

Dynamics of barrier penetration in a thermal medium: Exact result for the inverted harmonic oscillator

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The time evolution of quantum tunneling is studied when the tunneling system is immersed in a thermal medium. We analyze in detail the behavior of the system after integrating out the environment. An exact result for the inverted harmonic oscillator of the tunneling potential is derived and the barrier penetration factor is explicitly worked out as a function of time. The quantum mechanical formula for the case without environment is modified both by the potential renormalization effect and by a dynamical factor which may differ appreciably from the one previously obtained in the time range of $1/(\text{curvature at the top of potential barrier})$.

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I. INTRODUCTION

Tunneling phenomena in thermal media are of both theoretical and practical interest in many areas of physics. For instance, in cosmology there are a variety of tunneling phenomena that may have occurred during the evolution of our universe. If the phase transition related to electroweak gauge symmetry is of first order as assumed in the electroweak scenario of baryogenesis [1], then the tunneling from a metastable state to the true ground state of the electroweak theory must occur through either a quantum effect or thermally activated barrier crossing. Another possible first order phase transition in cosmology is the quark-hadron phase transition. We should not fail to mention also the classic example of a tunneling phenomenon that takes place in the central core of stars: a thermonuclear reaction [2].

A common circumstance for all these is the presence of an environment: the tunneling we are interested in does not take place for the system in isolation. Thus we are very interested in how substantially the quantum mechanical formula for the tunneling rate is modified by dissipative interaction with the surrounding medium. Despite this obvious interest, many past works in cosmology and astrophysics have relied on simple methods to deal with the tunneling problem, either using the bounce solution in the Euclidean approach [3–6] or exploiting some variant of the classical van't Hoff–Arrhenius law [7,8].

On the other hand, since the pioneering work [9] on quantum dissipation to tunneling phenomena at zero temperature, there have appeared many extended works in condensed matter and statistical physics (a partial list of these works is given in [10–12]). The intensive theoretical activity in this field is presumably related to the experimental possibility of observing macroscopic quantum tunneling in various areas of condensed matter physics. The problem is not simple, however, and only a limited class of problems has been addressed. Thus even in idealized models one often assumes that the entire system is in thermal equilibrium and attempts to derive quantities of limited value such as the decay rate of the metastable state by an extension of bounce analysis [4,5]. In some of these works [10,11], the key quantity is the

imaginary part of the free energy, which may be interpreted as the decay rate. However, since the equilibrium value of the free energy of the entire system is necessarily real, one must extract the imaginary part by projecting to the initial metastable state. In some discussions in the literature it is not clear how this projection is performed on rigorous grounds, although some of its physical consequences are reasonable. There is indeed some criticism of this type of approach [12,13]. It seems that a more fundamental microscopic approach to deal with the tunneling in a dissipative medium is needed.

With this background in mind, our aim in the present work is to clarify dynamical aspects of tunneling in a medium: how the barrier penetration basic to quantum tunneling proceeds in real time. The key idea is separation of a small system from a larger environment, and we would like to determine the reduced density matrix for the small system by integrating out environment variables [14]. This makes it easy to compute the penetrating flux factor for an energy eigenstate of the small subsystem. Our approach does not use the Euclidean technique, which in our opinion obscures the dynamics of time evolution. Neither do we assume that the tunneling system is in thermal equilibrium with the environment, although we can discuss this case using our fundamental formula. Moreover, we are able to deal with both the quantum and the thermally activated regions in a unified way.

The model we use to extract exact results for the barrier penetration is the inverted harmonic oscillator (IVHO). Since the form of the potential we use for exact results is very specialized, we cannot discuss the tunneling for general cases with full confidence. Nevertheless, we believe that the method employed in the present work, especially the integral transform of the Wigner function, should be useful in deriving approximate yet valuable results for the general potential in the semiclassical approach. We hope to return to a general tunneling potential in our subsequent work.

We take for the environment infinitely many harmonic oscillators of arbitrary spectrum. This is a standard case studied by many people in the field. The system of a normal harmonic oscillator coupled to this environment is analytically solvable, as discussed in [15–17]. Our barrier penetra-

tion model corresponds to the case of imaginary frequency. In the present work we shall employ and extend some techniques we developed in the case of the normal oscillator.

The main result of the present work is summarized by a formula for barrier penetration:

$$f(t)|T(E)|^2, \quad f(t) = \frac{p_0(t)}{\omega_B q_0(t)} = \frac{1}{\omega_B} \frac{d}{dt} \ln|q_0(t)|. \quad (1)$$

This formula is applied to an eigenstate of energy E taken for the initial IVHO subsystem. The well known quantum mechanical penetration formula is modified by the environment effect in two ways; first, via a change of the original curvature ω_0 (bare parameter) to the renormalized, pole curvature ω_B ,

$$|T(E)|^2 = \frac{1}{1 + e^{2\pi|E|/\omega_0}} \rightarrow \frac{1}{1 + e^{2\pi|E|/\omega_B}}, \quad (2)$$

with E the energy measured from the top of the potential barrier. This effect is essentially similar to, but numerically different from, the curvature renormalization effect much emphasized by Caldeira and Leggett [9]. In their work two cases with and without the friction term, but both including the curvature renormalization given by ω_R (which is larger than ω_B), are compared. The result of Caldeira and Leggett is understood when one writes ω_B in terms of ω_R .

The second environment effect is the time dependent factor $f(t)$ which is the ratio of the momentum $p_0(t) = \dot{q}_0(t)$ to the rescaled coordinate trajectory $q_0(t)$. This trajectory function $q_0(t)$ obeys the homogeneous Langevin equation, Eq. (43) below, under a thermal environment, being characterized by an initial energy corresponding to the top of the potential barrier. When the dynamical function $f(t) = 1$, the IVHO subsystem has the energy of the barrier top, and its deviation from unity is a measure of energy flow from the environment. When $f(t) > 1$, namely, $|p_0(t)| > \omega_B |q_0(t)|$, the IVHO system is excited by an energy inflow from the environment. On the other hand, when $f(t) < 1$, the system is deexcited by an energy outflow. The factor $f(t)$ deviates from unity within a time range of order $1/\omega_B$, and both for $t \ll 1/\omega_B$ and for $t \gg 1/\omega_B$ the effect is small: $f(t) \approx 1$. We find interesting examples in which this dynamical function exceeds unity, thus implying enhanced penetration, albeit for a short period of time of order $1/\omega_B$.

The rest of this paper is organized as follows. In Sec. II we explain how we model the environment and its interaction with a quantum system, and introduce the influence functional. The quantum Langevin equation is also briefly touched upon. In Sec. III we work out exact consequences for the inverted harmonic oscillator, and give the barrier penetration factor, taking an energy eigenstate for the initial state. This section is somewhat long, but we explain mathematical details to the extent that the paper is clearly presented and self-contained. Our general result includes an integral transform of the Wigner function from the initial to the final one, as explained in Appendix A. The fundamental formula (1) is derived along with an explicit form of

$p_0(t)/q_0(0)$, Eq. (77). The Ohmic or local approximation (the inherently nonlocal term of the environment interaction in the full Langevin equation being replaced by a few expansion terms) is shown to lead to some anomalous behavior of the dynamical factor. In Sec. IV some applications to a mixed initial state are discussed using the exact result for the inverted harmonic oscillator. Our understanding of the result of Ref. [9] is also shown in terms of the diagonalized curvature parameter ω_B . Three appendixes explain technical points somewhat off the main stream of arguments in the text. Appendix A gives the interesting form of the integral transform of the Wigner function, while Appendix B gives the differential form of the Fokker-Planck equation, both derived for the harmonic model of the environment. Appendix C explains parameters necessary for our numerical computation of the dynamical function.

