Dynamical norm method for nonadiabatic macroscopic quantum tunneling

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We present a method for macroscopic quantum tunneling, named dynamical norm method, which works over a very wide range of situations between the adiabatic and the sudden limits. We examine the validity of the method by studying the effects of linear oscillator coupling on the tunneling rate through an Eckart barrier. We then apply the method to discussing the effects of a nuclear intrinsic excitation on fission. This method shows that the adiabaticity of the tunneling process is governed not only by the relative time scale of the tunneling degree of freedom and of environmental degrees of freedom, but also by the properties of the coupling between them. We also show that the dynamical norm factor which represents nonadiabatic effects in our method is closely related to the dissipation factor in the Caldeira-Leggett theory for dissipative quantum tunneling.

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I. INTRODUCTION

The quantum tunneling in a multidimensional system, which is often called macroscopic quantum tunneling, has been a very popular subject during the past decade in many fields of physics and chemistry [1,2]. In nuclear physics, heavy-ion fusion reactions at energies below the Coulomb barrier are caused by a quantum tunneling of the relative motion between heavy ions. It is now well established that the fusion probability is enhanced by several orders of magnitude by the coupling of the relative motion to nuclear intrinsic motions such as surface vibrations of spherical nuclei, rotations of deformed nuclei, and the neck formation between the colliding nuclei [3]. Spontaneous fission is a typical example of a quantum tunneling in multidimensional space consisted of appropriate shape degrees of freedom [4].

One of the major interests in macroscopic quantum tunneling is to assess the effects of environmental degrees of freedom on the tunneling rate of a macroscopic variable. If the time scale of the tunneling degree of freedom and that of environments considerably differ, one can apply either the adiabatic or the sudden approximation, and the problem can be reduced to a one-dimensional problem by introducing the concepts of potential and mass renormalizations or a barrier distribution [5-8]. In most of the realistic cases, however, deviations from these limits play an important role. In heavy-ion fusion reactions, one can use a direct numerical solution of the coupled-channels equations to handle such intermediate situations. However, this method can be applied to limited problems such as to studying the effects of vibrational excitations.

In this paper we present a method which can be applied to the problems lying between the adiabatic and the sudden tunneling. In this method, we use the adiabatic tunneling as a reference, and represent the deviation from that limit in terms of the reduction of the norm of the environmental space during the tunneling process. We call our method the *dynamical norm method*. The idea of this method has been introduced by Brink, Nemes, and Vautherin [9] by using an extended WKB method [10–12]. Here, we reformulate their approach based on the path integral method. This approach clarifies the underlying assumptions of the method.

The paper is organized as follows. In Sec. II, we briefly review the path integral approach [5] and introduce the dynamical norm factor, which plays the central role in our method. We show that the dynamical norm factor reduces the penetration probability estimated in the adiabatic approximation. In Sec. III, we give an exact expression of the dynamical norm factor for the case of linear oscillator coupling. In Sec. IV, we consider a nearly adiabatic situation and show that the adiabaticity of the tunneling process is governed by both the time scale and the details of the coupling. In Sec. V, we investigate the applicability of our method by considering the effect of linear oscillator coupling on the tunneling probability through an Eckart potential barrier. Comparison with direct numerical solution shows that our method works very well when the energy is much below the barrier. In Sec. VI, we apply our method to studying the effects of a vibrational excitation on the rate of spontaneous fission of 234 U. We also compare the fission rate calculated by the dynamical norm method with that calculated by an alternative approach, i.e., in terms of a tunneling in multidimensional space [13]. In Sec. VII, we show that a constant coupling approximation can provide a good prescription for some cases at energies near and above the barrier, where our method loses its accuracy. In Sec. VIII, we consider the Caldeira-Leggett model in condensed matter physics and show that the dynamical norm factor in our method is very closely related to the dissipation factor found in Ref. [14]. We summarize our paper in Sec. IX.

II. DYNAMICAL NORM FACTOR

Our interest is to calculate the tunneling rate of a macroscopic variable in the presence of environments. We denote the macroscopic variable by R and consider the case where the environment has only one degree of freedom, which is denoted by ξ . It is straightforward to generalize the results to the cases where the environments have many degrees of freedom. In heavy-ion fusion reactions, R and ξ correspond to the coordinate of the relative motion between heavy ions and that of a nuclear intrinsic motion, respectively. We assume the following Hamiltonian:

$$H(R,\xi) = -rac{\hbar^2}{2M}rac{\partial^2}{\partial R^2} + U(R) + H_0(\xi) + V(R,\xi) \;. \;\; (1)$$

Here, M is the mass for the macroscopic motion, U(R)which we call the bare potential is the potential in the absence of the coupling, $H_0(\xi)$ is the nonperturbative Hamiltonian for the internal motion, and $V(R,\xi)$ is the coupling between them.

We are interested in the inclusive process. The barrier transmission probability from the initial position R_i on the right side of the barrier to the final position R_f on the left side is then given by [5]

$$P(E) = \lim_{\substack{R_i \to \infty \\ R_f \to -\infty}} \left(\frac{P_i P_f}{M^2} \right) \int_0^\infty dT \, e^{(i/\hbar)ET} \int_0^\infty d\tilde{T} \, e^{-(i/\hbar)E\tilde{T}} \\ \times \int \mathcal{D}[R(t)] \int \mathcal{D}[\tilde{R}(\tilde{t})] e^{(i/\hbar)[S_t(R,T) - S_t(\tilde{R},\tilde{T})]} \rho_M(\tilde{R}(\tilde{t}),\tilde{T};R(t),T) , \qquad (2)$$

where E is the total energy of the system, P_i and P_f are the classical momenta at R_i and R_f , respectively. We assumed that the energy dissipation is small compared with the total energy and ignored the change of P_f with respect to each final state. $S_t(R,T)$ is the action for the translational motion along a path R(t), and is given by

$$S_t(R,T) = \int_0^T dt [\frac{1}{2} M \dot{R}(t)^2 - U(R(t))] . \qquad (3)$$

The effects of the internal degree of freedom are included in the two time influence functional ρ_M , which is defined by

$$\rho_M(\tilde{R}(\tilde{t}), \tilde{T}; R(t), T) = \sum_{n_f} \langle n_i | \hat{u}^{\dagger}(\tilde{R}(\tilde{t}), \tilde{T}) | n_f \rangle \\ \times \langle n_f | \hat{u}(R(t), T) | n_i \rangle$$
(4)

with

$$i\hbar\frac{\partial}{\partial t}\hat{u}(R,t) = [H_0(\xi) + V(R,\xi)]\hat{u}(R,t) .$$
(5)

 $\hat{u}(R,t)$ is the time evolution operator of the internal motion along a given path R(t). n_i and n_f are the initial and final states of the internal motion at position R_i and R_f , respectively.

