k_\beta k_\alpha}{\mu^2}\left|\left\langle r_f\beta\left|\frac{1}{H-E}\right|r_i\alpha\right\rangle\right|^2 \quad (2a)$$

$$=\sum_\beta \frac{k_\beta k_\alpha}{\mu^2}\left|\lim_{\epsilon\to 0^+}\int_0^\infty dt\, e^{i(E+i\epsilon)t}\langle r_f\beta|e^{-iHt}|r_i\alpha\rangle\right|^2 \ . \quad (2b)$$

The sum runs over all final states β of the intrinsic degrees of freedom. We disregard the variation of the momentum k_β from the initial momentum k_α, which is not so large in the problem to be considered in the present work. We also approximate the time integral by the saddle point method.[20] We then consider the following path integral representation[4] of the transition probability from the initial position r_i to the final position r_f during the imaginary time lapse from $t_i=-i\tau_i=0$ to $t_f=-i\tau_f=-iT$:

$$\sum_\beta |\langle r_f\beta|e^{-HT}|r_i\alpha\rangle|^2=J(r_fT;r_i0) \quad (3a)$$

$$=J_R(r_f,r_i;T)J_\eta \ , \quad (3b)$$

where

$$J_R=\int \mathscr{D}R(\tau)\exp\left[-2\int_0^T\left(\frac{\mu}{2}\dot{R}^2+U(R)-E_{\rm c.m.}\right)d\tau/\hbar\right]\times\exp\left(-2\int_0^T W_R(\tau)\,d\tau/\hbar\right) \ , \quad (4)$$

with

$$W_R(\tau)=-\frac{1}{\hbar}\sigma^2(1+e^{-2\omega(T-\tau)})f[R(\tau)]e^{-\omega\tau}\times\int_0^\tau d\tau_1 f[R(\tau_1)]e^{\omega\tau_1} \quad (5)$$

and

$$J_\eta=\int \mathscr{D}\eta(\tau)\exp\{-[\eta(\tau)]^2\ldots\} \ . \quad (6)$$

In these equations we have used the average and the difference, $R(\tau)$ and $\eta(\tau)$, of two paths to determine the transition probability.[4] The influence potential W_R in Eq. (4) takes into account the effect of the linear oscillator coupling on the tunneling probability. In the formulas we derive below, we ignore the factor J_η, which is associated with a quantal effect.[22]

The integral over the average path $R(\tau)$ will be dominated by the saddle point path $\bar{R}(\tau)$. It obeys the following classical equation of motion:[4]

$$\mu\ddot{\bar{R}}(\tau)=\frac{dU}{d\bar{R}}+F(\tau) \ , \quad (7)$$

where

$$F(\tau)=-\frac{\sigma^2}{\hbar}\left(\frac{df}{d\bar{R}}\right)_\tau\left[\left(e^{-\omega\tau}\int_0^\tau d\tau_1 f[\bar{R}(\tau_1)]e^{\omega\tau_1}+e^{\omega\tau}\int_\tau^T d\tau_1 f[\bar{R}(\tau_1)]e^{-\omega\tau_1}\right)+e^{-2\omega T+\omega\tau}\int_0^T d\tau_1 f[\bar{R}(\tau_1)]e^{\omega\tau_1}\right] \ . \quad (8)$$

There is no dissipation effect in the case of $\omega=0$. In this limit, therefore, the effect of coupling can be represented exactly in terms of a renormalization of the potential. The resultant effective tunneling potential barrier $U^{\mathrm{eff}}_{\omega=0}(R)$ is given by

$$U^{\mathrm{eff}}_{\omega=0}(R)=U(R)-\frac{2\sigma^2}{\hbar}f(R)\int_0^T d\tau_1 f[R(\tau_1)] \ . \tag{9}$$