II. MODEL OF THE ENVIRONMENT AND INFLUENCE FUNCTIONAL METHOD

We expect that the behavior of a small system immersed in a thermal environment is insensitive to detailed modeling of the environment and the form of its interaction with the system. Only global quantities such as the environment temperature, the friction, and the threshold of the environment spectrum are expected to be important. Since the pioneering work of Feynman-Vernon [14] and Caldeira-Leggett [9], the standard model uses an infinite set of harmonic oscillators [its coordinate variable denoted by $Q(\omega)$] for the environment and a bilinear interaction with the small system (denoted by q),

$$L_Q = \frac{1}{2} \int_{\omega_c}^{\infty} d\omega [\dot{Q}^2(\omega) - \omega^2 Q^2(\omega)],$$

$$L_{\text{int}} = -q \int_{\omega_c}^{\infty} d\omega c(\omega) Q(\omega). \quad (3)$$

We assume the existence of a threshold $\omega_c > 0$. The coupling strength to the environment is specified by $c(\omega)$. In the present section we do not assume any special form for the potential of the q system, $V(q)$.

It is now appropriate to explain the influence functional method [14]. The influence functional denoted by $\mathcal{F}[q(\tau), q'(\tau)]$ results after integration of the environment variable $Q(\omega)$ when one computes the density matrix of the entire system. Since the density matrix is a product of the transition amplitude and its conjugate, the path integral formula resulting from the environment integration has a functional dependence on both the system path $q(\tau)$ and its conjugate path $q'(\tau)$. We thus define, when the initial environment is in a mixed state given by a density matrix $\rho_i(Q_i, Q'_i)$, the influence functional

$$\mathcal{F}[q(\tau), q'(\tau)] \equiv \int \mathcal{D}Q(\tau) \int \mathcal{D}Q'(\tau) \int dQ_i \int dQ'_i$$

$$\times \int dQ_f \int dQ'_f \delta(Q_f - Q'_f) K(q(\tau), Q(\tau))$$

$$\times K^*(q'(\tau), Q'(\tau)) \rho_i(Q_i, Q'_i), \quad (4)$$

$$K(q(\tau), Q(\tau)) = \exp(iS_Q[Q] + iS_{\text{int}}[q, Q]), \quad (5)$$

$$S_Q[Q] + S_{\text{int}}[q, Q] = \int_0^t d\tau (L_Q[Q] + L_{\text{int}}[q, Q]), \quad (6)$$

$$\rho_i(Q_i, Q'_i) = \sum_n w_n \psi_n^*(Q'_i) \psi_n(Q_i), \quad (7)$$

where w_n is the probability of finding a pure state n in the initial environment. The fact that there is a $\delta(Q_f - Q'_f)$ for the environment variable at the final time t indicates that one does not observe the environment part at t . Throughout this discussion we consider a definite time interval $0 < \tau < t$.

For the thermal ensemble of a Q harmonic oscillator of frequency ω ($\beta = 1/T$ being the inverse temperature), the density matrix is

$$\rho_\beta(Q, Q') = \left(\frac{\omega}{\pi \coth(\beta\omega/2)} \right)^{1/2} \exp \left[- \frac{\omega}{2 \sinh(\beta\omega)} \right. \\ \left. \times [(Q^2 + Q'^2) \cosh(\beta\omega) - 2QQ'] \right], \quad (8)$$

and one can explicitly perform the $Q(\omega)$ path integration in Eq. (4), since the $Q(\omega)$ integration is Gaussian. The result is a nonlocal action

$$\mathcal{F}[q(\tau), q'(\tau)] = \exp \left(- \int_0^t d\tau \int_0^\tau ds [\xi(\tau) \alpha_R(\tau-s) \xi(s) \right. \\ \left. + i\xi(\tau) \alpha_I(\tau-s) X(s) \right], \quad (9)$$

with

$$\xi(\tau) = q(\tau) - q'(\tau), \quad X(\tau) = q(\tau) + q'(\tau), \quad (10)$$

$$\alpha(\tau) \equiv \alpha_R(\tau) + i\alpha_I(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{\alpha}(\omega) e^{-i\omega\tau}, \quad (11)$$

$$\tilde{\alpha}(\omega) = i \int_{\omega_c}^{\infty} d\omega' c^2(\omega') \left(\frac{1}{\omega^2 - \omega'^2 + i0^+} - \frac{2\pi i}{e^{\beta\omega'} - 1} \right) \\ \times \delta(\omega'^2 - \omega^2). \quad (12)$$

Both α_R and α_I are real functions. A complex combination of these, the kernel function $\alpha(\tau)$ that appears in the exponent of the influence functional, is the real-time thermal Green's function for a collection of harmonic oscillators $Q(\omega)$, which makes clear the relation to thermal field theory.

The reduced density matrix $\rho^{(R)}$ for the q system is defined as follows. For simplicity we take for the initial system a pure quantum state given by a wave function $\psi(q_i)$,

$$\rho^{(R)}(q_f, q'_f) = \int \mathcal{D}q(\tau) \int \mathcal{D}q'(\tau) \\ \times \int dq_i \int dq'_i \psi^*(q'_i) \\ \times \mathcal{F}[q(\tau), q'(\tau)] e^{iS_q[q] - iS_q[q']} \psi(q_i). \quad (13)$$

Here $S_q[q]$ is the action for the q system. This density matrix $\rho^{(R)}$ may be used to compute the physical quantities of one's interest.

It is sometimes convenient to introduce the Wigner function by

$$f_W^{(R)}(x, p) = \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{2\pi}} \rho^{(R)} \left(x + \frac{\xi}{2}, x - \frac{\xi}{2} \right) e^{-ip\xi}. \quad (14)$$

We shall later mention the master equation for $f_W^{(R)}$. Here we quote for comparison a master equation for the Wigner function when the entire system is in a pure quantum state:

$$\frac{\partial f_W}{\partial t} = -p \frac{\partial f_W}{\partial x} + \frac{1}{i\hbar} \left[V \left(x + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) - V \left(x - \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) \right] f_W. \quad (15)$$

It takes the form of an infinite dimensional differential equation.

The master equation is simplified in the semiclassical limit of $\hbar \rightarrow 0$ to

$$\frac{\partial f_W}{\partial t} = -p \frac{\partial f_W}{\partial x} + \frac{\partial V}{\partial x} \frac{\partial f_W}{\partial p}. \quad (16)$$

A great virtue of the Wigner function is that this semiclassical equation coincides with the Liouville equation for the distribution function of a classical statistical system in the phase space (x, p) . It is thus easy to write down the semiclassical solution in the form of an integral transform,

$$f_W(x, p) = \int_{-\infty}^{\infty} dx_i \int_{-\infty}^{\infty} dp_i f_W^{(i)}(x_i, p_i) \\ \times \delta(x - \tilde{x}_{\text{cl}}(t)) \delta(p - \tilde{p}_{\text{cl}}(t)), \quad (17)$$

where the classical deterministic flow $(x_i, p_i) \rightarrow (\tilde{x}_{\text{cl}}, \tilde{p}_{\text{cl}})$ is defined by the classical mapping satisfying

$$\tilde{p}_{\text{cl}} = \frac{d\tilde{x}_{\text{cl}}}{dt}, \quad \frac{d\tilde{p}_{\text{cl}}}{dt} = - \left(\frac{\partial V}{\partial x} \right)_{x=\tilde{x}_{\text{cl}}}. \quad (18)$$