The path integral in Eq. (2) cannot be evaluated exactly except for some simple cases or limiting situations, where the excitation energy is strictly zero, i.e., sudden tunneling limit, or where the quantum tunneling occurs infinitely slowly, i.e., adiabatic tunneling limit. A first step towards evaluating the barrier penetrability in general cases is provided by finding the dominant tunneling path R(t) in the stationary phase approximation without regarding the influence functional, and then calculating it along the dominant path. We should, however, like to take the effects of coupling on the tunneling path into account.

To this end, we first introduce the adiabatic states by

$$[H_0(\xi) + V(R,\xi)]\varphi_n(R,\xi) = \epsilon_n(R)\varphi_n(R,\xi) .$$
 (6)

We then redefine the action for the translational motion by incorporating the adiabatic potential shift $\epsilon_0(R(t))$, such that

$$S_t^{\rm ad}(R,T) = \int_0^T dt [\frac{1}{2}M\dot{R}(t)^2 - U(R(t)) - \epsilon_0(R(t))] .$$
(7)

Correspondingly, the time evolution operator for the intrinsic motion and the influence functional in the adiabatic frame are defined by

$$i\hbar \frac{\partial}{\partial t} \hat{u}_{A}(R(t),t) = [H_{0}(\xi) + V(R,\xi) - \epsilon_{0}(R)] \\ \times \hat{u}_{A}(R(t),t) , \qquad (8)$$

$$\rho_{A}(\tilde{R}(\tilde{t}), \tilde{T}; R(t), T) = \sum_{n_{f}} \langle n_{i} | \hat{u}_{A}^{\dagger}(\tilde{R}(\tilde{t}), \tilde{T}) | n_{f} \rangle$$
$$\times \langle n_{f} | \hat{u}_{A}(R(t), T) | n_{i} \rangle . \tag{9}$$

We then rewrite the barrier penetrability as

$$P(E) = \lim_{\substack{R_i \to \infty \\ R_f \to -\infty}} \left(\frac{P_i P_f}{M^2} \right) \int_0^\infty dT \, e^{(i/\hbar)ET} \int_0^\infty d\tilde{T} \, e^{-(i/\hbar)E\tilde{T}} \\ \times \int \mathcal{D}[R(t)] \int \mathcal{D}[\tilde{R}(\tilde{t})] e^{(i/\hbar)[S_t^{\mathrm{ad}}(R,T) - S_t^{\mathrm{ad}}(\tilde{R},\tilde{T})]} \rho_A(\tilde{R}(\tilde{t}),\tilde{T};R(t),T) \,.$$
(10)

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We introduce the stationary phase approximation at this stage by disregarding the effects of the modified influence functional ρ_A on the dominant tunneling path. The influence functional evaluated along the dominant path $R_{s.p.}(t)$ now becomes

$$\rho_A(R_{\rm s.p.}, T^*_{\rm s.p.}; R_{\rm s.p.}, T_{\rm s.p.}) = \sum_{n_f} |\langle n_f | \hat{u}_A(R_{\rm s.p.}, \xi) | n_i \rangle|^2 \tag{11}$$

$$= \int_{-\infty}^{\infty} d\xi |\langle \xi | \hat{u}_A(R_{\mathbf{s}.\mathbf{p}.},\xi) | n_i \rangle|^2 .$$
(12)

This is nothing but the norm of the internal wave function at the time when the tunneling process is completed. We therefore call it "dynamical norm factor" and denote it by \mathcal{N}_b ; i.e.,

$$\mathcal{N}_{b} = \rho_{A}(R_{\rm s.p.}, T^{*}_{\rm s.p.}; R_{\rm s.p.}, T_{\rm s.p.}) .$$
(13)

The barrier penetrability for the inclusive process is finally given by

$$P(E) = \left| \lim_{\substack{R_i \to \infty \\ R_f \to -\infty}} \left(\frac{P_i P_f}{M^2} \right)^{1/2} \int_0^\infty dT e^{iET/\hbar} \int \mathcal{D}[R(t)] \exp\left[\frac{i}{\hbar} \int_0^T dt \left(\frac{1}{2} M \dot{R}^2 - U(R(t)) - \epsilon_0(R(t)) \right) \right] \right|^2 \mathcal{N}_b \quad (14)$$
$$= P_0(E; U_{ad}) \mathcal{N}_b, \tag{15}$$

where $P_0(E; U_{ad})$ is the barrier penetrability through the one-dimensional adiabatic potential barrier $U(R) + \epsilon_0(R)$ with the total energy E. Nonadiabatic effects are taken into account by the dynamical norm factor.