In the opposite limit of high frequency, the effect of linear oscillator coupling can be well represented in terms of a renormalization of the potential. For application to the nuclear fusion problem, this adiabatic limit requires $\omega >> \Omega_0$, where $\hbar\Omega_0 \sim 4$ MeV is the energy scale of the curvature of the potential barrier. The effective potential in this case $U^{\mathrm{eff}}_{\mathrm{ad}}(R)$ is given by[4]

$$U^{\mathrm{eff}}_{\mathrm{ad}}(R)=U(R)-\sigma^2[f(R)]^2/\hbar\omega \ . \tag{10}$$

To make a specific model of the entrance channel potential $U(r)$ and the coupling form factor $f(r)$, we have expanded the Hamiltonian used in Ref. 6 with respect to the coordinate of the harmonic oscillator and truncated by the first order term. This truncation is required because the derivation of the influence potential W_R in Eq. (5) is based on linear coupling.[4] The explicit forms of $U(r)$ and $f(r)$ are as follows:

$$U(r)=U_N(r)+\frac{Z_1Z_2e^2}{r} \ , \tag{11}$$

with

$$U_N(r)=-\frac{U_0}{2}\frac{R_1R_2}{R_1+R_2}\,\mathrm{Erfc}\left[\frac{r-R_1-R_2-\Delta R}{a}\right] \tag{12}$$

and

$$f(r)=-\frac{U_0}{2}\frac{R_1R_2}{R_1+R_2}\frac{1}{a}\frac{2}{\sqrt{\pi}}\exp\left[-\left[\frac{r-R_1-R_2-\Delta R}{a}\right]^2\right] \ . \tag{13}$$

The values of parameters were chosen to be

$$U_0=31.67 \ \ \mathrm{MeV\,fm^{-1}} \ , \tag{14a}$$

$$R_i=1.233A_i^{1/3}-0.98A_i^{-1/3} \ \ \mathrm{fm} \ , \tag{14b}$$

$$\Delta R=0.290 \ \ \mathrm{fm} \ , \tag{14c}$$

and

$$a=0.63\times 4/\sqrt{\pi}=1.422 \ \ \mathrm{fm} \ , \tag{14d}$$

where A_i is the mass number of the projectile or the target.

We have then determined the dominant tunneling path by solving Eq. (7) by iteration. We have ignored the excitation prior to tunneling. This is consistent with Eq. (5), which assumes that the harmonic oscillator is in the ground state at the beginning of the tunneling process, i.e., $|\alpha\rangle=|0\rangle$. Accordingly, we have chosen the initial condition to solve Eq. (7) such that $\bar{R}_i$ equals the outer turning point for the bare tunneling process and the initial velocity is zero. The transmission time $\tau_f=T$ has been identified with the time when the velocity again becomes zero, namely, when it changes sign. The transmission point $\bar{R}_f$ is the corresponding reflection point.

Our approximation to the tunneling probability is the integral J_R evaluated on the dominant path:

$$P_\omega(E_{\mathrm{c.m.}})=\exp\left[-2\int_0^T\left(\frac{\mu}{2}\dot{\bar{R}}^2+U(\bar{R})+W_{\bar{R}}(\tau)-E_{\mathrm{c.m.}}\right)d\tau/\hbar\right] \ . \tag{15}$$

The uniform approximation provides an improved formula for the tunneling probability[20] that we shall use in our calculations:

$$\tilde{P}_\omega(E_{\mathrm{c.m.}})=P_\omega(E_{\mathrm{c.m.}})/[1+P_\omega(E_{\mathrm{c.m.}})] \ . \tag{16}$$

The dependence of the tunneling probability on the oscillator frequency is implicit in the influence potential W.