Although it is not our main tool of analysis, it might be of some use to recall the quantum Langevin equation for the model of Eq. (3) [18]. By eliminating the environment variable $Q(\omega, t)$ one derives the operator equation for the q variable,

$$\frac{d^2q}{dt^2} + \frac{\partial V}{\partial q} + 2 \int_0^t ds \alpha_I(t-s)q(s) = F_Q(t), \quad (19)$$

$$F_Q(t) = - \int_{\omega_c}^{\infty} d\omega c(\omega) \left(Q(\omega, 0) \cos(\omega t) + \frac{P(\omega, 0)}{\omega} \sin(\omega t) \right), \quad (20)$$

$$\langle F_Q(\tau) F_Q(s)^{\text{sym}} \rangle_{\text{env}} = \int_{\omega_c}^{\infty} d\omega r(\omega) \cos \omega(\tau-s) \coth \left(\frac{\beta\omega}{2} \right), \quad (21)$$

where $r(\omega) = c^2(\omega)/(2\omega)$ and $\langle \rangle_{\text{env}}$ is the thermal average over the environment variables. Thus, the kernel function $\alpha_I(\tau)$ describes a nonlocal action from the environment, while $F_Q(t)$ is a random force from the environment. The local approximation to α_I , taking the form of $\alpha_I(\tau) = \delta\omega^2 \delta(\tau) + \eta \delta'(\tau)$, gives

$$\frac{d^2q}{dt^2} + \frac{\partial V}{\partial q} + \delta\omega^2 q + \eta \frac{dq}{dt} = F_Q(t). \quad (22)$$

The parameter $\delta\omega^2$ in this case is the frequency shift due to the presence of the environment, and η is the Ohmic friction. We call this approximation the Ohmic approximation. Perhaps more suitably, it might better be called the local approximation.

On the other hand, the real part of the kernel function α_R describes fluctuation, and it is related to the dissipation α_I by the fluctuation-dissipation theorem; for their Fourier components

$$\tilde{\alpha}_I(\omega) = \frac{1}{\pi} \text{P} \int_{\omega_c}^{\infty} d\omega' \frac{2\omega' \tilde{\alpha}_R(\omega') \tanh(\beta\omega'/2)}{\omega^2 - \omega'^2}, \quad (23)$$

where P denotes the principal part of the integration.

III. EXACT RESULTS FOR INVERTED HARMONIC OSCILLATOR

A. Formalism

We specialize the system dynamics of barrier penetration to that of the inverted harmonic oscillator given by the Lagrangian density

$$L_q = \frac{1}{2} \dot{q}^2 - V_q(q), \quad V_q(q) = -\frac{1}{2} \omega_0^2 q^2, \quad \omega_0^2 > 0. \quad (24)$$

There are similarities to the case of a normal oscillator of $\omega_0^2 < 0$, and we can take over some of the results derived for the unstable ($|\omega_0|^2 > \omega_c^2$) [16,17] or the stable ($0 < |\omega_0|^2 < \omega_c^2$) harmonic oscillator.

The Gaussian nature of the system is a great simplification, as demonstrated by Eq. (4), and one may write an effective action for the q system including the environment effect:

$$iS_{\text{eff}} = i \int_0^t d\tau \left(\frac{1}{2} \dot{\xi} \dot{X} + \frac{\omega_0^2}{2} \xi X \right) - \int_0^t d\tau \int_0^\tau ds [\xi(\tau) \alpha_R(\tau-s) \xi(s) + i \xi(\tau) \alpha_I(\tau-s) X(s)]. \quad (25)$$

The linearity in the $X(\tau)$ variable here gives a trivial $X(\tau)$ path integration in the form of a δ functional; it determines the $\xi(\tau)$ path as

$$\frac{d^2\xi}{d\tau^2} - \omega_0^2 \xi(\tau) + 2 \int_\tau^t ds \xi(s) \alpha_I(s-\tau) = 0. \quad (26)$$

The final ξ path integration then leads to

$$- \int_0^t d\tau \int_0^\tau ds \xi(\tau) \alpha_R(\tau-s) \xi(s) \quad (27)$$

for the exponent factor, plus a surface term resulting after the $X(\tau)$ partial integration. The function $\xi(\tau)$ here is the solution of Eq. (26) and the result of the path integral must be written with a specified boundary condition $\xi(0) = \xi_i$, $\xi(t) = \xi_f$.

The standard technique of solving this type of integro-differential equation for $\xi(\tau)$ is the Laplace transform [16]. We shall summarize only the final result. Two fundamental solutions to this equation are $g(t-\tau)$ and its time derivative $\dot{g}(t-\tau)$ given by

$$g(\tau) = \frac{N}{\omega_B} \sinh(\omega_B \tau) + 2 \int_{\omega_c}^{\infty} d\omega H(\omega) \sin(\omega \tau), \quad (28)$$

$$N = 1 - 2 \int_{\omega_c}^{\infty} d\omega \omega H(\omega) < 1. \quad (29)$$

The important properties are that $g(\tau)$ is odd and $\dot{g}(\tau)$ is even with $g(0) = 0$ and $\dot{g}(0) = 1$, which gives the relation fixing N . In terms of this basic function $g(\tau)$ a general solution to the integro-differential equation with the given boundary condition [16,19] is

$$\xi(\tau) = \frac{g(t-\tau)}{g(t)} \xi_i + \left(\dot{g}(t-\tau) - \frac{\dot{g}(t)}{g(t)} g(t-\tau) \right) \xi_f. \quad (30)$$

The weight function H here is a discontinuity of some analytic function $[F(z)$ of a complex variable $z = \omega$] across the branch-point singularity along the real axis at $\omega > \omega_c$, and is given by

$$H(\omega) = \frac{r(\omega)}{[\omega^2 + \omega_0^2 - \Pi(\omega)]^2 + [\pi r(\omega)]^2}, \quad r(\omega) = \frac{c^2(\omega)}{2\omega}, \quad (31)$$

$$\Pi(\omega) = \text{P} \int_{\omega_c}^{\infty} d\omega' \frac{2\omega' r(\omega')}{\omega^2 - \omega'^2}, \quad (32)$$

where the integral for Π stands for its principal part. The value ω_B in Eq. (28) is determined as a solution for the isolated pole on the real axis at $\omega^2 = -\omega_B^2 < 0$:

$$-\omega_B^2 + \omega_0^2 + \int_{\omega_c}^{\infty} d\omega \frac{2\omega r(\omega)}{\omega_B^2 + \omega^2} = 0. \quad (33)$$

In general, one has

$$\omega_B^2 > \omega_0^2. \quad (34)$$

Since many workers in this field use a renormalized potential according to Ref. [9], we also introduce these:

$$V_q + V_{qQ} = V_q^{(\text{ren})}(q) + V_{qQ}^{(\text{ren})}(q, Q), \quad (35)$$

$$V_q^{(\text{ren})}(q) = V - q^2 \int_{\omega_c}^{\infty} d\omega \frac{r(\omega)}{\omega} \equiv -\frac{1}{2} \omega_R^2 q^2, \quad (36)$$

$$\begin{aligned} V_{qQ}^{(\text{ren})}(q, Q) &= V_{qQ}(q, Q) + q^2 \int_{\omega_c}^{\infty} d\omega \frac{r(\omega)}{\omega} \\ &\equiv V_{qQ}(q, Q) + \frac{1}{2} \delta\omega^2 q^2. \end{aligned} \quad (37)$$