The norm of the internal wave function is, of course, normalized to one in the classically allowed region. This is, however, not the case during the tunneling process. This is because the stationary phase evaluations of the integrals over the path and the time in Eq. (10) lead to the evolution of the tunneling process along the imaginary time axis. The time evolution operator for the internal degree of freedom thus obeys

$$-\hbar \frac{\partial}{\partial \tau} \hat{u}_{A}(R(\tau),\xi) = [H_{0}(\xi) + V(R(\tau),\xi) - \epsilon_{0}(R(\tau))] \\ \times \hat{u}_{A}(R(\tau),\xi) .$$
(16)

The time derivative of the norm of the space of the internal motion is then given by

$$\frac{\partial \mathcal{N}}{\partial \tau} = -\frac{2}{\hbar} \langle n_i | \hat{u}_A^{\dagger} (H_0 + V - \epsilon_0) \hat{u}_A | n_i \rangle .$$
 (17)

If we expand the internal wave function by the adiabatic basis defined by Eq. (6)

$$\hat{u}_{A}|n_{i}\rangle = \sum_{n} a_{n}(\tau) \exp\left\{-\hbar^{-1} \int_{0}^{\tau} d\tau' [\epsilon_{n}(\tau') - \epsilon_{0}(\tau')]\right\} \\ \times |\varphi_{n}(R(\tau))\rangle , \qquad (18)$$

we can obtain

$$\frac{\partial \mathcal{N}}{\partial \tau} = -\frac{2}{\hbar} \sum_{n} \left| a_{n}(\tau) \right| \\ \times \exp\left\{ -\hbar^{-1} \int_{0}^{\tau} d\tau' [\epsilon_{n}(\tau') - \epsilon_{0}(\tau')] \right\} \right|^{2} \\ \times [\epsilon_{n}(R) - \epsilon_{0}(R)] \leq 0 .$$
(19)

Hence the norm keeps on decreasing during the tunneling process except for the case of extreme adiabatic limit, where the internal state always remains in the ground state during the tunneling process. In general, $\mathcal{N}_b < 1$ when the tunneling process is accomplished. The dynamical norm factor therefore reduces the barrier penetration probability estimated in the adiabatic limit.

III. ANALYTIC EXPRESSION OF DYNAMICAL NORM FACTOR FOR LINEAR OSCILLATOR COUPLING

A popular example of the macroscopic quantum tunneling is the linear oscillator coupling. In this case one can obtain an analytic expression of the dynamical norm factor in terms of the coupling form factor.

Let us express the Hamiltonian for the internal motion and the coupling Hamiltonian as

$$H_0(\xi) + V(R,\xi) = \hbar\omega(a^{\dagger}a + \frac{1}{2}) + \alpha_0 f(R)(a^{\dagger} + a) ,$$
(20)

where $\hbar \omega$, a (a^{\dagger}) , α_0 , and f(R) are the oscillator quanta, the annihilation (creation) operator of the oscillator, the amplitude of the zero point motion of the oscillator, and the coupling form factor, respectively.

The two time influence functional for this problem is given by [5]

$$\rho_M(\tilde{R}(\tilde{t}), \tilde{T}; R(t), T) = e^{-i\omega(T-\tilde{T})/2} \\ \times \exp\left(-\frac{\alpha_0^2}{\hbar^2}(y_1 + y_2 + y_3)\right) \quad (21)$$

with

$$y_{1} = \int_{0}^{T} dt \int_{0}^{t} ds f(R(t)) f(R(s)) e^{-i\omega(t-s)} , \qquad (22)$$

$$y_2 = \int_0^{\tilde{T}} d\tilde{t} \int_0^{\tilde{t}} d\tilde{s} f(\tilde{R}(\tilde{t})) f(\tilde{R}(\tilde{s})) e^{i\omega(\tilde{t}-\tilde{s})} , \qquad (23)$$

$$y_{3} = -e^{i\omega(\tilde{T}-T)} \int_{0}^{T} dt f(R(t)) e^{i\omega t}$$
$$\times \int_{0}^{\tilde{T}} d\tilde{t} f(\tilde{R}(\tilde{t})) e^{-i\omega \tilde{t}} .$$
(24)

By performing a partial integration once, we obtain

$$y_{1} = \frac{1}{i\omega} \int_{0}^{T} dt f(R(t))^{2} -\frac{1}{i\omega} \int_{0}^{T} dt \int_{0}^{t} ds f(R(t)) \frac{df(R(s))}{ds} e^{-i\omega(t-s)} , \quad (25)$$
$$y_{2} = -\frac{1}{i\omega} \int_{0}^{\tilde{T}} d\tilde{t} f(\tilde{R}(\tilde{t}))^{2}$$

$$+\frac{1}{i\omega}\int_{0}^{\tilde{T}}d\tilde{t}\int_{0}^{\tilde{t}}d\tilde{s}f(\tilde{R}(\tilde{t}))\frac{df(\tilde{R}(\tilde{s}))}{d\tilde{s}}e^{i\omega(\tilde{t}-\tilde{s})}.$$
 (26)

The first term in Eqs. (25) and (26) contributes to the adiabatic potential renormalization. The influence functional in the adiabatic frame is therefore obtained by

$$\rho_A(\tilde{R}(\tilde{t}), \tilde{T}; R(t), T) = \exp\left(-\frac{\alpha_0^2}{\hbar^2}(z_1 + z_2 + z_3)\right) \quad (27)$$

with

$$z_{1} = -\frac{1}{i\omega} \int_{0}^{T} dt \int_{0}^{t} ds f(R(t)) \frac{df(R(s))}{ds} e^{-i\omega(t-s)} , \quad (28)$$

$$z_2 = \frac{1}{i\omega} \int_0^T d\tilde{t} \int_0^t d\tilde{s} f(\tilde{R}(t)) \frac{df(\tilde{R}(\tilde{s}))}{d\tilde{s}} e^{i\omega(\tilde{t}-\tilde{s})} , \qquad (29)$$

$$z_3 = y_3$$
 . (30)

Since we are considering a tunneling process, we replace the real time with the imaginary time, and assume that the tunneling time is uniquely determined to be T_0 :

$$t \to -i\tau_1, \quad s \to -i\tau_2, \quad T \to -iT_0 \quad ,$$
 (31)

$$\tilde{t} \to i\tau_i, \quad \tilde{s} \to i\tau_2, \quad T \to iT_0 \;.$$
 (32)

We thus obtain

$$\mathcal{N}_{b} = \exp\left[-2\left(\frac{\alpha_{0}}{\hbar}\right)^{2}\frac{1}{\omega}\int_{0}^{T_{0}}d\tau_{1}f(R(\tau_{1}))e^{-\omega\tau_{1}}\int_{0}^{\tau_{1}}d\tau_{2}\left(\frac{df(R(\tau_{2}))}{d\tau_{2}}e^{\omega\tau_{2}}\right)\right]$$
$$\times \exp\left[\left(\frac{\alpha_{0}}{\hbar}\right)^{2}e^{-2\omega T_{0}}\left(\int_{0}^{T_{0}}d\tau_{1}f(R(\tau_{1}))e^{\omega\tau_{1}}\right)^{2}\right].$$
(33)

This is the analytic expression of the dynamical norm factor which we tried to derive. We will use Eq. (33) in Sec. VI to discuss the effects of a vibrational mode of excitation on fission.