In Fig. 1 we compare the enhancement factor,

$$\zeta_\omega(E_{\mathrm{c.m.}})=\frac{\tilde{P}_\omega(E_{\mathrm{c.m.}})}{\tilde{P}_{\mathrm{bare}}(E_{\mathrm{c.m.}})} \ , \tag{17}$$

calculated by the present path integral method (solid lines) with the results of coupled channel calculations (dashed lines). In Eq. (17), $\tilde{P}_{\mathrm{bare}}$ is the tunneling probability in the absence of coupling, i.e., when $\sigma=0$. The colliding system is $^{16}O+{}^{148}Sm$. The amplitude of the zero point oscillation has been fixed to be $\sigma=0.2$ fm. We show the results of the coupled channel calculations for the case of $\hbar\omega=0$ MeV and of $\hbar\omega=20$ MeV. We took only two channels for the

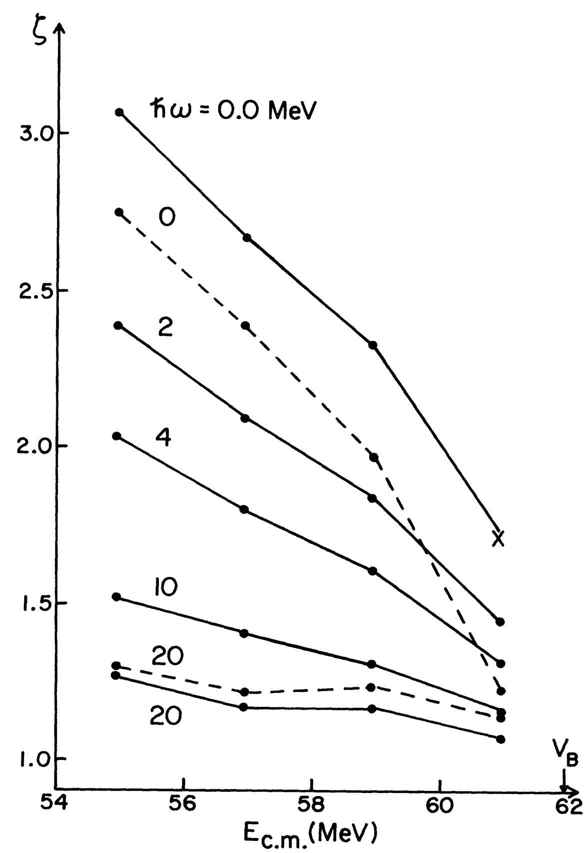

FIG. 1. The enhancement factor ζ is shown as a function of the incident energy. The solid lines are the result of the path integral method, while the dashed lines are the result of the coupled channel calculations. The numbers denote the energy quanta of the intrinsic harmonic oscillator.

latter case. The case of $\hbar\omega=0$ MeV is the case when the disagreement betweeen the path integral calculations and the coupled channel calculations is largest. The path integral method compares quite well with the coupled channel calculations except near the top of the potential barrier, $V_B=61.53$ MeV. The case marked by a cross ($E_{\rm c.m.}=60.93$ MeV, $\hbar\omega=0$ MeV) is beyond the scope of the present method. The imaginary time path integral method breaks down for this case because the effective potential becomes lower than the incident energy.

Under our assumption of a single dominant semiclassical path, the influence functional method can easily be generalized to many internal degrees of freedom.[5] If the internal degrees of freedom are oscillators that couple independently according to Eq. (1), the classical equation of motion (7) has independent contribution to the force from each internal degree of freedom. Practically, the equation can be solved just as easily as in the single oscillator case. The penetrability function will have a product of exponential factors, each of which is represented as the time integral of the influence potential. The approximate effect on the penetrability will thus be given as a product of enhancement factors for each intrinsic degree of freedom. In this respect, the semiclassical method is far superior to the coupled channel method, which is severely limited in the number of channels that can be treated.

Another advantage of the semiclassical method is that there is no limitation in the strength of the coupling. In contrast, the coupled channel method becomes numerically difficult for small ω when the amplitude is large, i.e., for $\sigma \gtrsim 0.4$.