We shall redefine the q system potential using $V_q^{(\text{ren})}(q)$. This renormalized potential gives an inverted harmonic oscillator with the curvature parameter ω_R . This renormalized curvature differs from the pole location of the spectral function $H(\omega)$, namely, ω_B , by a factor of order of the interaction coupling. In the weak coupling limit these two quantities are given by

$$\omega_R^2 = \omega_0^2 + 2 \int_{\omega_c}^{\infty} d\omega \frac{r(\omega)}{\omega}, \quad (38)$$

$$\omega_B^2 \approx \omega_0^2 + 2 \int_{\omega_c}^{\infty} d\omega \frac{\omega r(\omega)}{\omega^2 + \omega_0^2}. \quad (39)$$

The equation for ω_R^2 gives a precise relation, while the equation for ω_B^2 is an approximate relation valid for weak coupling, the exact relation being given by Eq. (33). In general, one can prove that

$$\omega_B^2 < \omega_R^2, \quad (40)$$

beyond the weak coupling approximation. To give an example, in the Ohmic model that will be discussed shortly, the relation becomes

$$\omega_B \approx \omega_R - \frac{1}{2} \eta, \quad (41)$$

where η is the Ohmic friction. A more precise relation in this case is Eq. (86) below. The relation to the bare quantity ω_0 is

$$\omega_R \approx \omega_0 + k \eta, \quad k \approx \frac{\Omega}{\pi \omega_0}. \quad (42)$$

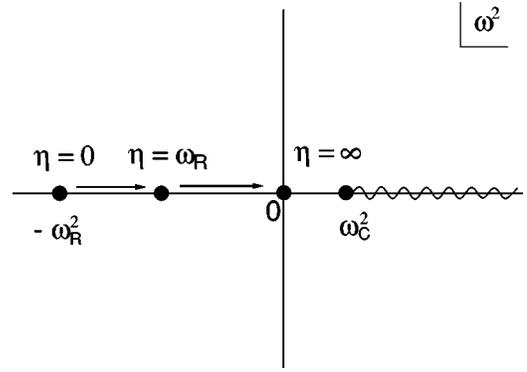


FIG. 1. Analytic structure of $F(\omega^2)$ as a function of the complex ω^2 variable. The pole at $-\omega_B^2$ moves as indicated when the friction η becomes large with the parameter ω_R^2 fixed. The continuous branch cut starts from a threshold at ω_c^2 .

In the infinite cutoff limit, $\Omega \rightarrow \infty$, the quantity k is divergent.

In Fig. 1 we show schematically the analytic structure of the function $F(z^2)$, basic to the determination of the discontinuity function $H(\omega)$. Unlike the case of the normal harmonic oscillator for which the pole location may have an imaginary part, the pole at $z^2 = -\omega_B^2$ appears exactly on the real axis. The other singularity is the branch cut starting from the threshold $z^2 = \omega_c^2$.

The physical meaning of the basic function $g(\tau)$ is better understood by solving the operator Langevin equation for this system:

$$\frac{d^2 q}{dt^2} - \omega_0^2 q + 2 \int_0^t d\tau \alpha_I(t-\tau) q(\tau) = F_Q(t). \quad (43)$$

The quantity ω_0^2 here should be understood as a function of ω_B^2 after eliminating ω_0^2 with Eq. (33). The homogeneous solution to this Langevin equation is given by using $g(t)$ and $\dot{g}(t)$; with the initial data of $q(0)$, $\dot{q}(0) = p(0)$,

$$q(t) = q(0)\dot{g}(t) + p(0)g(t). \quad (44)$$

The main term $g(t) \approx N \sinh(\omega_B t)/\omega_B$ and $\dot{g}(t) \approx N \cosh(\omega_B t)$ describes an average motion $\langle q(t) \rangle$ under the renormalized, inverted harmonic oscillator modified by the environment, for which the original parameter $|\omega_0^2|$ is replaced by the new shifted ω_B^2 . The correction to this classical motion given by the second term in Eq. (28) describes a damped oscillation with an amplitude decreasing as an inverse power of time at large times.

A straightforward calculation of X and ξ path integration finally gives an effective action valid for any initial state of the q system. We first define new functions by

$$h(\omega, t) = \int_0^t d\tau g(\tau) e^{-i\omega\tau}, \quad (45)$$

$$k(\omega, t) = \int_0^t d\tau \dot{g}(\tau) e^{-i\omega\tau} = i\omega h(\omega, t) + g(t) e^{-i\omega t}. \quad (46)$$

With the normalization fixed by unitarity, one has for the effective action J defined by $\rho^{(R)} = \text{tr}(J\rho_i)$

$$J(X_f, \xi_f; X_i, \xi_i; t) = \frac{1}{2\pi g(t)} e^{iS_{\text{cl}}}, \quad (47)$$

where S_{cl} is given by [19]

$$iS_{\text{cl}} = -\frac{U}{2}\xi_f^2 - \frac{V}{2}\xi_i^2 - W\xi_i\xi_f + \frac{i}{2}X_f\dot{\xi}_f - \frac{i}{2}X_i\dot{\xi}_i, \quad (48)$$

$$U = \left(\frac{\dot{g}}{g}\right)^2 I_1 + I_2 - 2\frac{\dot{g}}{g}I_3, \quad V = \frac{1}{g^2}I_1, \quad (49)$$

$$W = \frac{1}{g}I_3 - \frac{\dot{g}}{g^2}I_1 = \frac{1}{2}g\dot{V}, \quad (50)$$

$$I_1 = \int_{\omega_c}^{\infty} d\omega \coth \frac{\beta\omega}{2} r(\omega) |h(\omega, t)|^2, \quad (51)$$

$$I_2 = \int_{\omega_c}^{\infty} d\omega \coth \frac{\beta\omega}{2} r(\omega) |k(\omega, t)|^2, \quad (52)$$

$$I_3 = \int_{\omega_c}^{\infty} d\omega \coth \frac{\beta\omega}{2} r(\omega) \text{Re}[h(\omega, t)k^*(\omega, t)], \quad (53)$$

$$\dot{\xi}(\tau) = -\xi_i \frac{\dot{g}(t-\tau)}{g(t)} - \xi_f \left(\ddot{g}(t-\tau) - \frac{\dot{g}(t-\tau)\dot{g}(t)}{g(t)} \right). \quad (54)$$

For the discussion of the barrier penetration factor, we take a pure initial state given by the wave function $\psi(x)$. The Wigner function in this case is

$$f_W^{(R)}(x, p) = \int \frac{dx_i d\xi_i}{2\pi\sqrt{C}} \psi^* \left(x_i - \frac{1}{2}\xi_i \right) \psi \left(x_i + \frac{1}{2}\xi_i \right) e^{-A}, \quad (55)$$

$$\begin{aligned} A = & \frac{\det I}{2C} [\xi_i + i(gJ_1 + \dot{g}J_3)(x - \dot{g}x_i) \\ & + i(\dot{g}J_2 + gJ_3)(p - \ddot{g}x_i)]^2 \\ & + \frac{1}{2} [J_1(x - \dot{g}x_i)^2 + J_2(p - \ddot{g}x_i)^2 \\ & + 2J_3(x - \dot{g}x_i)(p - \ddot{g}x_i)], \end{aligned} \quad (56)$$

$$C = \int_{\omega_c}^{\infty} d\omega \coth \frac{\beta\omega}{2} r(\omega) |\dot{g}h(\omega, t) - gk(\omega, t)|^2, \quad (57)$$

$$(J) = (I)^{-1}, \quad J_{1,2} = \frac{I_{2,1}}{I_1 I_2 - I_3^2}, \quad J_3 = -\frac{I_3}{I_1 I_2 - I_3^2}. \quad (58)$$

Although it is not used in the calculation of the flux factor in the next subsection, it is of great theoretical interest to

express our result as a transformation of the initial Wigner function $f_W^{(i)}$ to the final one $f_W^{(R)}$. We give this in Appendix A. This mapping $f_W^{(i)} \rightarrow f_W^{(R)}$ is an integrated form describing the dynamics of the q system. Its differential form is known as the Fokker-Planck equation, and we shall explain this briefly in Appendix B.