IV. PERTURBATIVE EXPRESSION OF DYNAMICAL NORM FACTOR AND CRITERION OF ADIABATICITY

A method to calculate the dynamical norm factor in general cases is to determine the expansion coefficients a_n in Eq. (18) by solving the coupled linear differential equations,

$$\frac{\partial a_n}{\partial \tau} - \sum_{m \neq n} a_m \frac{\partial R}{\partial \tau} \langle \varphi_n | \frac{\partial}{\partial R(\tau)} | \varphi_m \rangle \exp\left\{ -\hbar^{-1} \int_0^\tau d\tau' [\epsilon_m(\tau') - \epsilon_n(\tau')] \right\} = 0 .$$
(34)

In this section we solve this equation perturbatively by considering a nearly adiabatic situation. We then use the resultant expression of the dynamical norm factor to discuss the parameters governing the adiabaticity of the tunneling process.

The first order solution of Eq. (34) is given by [8]

$$a_{n}^{(1)}(\tau) = \delta_{n,0} + (1 - \delta_{n,0})\dot{R}(\tau) \\ \times \langle \varphi_{n}(R(\tau),\xi) | \frac{\partial}{\partial R(\tau)} | \varphi_{0}(R(\tau),\xi) \rangle \frac{-\hbar}{\epsilon_{n}(\tau) - \epsilon_{0}(\tau)} \exp\left(\int_{0}^{\tau} d\tau' [\epsilon_{n}(\tau') - \epsilon_{0}(\tau')]/\hbar\right) , \qquad (35)$$

where the matrix element on the right-hand side of Eq. (35) can be rewritten as

$$\langle \varphi_n(R(\tau),\xi) | \frac{\partial}{\partial R(\tau)} | \varphi_0(R(\tau),\xi) \rangle = -\frac{1}{\epsilon_n(\tau) - \epsilon_0(\tau)} \langle \varphi_n(R(\tau),\xi) | \frac{\partial V(R(\tau),\xi)}{\partial R(\tau)} | \varphi_0(R(\tau),\xi) \rangle .$$
(36)

If the coupling Hamiltonian is separable

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$$V(R,\xi) = f(R)g(\xi) , \qquad (37)$$

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then this matrix element reads

$$\langle \varphi_n(R(\tau),\xi) | \frac{\partial}{\partial R(\tau)} | \varphi_0(R(\tau),\xi) \rangle = -\frac{1}{\epsilon_n(\tau) - \epsilon_0(\tau)} \frac{\partial f(R(\tau))}{\partial R(\tau)} g_{n0}$$
(38)

with

$$g_{n0} = \langle \varphi_n(R(\tau), \xi) | g(\xi) | \varphi_0(R(\tau), \xi) \rangle .$$
(39)

The first order solution is therefore given by

$$a_n^{(1)}(\tau) = \delta_{n,0} + (1 - \delta_{n,0}) \frac{\hbar \dot{R}(\tau)}{[\epsilon_n(\tau) - \epsilon_0(\tau)]^2} \frac{\partial f(R(\tau))}{\partial R(\tau)} g_{n0} \exp\left(\int_0^\tau d\tau' [\epsilon_n(\tau') - \epsilon_0(\tau')]/\hbar\right)$$
(40)

Equations (19) and (40) lead to the following expression for the dynamical norm factor:

$$\mathcal{N}_{b} = 1 - \int_{0}^{T_{0}} d\tau \frac{2}{\hbar} \sum_{n} \left| a_{n} \exp\left(-\hbar^{-1} \int_{0}^{\tau} d\tau' [\epsilon_{n}(\tau') - \epsilon_{0}(\tau')] \right) \right|^{2} [\epsilon_{n}(\tau) - \epsilon_{0}(\tau)]$$

$$\tag{41}$$

$$= 1 - 2\hbar \sum_{n} g_{n0}^{2} \int_{0}^{T_{0}} d\tau \frac{R^{2}}{[\epsilon_{n}(\tau) - \epsilon_{0}(\tau)]^{3}} \left(\frac{df}{dR}\right)^{2}$$
(42)

$$\sim \exp\left[-2\hbar \sum_{n} g_{n0}^2 \int_0^{T_0} d\tau \frac{\dot{R}^2}{[\epsilon_n(\tau) - \epsilon_0(\tau)]^3} \left(\frac{df}{dR}\right)^2\right]$$
(43)

In order to more explicitly see the physical implications of Eq. (43), we consider now a problem of double linear oscillator coupling, i.e., the case where

$$H_0(\xi) + V(R,\xi) = \hbar\omega(a^{\dagger}a + \frac{1}{2}) + c\alpha_0 R(a^{\dagger} + a)$$
. (44)

The dynamical norm factor in the lowest order perturbation approximation is then given by

$$\mathcal{N}_{b} = \exp\left[-\frac{\pi}{2} \left(\frac{\alpha_{0} c R_{0}}{\hbar \omega}\right)^{2} \frac{\Omega}{\omega}\right] . \tag{45}$$

In obtaining Eq. (45) we approximated the bare potential barrier U(R) by a parabolic function $\frac{1}{2}M\Omega^2 R^2$ and the tunneling path $R(\tau)$ by $R_0 \cos\Omega\tau$, R_0 being the thickness of the tunneling region.