Figure 1 compares also the enhancement factor $\zeta_\omega(E_{\rm c.m.})$ for five different values of ω. The figure shows that the enhancement is larger when the tunneling degree of freedom couples to a harmonic oscillator with lower frequency. This agrees with what has been found in Ref. 6. This frequency dependence of the enhancement can be attributed to the strong ω dependence of the renormalization of the potential barrier. As an example, Fig. 2 compares the effective potential $U^{\rm eff}_{\omega=0}(r)$, Eq. (9), for the case of $E_{\rm c.m.}=56.93$ MeV with the entrance channel potential and the adiabatic potential for $\hbar\omega=20$ MeV. The effective potential $U^{\rm eff}_{\omega=0}(r)$ for different incident energies does not differ so much from that for $E_{\rm c.m.}=56.93$ MeV except when $E_{\rm c.m.}$ is very close to the barrier top energy V_B. Figure 2 shows that the potential renormalization is indeed much larger and favors the enhancement of the tunneling probability for the coupling to an harmonic oscillator with lower frequency.

Caldeira and Leggett[23] have discussed the importance of the dissipation effect in the quantum tunneling in open system problems. They have attributed the hindrance of the quantum tunneling of flux quanta across superconducting junctions to this effect. In order to learn the importance of the effect in the present case, we compared $P_\omega(E_{\rm c.m.})$ with the bare tunneling probability and the adiabatic approximation $P_{\rm ad}(E_{\rm c.m.})$ for the case of $\hbar\omega=20$ MeV. $P_{\rm ad}(E_{\rm c.m.})$ is the tunneling probability through a one-dimensional effective potential barrier $U^{\rm eff}_{\rm ad}(r)$. As is expected on physical grounds, we found that $P_{\rm ad}$ is always larger than the final tunneling probability $P_\omega(E_{\rm c.m.})$. It is, however, only slightly larger than $P_\omega(E_{\rm c.m.})$. This means that the dissipation effect plays a minor role in the adiabatic case. Obviously, there is no dissipation effect in the other extreme limit, i.e., when $\hbar\omega=0$. For small but finite values of ω, the total effect of the oscillator coupling on the collective quantum tunneling cannot be easily factorized into dissipation and potential renormalization effects.[4] Therefore the concept of a dissipation effect does not seem to be useful in discussing the quantum tunneling considered in the present work.

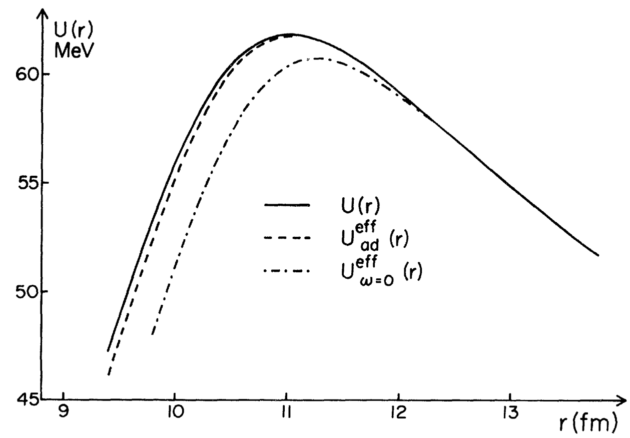

FIG. 2. Comparison of the bare and the renormalized potentials. The solid, dashed, and dot-dashed lines represent the entrance channel potential, the adiabatic potential for $\hbar\omega=20$ MeV, and the effective potential $U^{\rm eff}_{\omega=0}(r)$ for $E_{\rm c.m.}=57$ MeV, respectively.

Finally, we wish to comment on the strong sensitivity of the potential renormalization to the form of the coupling. The integral on the right-hand side of Eq. (9) will almost cancel out if the coupling form factor changes sign during the tunneling process. The corresponding potential renormalization for the case of $\omega=0$ will thus be much smaller in this case than where the sign of the coupling form factor is fixed, as is assumed in this work. Quantum tunneling has often been discussed in the framework of a model having a linear coupling potential in the tunneling degree of freedom.[4,23,24] The above observation is a warning that such a model could give totally different behavior compared with models with physically reasonable coupling potentials.

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*Permanent address: Department of Physics, Tohoku University, 980 Sendai, Japan.

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