B. Barrier penetration factor

The flux at position x is computed from the formula

$$I(x, t) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} p f_W^{(R)}(x, p; t) \quad (59)$$

to give

$$\begin{aligned} I(x, t) = & \int \frac{dx_i d\xi_i}{2\pi g} \psi^* \left(x_i - \frac{\xi_i}{2} \right) \psi \left(x_i + \frac{\xi_i}{2} \right) \\ & \times \left[\frac{\dot{g}}{g}x + \left(\ddot{g} - \frac{\dot{g}^2}{g} \right) x_i + iW\xi_i \right] \\ & \times \exp \left[-\frac{V}{2} \left(\xi_i + \frac{i}{gV}(x - \dot{g}x_i) \right)^2 \right. \\ & \left. - \frac{1}{2g^2V}(x - \dot{g}x_i)^2 \right]. \end{aligned} \quad (60)$$

We use the WKB formula for energy eigenstates of the IVHO. Considering the incident left mover at $x < 0$ with unit flux, we take as the wave function at $x > x_*$ (the right turning point)

$$\psi(x) \approx \frac{T(E)}{\sqrt{p(x)}} \exp \left(i \int_{x_*}^x dx' p(x') \right), \quad p(x) = \sqrt{2E + \omega_B^2 x^2}, \quad (61)$$

where $x_* = \sqrt{2|E|}/\omega_B$ and $T(E)$ is the transmission coefficient as a function of the energy E in a pure quantum state. This choice of the wave function gives the transmission coefficient

$$|T(E)|^2 \approx \frac{1}{1 + e^{-2\pi E/\omega_B}}. \quad (62)$$

A point that becomes important when we compare our result with those of other papers is how one prepares the initial state. In much past work a thermal equilibrium between the subsystem and the environment is often assumed, and in this context it is natural to take for our choice of the pure state the reference system characterized by the curvature ω_B , the exact pole curvature. The choice of the WKB wave function, using the curvature parameter ω_B , fits with this picture. But it should be kept in mind that we may in

principle take any reference curvature (hereafter denoted by $\tilde{\omega}$) and in these cases we replace ω_B below by $\tilde{\omega}$.

Expanding wave functions in ξ_i , we derive a general formula for the dynamical factor. This involves an infinite series of the expansion in ξ of the initial density matrix element,

$$\psi(x_i + \xi_i/2)\psi^*(x_i - \xi_i/2) = \sum_{n=0}^{\infty} \mathcal{A}_n(x_i)\xi_i^n. \quad (63)$$

The first few terms of this series are

$$\mathcal{A}_0(x_i) = |\psi(x_i)|^2, \quad \mathcal{A}_1(x_i) = \frac{1}{2}(\psi^* \partial \psi - \psi \partial \psi^*)(x_i), \quad (64)$$

$$\mathcal{A}_2(x_i) = \frac{1}{8}[(\psi^* \partial^2 \psi + \psi \partial^2 \psi^*)(x_i) + |\partial \psi|^2(x_i)]. \quad (65)$$

Computation of the flux factor is then given by

$$I(x, t) = \sum_{n=0}^{\infty} I_n(x, t), \quad (66)$$

$$\begin{aligned} I_n(x, t) &= \int \frac{dx_i d\xi_i}{2\pi g} \mathcal{A}_n(x_i) \xi_i^n \left[\frac{\dot{g}}{g} x + \left(\ddot{g} - \frac{\dot{g}^2}{g} \right) x_i + i \left(\frac{I_3}{g} - \frac{\dot{g} I_1}{g^2} \right) \xi_i \right] \exp \left[-\frac{V}{2} \left(\xi_i + \frac{i}{gV} (x - \dot{g} x_i) \right)^2 - \frac{1}{2g^2 V} (x - \dot{g} x_i)^2 \right] \\ &= \left(\frac{g}{\sqrt{I_1}} \right)^n \int \frac{d\alpha}{2\pi g} \mathcal{A}_n \left(\frac{x}{\dot{g}} + \frac{\sqrt{I_1}}{\dot{g}} \alpha \right) e^{-\alpha^2/2} \int d\beta (\beta + i\alpha)^n \left\{ \frac{\ddot{g}}{\dot{g}} x + \left(\frac{\ddot{g} \sqrt{I_1}}{\dot{g}} - \frac{I_3}{\sqrt{I_1}} \right) \alpha + i \left(\frac{I_3}{g} - \frac{\dot{g} I_1}{g^2} \right) \frac{g}{\sqrt{I_1}} \beta \right\} e^{-\beta^2/2}. \end{aligned} \quad (67)$$

The second equality follows by a trivial scale change of the integration variables x_i, ξ_i .

One may use the expansion of $\mathcal{A}_n(x/\dot{g} + \sqrt{I_1}\alpha/\dot{g})$ in powers of the coupling:

$$\begin{aligned} \mathcal{A}_n \left(\frac{x}{\dot{g}} + \frac{\sqrt{I_1}}{\dot{g}} \alpha \right) &= \mathcal{A}_n \left(\frac{x}{\dot{g}} \right) + \mathcal{A}'_n \left(\frac{x}{\dot{g}} \right) \frac{\sqrt{I_1}}{\dot{g}} \alpha + \dots \\ &\quad + \frac{1}{(k-1)!} \mathcal{A}_n^{(k-1)} \left(\frac{x}{\dot{g}} \right) \\ &\quad \times \left(\frac{\sqrt{I_1}}{\dot{g}} \alpha \right)^{k-1} + \dots \end{aligned} \quad (68)$$

For calculation of the penetration factor one needs only the $x \rightarrow \infty$ limit of the flux function. From the WKB formula

$$\begin{aligned} \mathcal{A}_n(x_i) &= \frac{|T(E)|^2}{n!} \frac{d^n}{d\xi_i^n} \frac{1}{\sqrt{p(x_i - \xi_i/2)p(x_i + \xi_i/2)}} \\ &\quad \times \exp \left(i \int_{x_i - \xi_i/2}^{x_i + \xi_i/2} dx' p(x') \right) \Big|_{\xi_i=0}, \end{aligned} \quad (69)$$

one has

$$\mathcal{A}_n(x_i) \rightarrow |T(E)|^2 \left\{ i \frac{(i\omega_B x_i)^{n-1}}{n!} + O(x_i^{n-3}) \right\}. \quad (70)$$

Only the term containing $[(\sqrt{I_1}/\dot{g})\alpha]^{n-1}$ remains here. One may then derive

$$I_n(x, t) \rightarrow |T(E)|^2 (-1)^n \left(\frac{\omega_B \ddot{g}}{\dot{g}} \right)^{n-1} \left(\frac{g \ddot{g}}{\dot{g}^2} - 1 \right) \quad (n \geq 1). \quad (71)$$

This along with

$$I(\infty, t) = |T(E)|^2 f(t) \quad (72)$$

gives a general formula for the dynamical factor:

$$f(t) = \frac{\ddot{g}}{\omega_B \dot{g}} - \left(\frac{g \ddot{g}}{\dot{g}^2} - 1 \right) \sum_{n=1}^{\infty} \left(-\frac{\omega_B \ddot{g}}{\dot{g}} \right)^{n-1} = \frac{\ddot{g} + \omega_B \dot{g}}{\omega_B (\dot{g} + \omega_B \ddot{g})}. \quad (73)$$

This is the main result of the present work.