Equation (45) implies that the adiabaticity of the tunneling process depends not only on the ratio of the energy scale Ω/ω , in other words the ratio of the time scales of the tunneling process and of the intrinsic motion, but also on the ratio of the coupling strength to the excitation energy of the nonperturbative system $\alpha_0 c R_0/\hbar\omega$. As we see in Eq. (43), the radial dependence of the coupling form factor is also an important factor to govern the adiabaticity of the tunneling process. This has been pointed out also in Ref. [15]. We will use Eq. (45) in Sec. VIII to show that the dynamical norm factor in our method is intimately related to the dissipation factor obtained by Caldeira and Leggett in their seminal work on the macroscopic quantum tunneling [14].

V. APPLICABILITY OF THE DYNAMICAL NORM METHOD

In this section we examine the accuracy and the usefulness of our dynamical norm method by applying it to a problem, where a macroscopic variable which tunnels through an Eckart potential barrier linearly couples to a harmonic oscillator [see Eq. (20)]. We assume that the coupling form factor is a square root of the Eckart potential. This makes our calculations simpler, because the adiabatic barrier then becomes also an Eckart potential. Notice that the barrier transmission probability can be written analytically for an Eckart potential [16].

The bare potential and the coupling form factor are given by

$$U(R) = \frac{U_0}{\cosh^2(R/a)} , \qquad (46)$$

$$f(R) = \frac{f_0}{\cosh(R/a_f)} , \qquad (47)$$

where the parameters were chosen such that, $U_0 = 10 \text{ MeV}$, a = 5 fm, $M = 2000 \text{ MeV}/c^2$, $f_0 = 1 \text{ MeV/fm}$, $a_f = 5 \text{ fm}$, and $\alpha_0 = 1 \text{ fm}$. The curvature of the potential barrier $\hbar\Omega$ is 2.8 MeV. The oscillator quanta of the intrinsic vibration was assumed to be $\hbar\omega = 1 \text{ MeV}$. Our example therefore corresponds to the case of a fast quantum tunneling, where the formula of the quantum

tunneling in the sudden limit will offer a good zeroth order estimate, but where a sizable deviation from it can be expected. The values of the intrinsic excitation energy and the barrier curvature correspond to typical values in realistic heavy ion fusion reactions. We notice that the comparison of the results of the exact analytic expression for the transmission probability through the bare Eckart potential with those in the WKB approximation confirms that semiclassical approach is accurate enough to describe the present problem.

In solving Eq. (34), to determine a_n we truncated at some maximum oscillator quanta N_{max} . Also, we assumed that the tunneling path can be well approximated by

$$\frac{\partial R}{\partial \tau} = -\sqrt{\frac{2}{M}[U(R) + \epsilon_0(R) - E]} .$$
(48)

Using the values of thus obtained expansion coefficients a_n at the end of the tunneling, i.e., at $\tau = T_0$, we calculated the dynamical norm factor by

$$\mathcal{N}_{b} = \sum_{n=0}^{N_{\max}} \left| a_{n}(T_{0}) \exp\left(-\hbar^{-1} \int_{0}^{T_{0}} d\tau [\epsilon_{n}(\tau) - \epsilon_{0}(\tau)] \right) \right|^{2} .$$

$$(49)$$

The result for the tunneling probability is shown in Fig. 1 as a function of the bombarding energy for energies below the potential barrier. The dotted line is the tunneling probability for the bare potential barrier, and corresponds to the case without coupling. The dot-dashed line represents the results of the direct numerical solution of the coupled-channels equations. The thin solid line is the result of the adiabatic approximation, where only the adiabatic potential renormalization due to the coupling was taken into account. It clearly overestimates the enhancement of the tunneling probability due to the coupling to the environment. By taking the dynamical norm factor into account, we obtain the thick solid line, which agrees very well with the exact numerical results. For comparison, the barrier penetrability calculated in the limit of sudden approximation (the dashed line) is also included in Fig. 1. As we remarked before, the present input parameters correspond to a sudden tunneling rather than to an adiabatic tunneling. Consequently, the result in the sudden approximation (the dashed line) is closer to the accurate result (the dot-dashed line) than that in the adiabatic approximation (the thin solid line), but still deviates significantly from the accurate result. It is remarkable that the dynamical norm method provides a much better reproduction of the accurate result than that in the sudden approximation even in an unfavorable situation, which belongs to a fast quantum tunneling rather than to an adiabatic tunneling.

The convergence of solving Eq. (34) with respect to the maximum oscillator state, i.e., N_{\max} , was fairly fast. This convergence feature is shown in Fig 2 by taking the barrier penetrability and N_{max} as the ordinate and the abscissa, respectively. The corresponding bombarding energy is 7.1 MeV in the center of mass system. The results of our dynamical norm method are shown by filled circles and are connected by thick solid lines. The penetrability obtained by the adiabatic approximation is denoted by the dotted line and the result of the exact numerical integration of the coupled-channels equations is denoted by the cross. This figure shows that only two states are needed to converge the calculation of Eq. (34). It also shows that the excited states with oscillator quanta higher than three do not play a very important role in enhancing the tunneling probability at this energy [17]. This example clearly shows the power of our dynamical norm method to obtain an accurate estimate of the tunneling rate under influence of environments.



FIG. 1. Barrier penetration probability as a function of the center of mass energy. The dotted line is the barrier penetrability in the potential model without coupling, while the dot-dashed line is the results of the direct numerical solution of the coupled-channels equations. The thin solid line and the dashed line are the results in the adiabatic and in the sudden approximations, respectively. The results of the dynamical norm method are given by the thick solid line.



FIG. 2. Convergence behavior of the barrier penetrability calculated by the dynamical norm method (the solid circles) as a function of the number of included states N_{\max} , where $N_{\max} = 0$ corresponds to the case without coupling. The bombarding energy is 7.1 MeV. The barrier penetrability calculated in the adiabatic approximation is denoted by dots, and the result of the exact numerical integration of the coupled-channels equations is given by the cross.

VI. APPLICATION TO SPONTANEOUS FISSION OF ²³⁴U

As an application of our method, we study in this section the model of Brink et al. for the spontaneous fission of 234 U [9] by our dynamical norm method. In this nucleus there is a series of low lying excited states, which could be understood as a beta-vibrational band built on the 0^+ state at 0.85 MeV. In addition, there are 0^+ and 2⁺ states at 1.05 MeV and at 1.09 MeV, respectively, which have appreciable transition strengths to the states in the beta-vibrational band [18]. Brink *et al.* considered these additional states to represent a vibrational mode of excitation orthogonal to the beta vibration, and discussed their effects on the spontaneous fission of $^{234}\mathrm{U}$ by treating the beta vibration and the additional states as the coordinate of the fission R and an environmental coordinate ξ , respectively. The Hamiltonian which they assumed reads

$$H(R,\xi) = -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial R^2} + U(R) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial \xi^2} + \frac{1}{2}m\omega^2\xi^2 + cR\xi, \qquad (50)$$

with

$$U(R) = \frac{1}{2}M\Omega^2 R^2 (1 - R/R_b) .$$
 (51)

Following Ref. [9] we assume that the beta band and the additional states mentioned above are originally degenerate to each other with the excitation energy $\hbar\Omega = \hbar\omega = 0.97$ MeV and are split by the coupling. The coupling strength is then determined to be $\hbar\sqrt{c^2/Mm\Omega^2} = 0.25$ MeV. The range of the tunneling region in the bare potential R_b was chosen to be 12.83 fm so as to reproduce the experimental spontaneous fission width in the case when one considers only the bare potential U(R), though more consistently, it should be determined by taking the effects of coupling into account. We consider the symmetric fission. The mass of the tunneling motion is therefore $M = 234M_N/4, M_N$ being the nucleon mass. We estimate the mass of the intrinsic motion ξ based on the liquid drop model to be

$$m = \frac{3}{8\pi} A M_N R_0^2, \tag{52}$$

where A is the atomic number of the parent nucleus 234 U and R_0 its equivalent sharp surface radius.

Figure 3 shows the fission rate plotted as the ratio to that in the absence of the coupling. The dotted line is the fission rate estimated in the adiabatic approximation. The results of our dynamical norm method are given by the solid circles and are connected by thick solid lines. The abscissa is the number of states used to solve the coupled linear differential equations (34) to determine the expansion coefficients a_n . For comparison, we also added the results of the perturbation solution (43) by an open square and of analytic expression (33) by an open triangle, respectively. One can draw several conclusions from this figure. It suggests that the fission rate is strongly



FIG. 3. The effects of environment on the spontaneous fission of 234 U. The fission rate calculated by the dynamical norm method is shown as a function of the number of states $(N_{\rm max})$ considered in solving Eq. (34) (the solid circles). It is plotted in the ratio to that without coupling. The result in the adiabatic approximation, that obtained by using the analytic expression of the dynamical norm factor Eq. (33), and that obtained in the perturbation theory Eq. (43) are denoted by the dots, the open triangle, and the open square, respectively. The cross denotes the fission rate calculated by the method of Schmid by treating the same problem as a two-dimensional quantum tunneling.

enhanced by nuclear intrinsic motions. It is important to take into account nonadiabatic effects in order to properly estimate the magnitude of this enhancement. The agreements between the solid circle at $N_{\text{max}} = 1$ with the open square and between the solid circles for large $N_{\rm max}$ with the open triangle ensure the accuracy of our numerical procedure to determine the dynamical norm factor. The figure also shows that the effect of the intrinsic motion ξ quickly saturates as a function of the maximum number of states N_{\max} incorporated in determining the dynamical norm factor. Incidentally, our estimate of the fission rate including the dynamical norm factor agrees very well with the result of Brink et al. obtained by a slightly different method. In calculating the exact dynamical norm factor (the open triangle), we used the parabolic approximation for the path of the macroscopic degree of freedom R.

One interesting thing is to compare our result with the result of a totally different way of estimating the fission rate, i.e., the fission rate estimated by considering the same problem as a quantum tunneling in the twodimensional space spanned by R and ξ . We use the method of Schmid [13,19,20] in order to obtain this alternative estimate of the fission rate. This is a generalization of the WKB method to the quantum tunneling in a multidimensional space.

In this method, the so-called escape path in the multidimensional space plays the central role. It is a kind of classical path. If we use generalized notations for the coordinates, such that $r_1 = R$ and $r_2 = \xi$ for our problem, then the escape path is obtained by solving

$$\frac{dr_i}{d\tau} = \frac{\partial H_0}{\partial p_i}, \quad \frac{dp_i}{d\tau} = -\frac{\partial H_0}{\partial r_i}, \tag{53}$$

where

$$H_0 = \sum_{i,j} p_i (\mathcal{M}^{-1})_{ij} p_j - V(\vec{r}) .$$
 (54)

The \mathcal{M} and V in Eq. (54) are the mass tensor and the potential in the multidimensional space. In the problem given by Eq. (50), \mathcal{M} is a diagonal 2×2 matrix and V is given by

$$V(\vec{r}) = U(R) + \frac{1}{2}m\omega^2\xi^2 + cR\xi .$$
 (55)

One often represents the decay width as a product of the exponential factor and a prefactor

$$\Gamma = A e^{-2S_{\rm EP}/\hbar} , \qquad (56)$$

where

$$S_{\rm EP} = \int_{\rm EP} \sum_{i,j} \dot{r}_i \mathcal{M}_{ij} \dot{r}_j d\tau . \qquad (57)$$

As indicated in these equations, the exponential factor is given by the action integral along the escape path. The procedure to find the prefactor A for multidimensional tunneling problems is much more complicated than the case for one-dimensional problems. In this paper, we approximated it by the prefactor for a one-dimensional problem along the escape path, which is further simulated by the escape path through a quadratic plus a cubic function potential. The actual formula which we used is given by [13]

$$A/\omega = 60^{1/2} \left(\frac{2S_{\rm EP}}{2\pi\hbar}\right)^{1/2} \,. \tag{58}$$

The result obtained by the method of Schmid is denoted in Fig. 3 by the cross. It agrees fairly well with the result obtained by the dynamical norm method. Figure 4 shows the potential energy surface and tunneling paths for our problem. We can see that only one escape path (the thick dashed line) is found. All the other paths are reflected before they reach the boundary to the classically allowed region, which is denoted by a thick solid line.