The salient feature of this result is factorization; the main suppression factor given by $|T(E)|^2$ is affected by the presence of the thermal environment only via the renormalization effect, as will be more fully discussed shortly. The other prefactor $f(t)$ carries dynamical information about the time evolution.

The basic functions $g(t)$ and $\dot{g}(t)$ that appear in the dynamical function $f(t)$ are the solution to the homogeneous part ($F_Q=0$) of the Langevin equation (43) with the initial condition, $g(0)=0$, $\dot{g}(0)=1$. More conveniently, one may rewrite the dynamical function as

$$f(t) = \frac{p_0(t)}{\omega_B q_0(t)}, \quad p_0(t) = \dot{q}_0(t). \quad (74)$$

Here $q_0(t)$ is the solution with the initial condition

$$\dot{q}(0) = \omega_B q(0). \quad (75)$$

This condition corresponds to zero energy at time $t=0$, since

$$H_q = \frac{1}{2} \dot{q}^2 - \frac{1}{2} \omega_B^2 q^2 = 0. \quad (76)$$

That is, the particle is on the top of the renormalized potential barrier. Note, however, that the exact pole curvature ω_B appears here instead of the renormalized ω_R . The ratio of the momentum to the coordinate for $f(t)$ is a measure of the energy flow from the thermal environment. Thus, the case of $f(t) > (<) 1$ corresponds to an energy inflow (outflow). Both at $t \ll 1/\omega_B$ and at $t \gg 1/\omega_B$ this function $f(t)$ is nearly unity and it deviates appreciably from unity only within the time range of $1/\omega_B$.

An explicit formula useful for detailed analysis of the dynamical function $f(t)$ is

$$q_0(t) = \dot{g}(t) + \omega_B g(t) = N e^{\omega_B t} + 2 \int_{\omega_c}^{\infty} d\omega H(\omega) (\omega \cos \omega t + \omega_B \sin \omega t). \quad (77)$$

The first term represents a simple classical motion under the potential, modified by the curvature renormalization, while the second term is a further deviation due to the environment interaction. The environment effect for $f(t)$ appears in two ways: the first via the definition of ω_B determined by the potential renormalization due to the environment interaction and the second the continuous part of the spectral integral in Eq. (77), and its associated deviation of the normalization factor N from unity.

Before we go on to specific models of the environment, it is appropriate to discuss some general results. First, both in the weak coupling region and at the asymptotic late time the dynamical function $f(t)$ behaves as

$$f(t) \approx f_{\text{asym}}(t),$$

$$f_{\text{asym}}(t) = 1 - \frac{2}{\omega_B N} e^{-\omega_B t} \int_{\omega_c}^{\infty} d\omega H(\omega) (\omega^2 + \omega_B^2) \sin \omega t. \quad (78)$$

This form has the correct asymptotic behavior $f(\infty) = 1$ as well as the correct initial behavior $f(0) = 1$ if the integral above is convergent.

On the other hand, one can prove for the initial-time behavior of $f(t)$ that

$$f(t) = 1 - \omega_B \left(1 - \frac{\ddot{g}(0)}{\omega_B^2} \right) t + \dots, \quad (79)$$

$$1 - \frac{\ddot{g}(0)}{\omega_B^2} = \frac{2}{\omega_B^2} \int_{\omega_c}^{\infty} d\omega H(\omega) \omega (\omega^2 + \omega_B^2) > 0. \quad (80)$$

The last inequality means that, for very small t , $f(t) < 1$, giving rise to suppression for barrier penetration. In order to

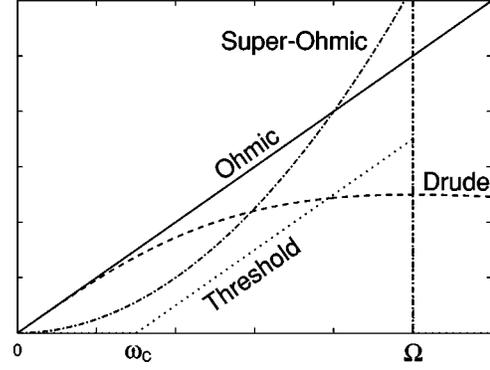


FIG. 2. Schematic form of model spectral weights. The spectral function $r(\omega) = c^2(\omega)/(2\omega)$ is plotted as a function of the frequency ω .

have a convergent integral (80) for the formula for $\ddot{g}(0)$ a physical cutoff Ω of the environment spectrum is necessary; thus the simple-minded Ohmic model without the cutoff should be treated with caution.

The asymptotic formula (78), as will be shown later, describes well, even numerically, the dynamical function at all times, including small times. For instance, the expansion in time t of Eq. (78) gives almost the same result as Eq. (79), except for the missing factor N .

We would like to stress that two properties, $f(t) < 1$ with $f(0) = 1$ for small t and $f(\infty) = 1$, are generic features for any model having a finite physical cutoff of the spectral weight $r(\omega)$. As shown later, however, some approximations or models with the infinite cutoff violate these general properties.

Although our fundamental formula (72) is derived for energy eigenstates, one may compute the barrier penetration factor for any mixed state by suitably weighting this rate for the energy eigenstate. A salient feature of our flux formula (72) is that the dependence on the initial (system) state is given by the well known quantum mechanical barrier penetration factor $|T(E)|^2$, the other factor $f(t)$ being independent of the initial state. This property of factorization is specific to the harmonic barrier. For a more general potential barrier the dynamical factor may depend on the energy of the initial state as $f(t; E)$.

We would like to stress that our result extends the result of [9] in several ways. First, we derived the tunneling rate for any energy eigenstate, while the authors of Ref. [9] deal with the zero temperature limit of the mixed state in complete equilibrium. Our method is also completely different from Caldeira-Leggett's Euclidean approach, and our method makes it possible to discuss the dynamics of the time evolution. The third point is that we derived the prefactor rigorously, unlike previous approximate calculations. In the next section we explicitly show how we effectively obtain the result of Caldeira and Leggett.