VII. CONSTANT COUPLING APPROACH TO NEAR AND ABOVE BARRIER PROBLEMS

We have shown in Sec. V that the dynamical norm method can accurately estimate the tunneling rate including the effects of environments at energies well below

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FIG. 4. The potential energy surface in the (R, ξ) space (the thin solid lines) and the escape path (the thick dashed line) for the spontaneous fission of ²³⁴U. Several classical paths are also shown by dotted lines. The thick solid line divides the classically allowed and the classically forbidden regions.

the potential barrier. We thus expect that it becomes a powerful method in treating especially those problems which cannot be easily handled by standard coupledchannels calculations.

We found, however, that the dynamical norm method loses accuracy at energies near and above the potential barrier. The problem is more serious at energies above the barrier. We derived our key formula Eq. (15) by assuming that there exists a dominant tunneling path, which is common to all the final states of the intrinsic motion. In principle, however, the dominant tunneling path will depend on each final state. It might become important to take this effect into account, especially at energies above the barrier, because the change of the energy of the macroscopic motion for each final state of the intrinsic motion delicately influences at energies above the barrier to make the barrier transmission either classically allowed or classically forbidden.

Another possible reason of the failure is that the multiple reflections under the barrier must be properly treated at energies near and above the potential barrier [21]. The uniform approximation [21] must be used there. However, the uniform approximation for multidimensional tunneling problems has not yet been developed.

A possible way to circumvent this difficulty is to resort to a constant coupling model, i.e., to approximate the coupling Hamiltonian by its value at a fixed position of the macroscopic variable $R = R_0$. The transition amplitude of the internal motion can then be calculated as

$$\langle n_f | \hat{u}_A(R(t),\xi) | n_i \rangle = \langle n_f | \exp\left((i/\hbar) \int_0^t dt [H_0(\xi) + V(R_0,\xi) - \epsilon(R_0)] \right) | n_i \rangle$$
 (59)

$$= \sum_{n} \langle n_f | n(R_0) \rangle \exp\left\{-(i/\hbar) [\epsilon_n(R_0) - \epsilon_0(R_0)]t\right\} \langle n(R_0) | n_i \rangle$$
(60)

We then obtain

$$P = \sum_{n} |\langle n(R_0) | n_i \rangle|^2 \times P_0(E - [\epsilon_n(R_0) - \epsilon_0(R_0)]; U_{ad}) .$$
(61)

In Fig. 5 we compare the barrier penetrability calculated by the exact numerical solution of the coupledchannels equations (the dot-dashed line), in the adiabatic approximation (the thin solid line), in the potential model without coupling (the thin dotted line), and in the constant coupling model (the thick dot-dashed line) for the same system as that for Fig 1. There could be two different versions of the constant coupling model. In one of them, which we call the adiabatic constant coupling model, we introduce the constant coupling approximation after we incorporate the adiabatic potential shift in redefining the potential barrier and hence after redefining the coupling Hamiltonian. In the other, which we call the bare constant coupling model, the constant coupling approximation is introduced for the original coupling Hamiltonian [22]. Since one cannot distinguish the results of the adiabatic and the bare constant coupling approximations on the scale of Fig 5 for this model, the figure contains only one of them. Figure 5 shows that the constant coupling models provide a fairly good description of the effects of channel coupling over the whole energy range. We have chosen R_0 to be the position of the potential barrier.

The quality of the two constant coupling approximations depends on the system. It is likely that the adiabatic constant coupling model has a wider applicability than the bare constant coupling model, because an important part of the coupling is included without approximation in renormalizing the potential barrier through the adiabatic potential shift. Figure 6 shows one such example, where the two constant coupling models have fairly different accuracy. The system is the same as that



FIG. 5. Comparison of the barrier penetrability calculated by several methods. The system is given by an Eckart potential barrier and a linear oscillator coupling. The thin dot-dashed line is the results of the exact numerical solution of the coupled-channels calculations. The thin dotted and the thin solid lines are the results in the potential model and in the adiabatic approximation, respectively. The results of the constant coupling approximation are shown by the thick dot-dashed line.

studied by Dasso *et al.* in Ref. [15] to discuss the adiabaticity of a tunneling process. The bare potential is given by a Gaussian function and the intrinsic motion has only two states. The coupling form factor is given also by a Gaussian function

$$U(R) = U_0 \exp(-R^2/2\sigma^2), \quad F(R) = F_0 \exp(-R^2/2\sigma_F^2) .$$

(62)

Following Dasso *et al.* we chose $U_0 = 10$ MeV, $F_0 = 3$ MeV, $\sigma = 3$ fm, and $\sigma_F = 2$ fm. The mass and the Q value, i.e., the splitting between the two intrinsic states, were chosen to be twice the proton mass and -1 MeV, respectively, to mimic the fusion of a light nuclear system [15].

Figure 6 shows that the adiabatic constant coupling approximation (the thick dot-dashed line) is more accurate than the bare constant coupling approximation (the thick dotted line). Namely, the former better reproduces the results of the exact numerical integration of the coupled-channels equations (the thin dot-dashed line). The figure also contains the results of the dynamical norm method (the thick solid line). Although it is the best among all the approximations in the energy range shown in the figure, it largely deviates from the results of the coupled-channels calculations at higher energies, while the agreement between the coupled-channels calculations and the results of the adiabatic constant coupling approximation persist even at high energies similarly to Fig 5. Figure 6 also contains the result of the sudden approximation (the dashed line). Though globally it is better than the result in the adiabatic approximation, it significantly deviates from the exact result. This is the same situation as in Fig. 1.



FIG. 6. Comparison of the barrier penetrability calculated by several methods. The system is given by a Gaussian potential barrier and an intrinsic motion with two levels. The thin dot-dashed line is the results of the exact numerical solution of the coupled-channels calculations. The thick solid line is the results of the dynamical norm method. The thin dotted line is the result in the potential model. The thin solid and the dashed lines are the results in the adiabatic and in the sudden approximations, respectively. The results of the adiabatic and the bare constant coupling approximations are shown by the thick dot-dashed and the thick dotted lines, respectively.