C. Some examples

We would like to compute this dynamical function for a few typical examples of the environment spectrum. The spectral function $r(\omega)$ is taken as

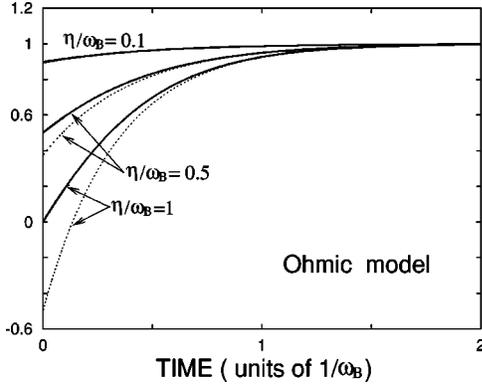


FIG. 3. Dynamical function $f(t)$ for the Ohmic model. Values of the friction η relative to the system curvature are given for each case. Dotted lines are calculated using the approximate, asymptotic formula $f_{\text{asym}}(t)$, Eq. (78) in the text.

$$(1) \quad r_O(\omega) = \frac{\eta}{\pi} \omega, \quad (81)$$

$$(2) \quad r_D(\omega) = \frac{\eta \omega}{\pi(1 + \omega^2/\Omega^2)}, \quad (82)$$

$$(3) \quad r_T(\omega) = \frac{\eta}{\pi} [\omega - \omega_c \epsilon(\omega)] \theta(|\omega| - \omega_c) \theta(\Omega - |\omega|), \quad (83)$$

$$(4) \quad r_S(\omega) = \frac{\eta}{\pi} \omega^2 \epsilon(\omega) \theta(\Omega - |\omega|). \quad (84)$$

As usual, $\theta(x)$ is the step function and $\epsilon(x)$ the signature function. The first example $r_O(\omega)$ is the Ohmic model (without physical cutoff of the environment spectrum), the second $r_D(\omega)$ the Drude model, and the fourth $r_S(\omega)$ a super-Ohmic model, while the third one $r_T(\omega)$ has a threshold at ω_c . In Fig. 2 these spectral weights are schematically depicted. In the last three cases Ω acts as a cutoff of the environment

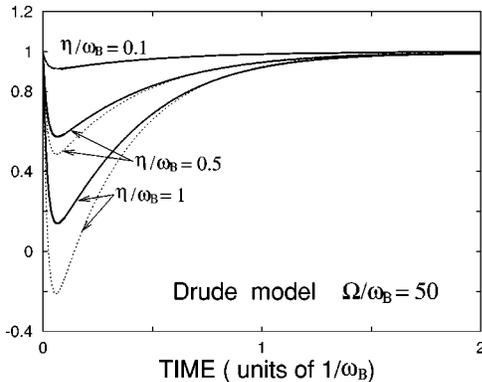


FIG. 4. Dynamical function $f(t)$ for the Drude model. Values of the friction and the cutoff relative to the system curvature are given for each case. Dotted lines are calculated using the approximate, asymptotic formula $f_{\text{asym}}(t)$, Eq. (78) in the text.

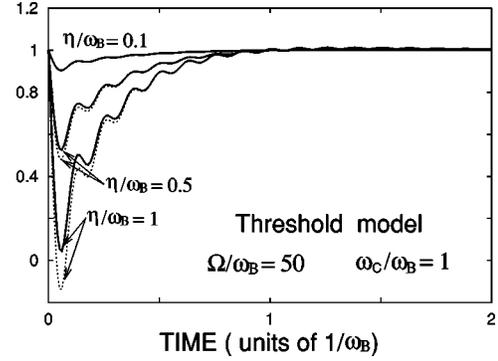


FIG. 5. Dynamical function $f(t)$ for the threshold model of low threshold. Values of the friction, the cutoff, and the threshold relative to the system curvature are given for each case. Dotted lines are calculated using the approximate, asymptotic formula $f_{\text{asym}}(t)$, Eq. (78) in the text.

spectrum. In Appendix C we give the parameters necessary to compute the dynamical function $f(t)$.

We note here that the Ohmic model defined here by the spectral weight $r_O(\omega)$ should, strictly speaking, be taken as some limit of the infinite cutoff. This cutoff could be given by a straightforward frequency cutoff like $|\omega| < \Omega$, or by a smoother function as in the case of the Drude model at large Ω . The method of introducing the cutoff does not matter provided a cutoff is there, but in some evaluations of the integral one should first introduce a finite cutoff and then take the infinite cutoff limit.

The dynamical factor $f(t)$ is plotted in Figs. 3–7 for these four cases. As the friction η becomes large, deviation of $f(t)$ from unity becomes appreciable, but only in a time range of order $1/\omega_B$. For physical reasons we always take $\eta \leq \omega_B$. We have found an interesting behavior of $f(t)$; some models can give enhancement over the usual quantum formula in the time range $t \approx 1/\omega_B$. These are the threshold model with a large ω_c and the super-Ohmic model, for which the dynamical factor can exceed unity. The super-Ohmic model also has the peculiar feature that the dynamical function $f(t)$ can even become negative for a short time interval. The use of the asymptotic or weak coupling expression for $f_{\text{asym}}(t)$, Eq. (78), is compared to the exact result in these figures. Except

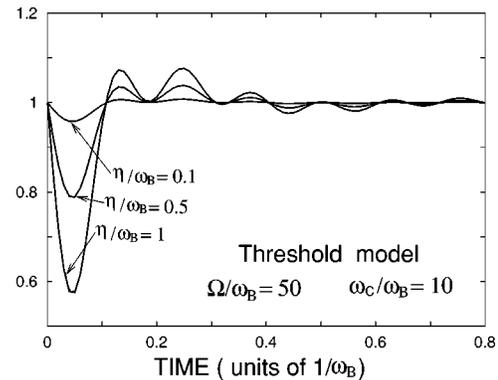


FIG. 6. The same as in Fig. 5, for the threshold model of high threshold.

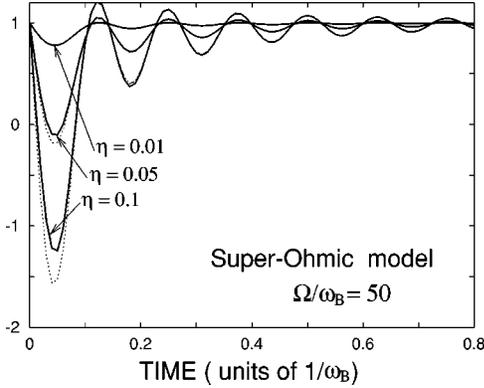


FIG. 7. Dynamical function $f(t)$ for the super-Ohmic model. Values of the friction and the cutoff are given for each case. Dotted lines are calculated using the approximate, asymptotic formula $f_{\text{asym}}(t)$, Eq. (78) in the text.

at initial times this approximate form gives a reasonable fit to more exact results. The presence of the normalization factor N in the formula is important to get a good agreement.

The initial-time behavior of the Ohmic model (81) does not reflect the necessary condition of $f(0) = 1$, since $f(t)$ at very small t is singular, having no smooth derivative at $t = 0$ (the left and the right derivatives do not meet) in the case of the infinite cutoff limit. This implies that $f(0) < 1$ in this case indicates an anomaly associated with the infinite cutoff, and should not be taken too seriously. On the other hand, the Drude model for a large but finite cutoff has the expected decrease of $f(t)$ from unity at small times. The larger the cutoff is, the more abrupt this decrease is, and a local minimum of $f(t)$ appears at a time proportional to $1/\Omega$.

Finally, we note how the dynamical function behaves in the Ohmic or local approximation. We wish to distinguish this Ohmic approximation from the Ohmic model we just discussed. First, write Eq. (22) for the IVHO:

$$\frac{d^2 q}{dt^2} + \eta \frac{dq}{dt} - \omega_R^2 q = F_Q(t). \quad (85)$$

There is a problem of how to interpret the zero energy solution since the ω_B we need for this is not well defined. One choice might be to use the relation obtained from $r_O(\omega)$ in the Ohmic model:

$$\omega_B = \sqrt{\omega_R^2 + \frac{\eta^2}{4}} - \frac{\eta}{2}. \quad (86)$$

This relation is derived by using two exact definitions, the one for ω_B [Eq. (33)] and another for ω_R [Eq. (38)], along with the form of the weight $r_O(\omega)$. In this case the dynamical function is trivial; $f(t) = 1$. But it is by no means obvious that this choice is unique, since without a specific form of the weight function there is no way to locate the pole curvature ω_B .