Figures 5 and 6 show that the constant coupling approximation is superior to the dynamical norm method at energies near and above the barrier. It also works fairly well at low energies. This seems to indicate that there is not much sense in using the dynamical norm method. The constant coupling approximation has, however, a serious drawback in that the results could strongly depend on the choice of R_0 , i.e., on the place at which we evaluate the strength of the coupling Hamiltonian. This problem becomes serious if the coupling form factor changes rapidly. This is the case in heavy-ion fusion reactions because of the cancellation between the Coulomb and the nuclear coupling. The dynamical norm method is free from this problem.

VIII. CONNECTION OF THE DYNAMICAL NORM FACTOR TO DISSIPATION FACTOR IN MACROSCOPIC QUANTUM TUNNELING

Before we close the paper it would be worth relating our dynamical norm method to other approaches to macroscopic quantum tunneling. Caldeira and Leggett have considered a model, where the environment consists of many harmonic oscillators having the spectral distribution of an Ohmic dissipation. They have thus shown that the tunneling rate is reduced from that in the adiabatic limit by a dissipation factor [14]. In this section, we consider the same model and discuss the connection between the dynamical norm factor in our method and the dissipation factor in Ref. [14].

Equation (45) leads to the following expression for the dynamical norm factor in the case where the environment consists of many independent harmonic oscillators:

$$\mathcal{N}_{b} = \exp\left[-\frac{\pi}{2}\sum_{i}\left(\frac{\alpha_{0i}c_{i}R_{0}}{\hbar\omega_{i}}\right)^{2}\frac{\Omega}{\omega_{i}}\right] .$$
 (63)

Following Caldeira and Leggett, we now consider the case of an Ohmic dissipation, where the spectral density is given by

$$J(\omega) = \sum_{i} \frac{\pi}{\hbar} c_i^2 \alpha_{0i}^2 \delta(\omega - \omega_i) = \eta \omega .$$
 (64)

The dynamical norm factor is then given by

$$\mathcal{N}_b = \exp\left(-\eta \frac{R_0^2 \Omega}{\hbar} \int_0^\infty d\omega \frac{1}{\omega^2}\right) \ . \tag{65}$$

The integration in Eq. (65) diverges at the lower limit. Here we introduce the cutoff $\omega = \omega_0$ at the low frequency side and set it to be Ω , because Eq. (65) has been derived based on the assumption that the tunneling is slow compared with the intrinsic motion. We thus obtain

$$\mathcal{N}_b = \exp\left(-\frac{\eta R_0^2}{\hbar}\right) \;.$$
 (66)

The dynamical norm factor in our method is thus inti-

mately related to the dissipation factor in Ref. [14]. They have the same dependence on the friction coefficient η and the range of the tunneling region R_0 . They differ only by a factor of the order of 1 in front of the ηR_0^2 in the argument of the exponential factor. A similar result has been obtained in Ref. [9] with again a slightly different coefficient of the order of 1.

IX. SUMMARY AND FURTHER DEVELOPMENTS

We presented a method to calculate the tunneling rate of a macroscopic variable which couples to other degrees of freedom resorting to neither the adiabatic nor the sudden approximations. We named this method the dynamical norm method. This method uses the adiabatic potential barrier as a reference to calculate the tunneling rate and takes the effects of deviation from the adiabatic limit into account through a dynamical norm factor.

Using an example, where a macroscopic variable tunnels through an Eckart potential barrier in the presence of a linear oscillator coupling, we have shown that the dynamical norm method provides an accurate estimate of the tunneling rate at energies well below the barrier. We have discussed the parameters which govern the adiabaticity of a tunneling process based on a perturbative solution of the dynamical norm factor. We have shown that the adiabaticity is governed not only by the ratio of the time scales of the tunneling process and of intrinsic motions, but also by the coupling strength, and have pointed out that the radial dependence of the coupling form factor influences the adiabaticity. The same arguments hold also for the validity of the sudden approximation and will be published elsewhere [23]. In this paper we have discussed also the connection between the dynamical norm factor in our method and the dissipation factor in macroscopic quantum tunneling by considering the Caldeira-Leggett model. As an example of the application of the dynamical norm method to realistic problems, we discussed the rate of the spontaneous fission of ²³⁴U and have shown that the fission rate is strongly influenced by high-lying states which strongly couple to the beta vibrational states. In this problem, we have also shown that the fission rate calculated by the dynamical norm method agrees very well with that calculated by treating the same problem as a quantum tunneling in two-dimensional space. To the latter end, we used the method of Schmid. A problem concerning the fission of ²³⁴U is that it is not clear whether our model following [9] to describe the high-lying vibrational states in terms of an additional oscillator is reasonable or not. A more realistic model is now under investigation.

In this paper, we considered problems to which standard coupled-channels calculations can be rather easily applied. This is because one of the main aims of this paper is to examine the accuracy of our method by comparing its result with that of the coupled-channels calculations. The real power of the dynamical norm method will be exhibited in problems where the standard coupledchannels calculations cannot be easily applied. There are many interesting problems, which could be tackled by the dynamical norm method. The muon catalyzed fusion [24], atomic screening effects in nuclear astrophysical reactions, alpha and heavy particle decays, and fusion of neutron rich nuclei, especially the molecular bond effects [25,26], are some of such examples. The effect of neck formation on heavy-ion fusion reactions is another example, which could be reexamined from quantitative point of view by the dynamical norm method. The extension of the microscopic adiabatic time dependent Hartree-Fock theory is also another example, which could be tackled by our method.

A problem is that the dynamical norm method in the present version does not work well at energies near and above the potential barrier. We have shown that the adiabatic constant coupling model can be an alternative for some problems. It is an interesting future problem to extend our method so that it can be applied to the whole energy range. In this paper, we used the adiabatic quantum tunneling as the reference, i.e., as the zeroth order approximation, by introducing the adiabatic action and the adiabatic influence functional in Eqs. (7) and (9). A better approximation will be obtained by optimizing the choice of the reference frame. This is another problem that requires further study.

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