Another choice is to take a more phenomenological view limited to the local Langevin equation, and define the zero energy condition by taking ω_R for ω_B ; namely, at time 0,

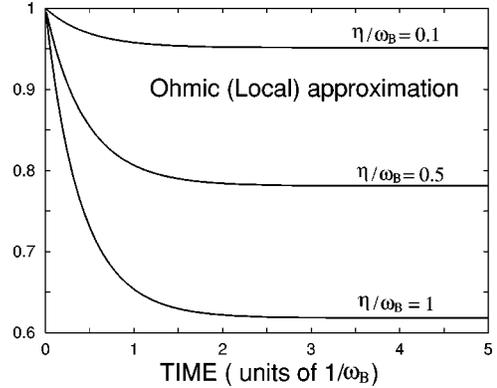


FIG. 8. Dynamical function $f(t)$ in the local, Ohmic approximation. Values of the friction are given for each case.

$$H_q = \frac{1}{2} \dot{q}^2 - \frac{1}{2} \omega_R^2 q^2 = 0. \quad (87)$$

The zero energy solution that is initially on the potential top is then

$$q_0(t) = N[(\omega_+ + \omega_R)e^{\omega_- t} + (\omega_- - \omega_R)e^{-\omega_+ t}]. \quad (88)$$

The parameters here are given by

$$\omega_{\pm} = \sqrt{\omega_R^2 + \frac{\eta^2}{4}} \pm \frac{\eta}{2}, \quad (89)$$

both of which are larger than ω_R . It is then easy to get

$$f(t) = \frac{\omega_- (\omega_+ + \omega_R) e^{\omega_- t} - \omega_+ (\omega_- - \omega_R) e^{-\omega_+ t}}{\omega_R [(\omega_+ + \omega_R) e^{\omega_- t} + (\omega_- - \omega_R) e^{-\omega_+ t}]}. \quad (90)$$

This function behaves reasonably at initial times, having $f(0) = 1$. More precisely,

$$f(t) \rightarrow 1 - \eta t. \quad (91)$$

Its asymptotic late time behavior is given by

$$f(t) \rightarrow f(\infty)(1 + C e^{-(\omega_+ + \omega_-)t}), \quad (92)$$

$$f(\infty) = \frac{\omega_-}{\omega_R} < 1, \quad C = \frac{(\omega_+ + \omega_-)(\omega_R - \omega_-)}{\omega_- (\omega_+ + \omega_R)} > 0. \quad (93)$$

The function $f(t)$ of Eq. (90) is plotted in Fig. 8. The property $f(\infty) < 1$ shows an anomalous behavior of this local approximation, which we regard as a defect inherent in the local approximation.

IV. APPLICATIONS

To illustrate the advantages of our approach, we take up two applications of our basic formula Eq. (72) along with Eq. (73). The first example is computation of the tunneling rate for the kind of potential depicted in Fig. 9. Qualitatively, a new normal harmonic oscillator is added in the left region of the previous inverted harmonic oscillator. The simplest example of this class of potential is a cubic form,

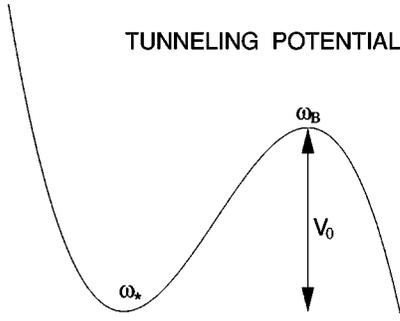


FIG. 9. Schematic form of a general potential as a function of position.

$$V(x) = -\frac{\omega_B^3}{3\sqrt{6}V_0}x^3 - \frac{\omega_B^2}{2}x^2. \quad (94)$$

Here V_0 is the barrier height measured from the left bottom of the potential, and ω_B is taken real and positive. The important quantity added, a new frequency ω_* in the left harmonic well, is equal to ω_B in this cubic potential. Below we generally distinguish the two, ω_B and ω_* , having a more general tunneling potential in mind.

The problem we set up is to compute the tunneling rate trapped in the metastable state in the left oscillator part at temperature T , the same temperature as the environment. The setting of this problem is the same as in the Euclidean approach of Grabert *et al.* [19]. We assume that the temperature $T \leq V_0$ with a further condition of $V_0 \gg \omega_*$. Under these circumstances the n th energy eigenstate of the left oscillator is distributed with the probability w_n of the Boltzmann-Gibbs ensemble,

$$w_n = \frac{e^{-n\beta\omega_*}}{\sum_m e^{-m\beta\omega_*}} = (1 - e^{-\beta\omega_*})e^{-n\beta\omega_*}. \quad (95)$$

We then convolute with this weight the barrier penetration factor, to get the tunneling probability Γ ,

$$\Gamma(T, t) = (1 - e^{-\beta\omega_*}) \sum_{n=0}^{\infty} e^{-n\beta\omega_*} \times |T[-V_0 + \omega_*(n + \frac{1}{2})]|^2 f(t). \quad (96)$$

We first discuss the infinite time limit, in which $f(t) \rightarrow 1$. This probability has the zero temperature limit

$$\Gamma(0, \infty) \approx \left| T\left(-V_0 + \frac{\omega_*}{2}\right) \right|^2 = \frac{1}{1 + e^{2\pi(V_0 - \omega_*/2)/\omega_B}}, \quad (97)$$

which is valid for $T \ll \omega_*$. On the other hand, for $T \gg \omega_*$, the discrete sum

$$\Gamma(T, \infty) = 2 \sinh \frac{\beta\omega_*}{2} e^{-\beta V_0} \sum_{n=0}^{\infty} \frac{e^{-\beta\omega_*(n+1/2-V_0/\omega_*)}}{1 + e^{-2\pi[(n+1/2)\omega_* - V_0]/\omega_B}} \quad (98)$$

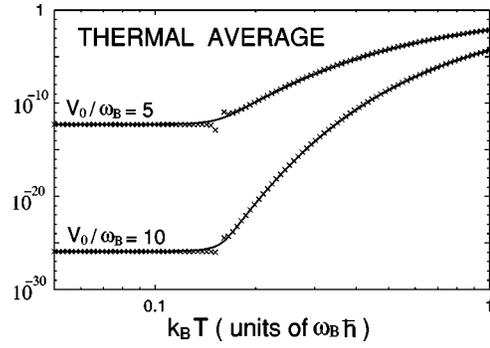


FIG. 10. Thermally averaged tunneling probability based on Eq. (96) with $f(t) = 1$ taking $\omega_* = \omega_B$. Points marked with crosses are calculated using the approximate formula (100).

holds. This approximately reduces to

$$\begin{aligned} \Gamma(T, \infty) &\approx 2 \frac{\beta\omega_*}{2} e^{-\beta V_0} \int_0^{\infty} \frac{dx}{\beta\omega_*} \frac{1}{1 + x^{2\pi/\beta\omega_B}} \\ &= \frac{\beta\omega_B e^{-\beta V_0}}{2 \sin(\beta\omega_B/2)} \approx e^{-\beta V_0}. \end{aligned} \quad (99)$$

The last formula holds for $T \gg \omega_B$. This is the expected classical formula for the barrier penetration at finite temperature. More quantitatively, we computed Eq. (96) numerically to compare with various approximate formulas. The quantity $\Gamma(T, \infty)$, computed from Eq. (96) with $f(t) = 1$, is plotted in Fig. 10. In this figure an approximate formula

$$\begin{aligned} \Gamma(T, \infty) &= \frac{\omega_B \sinh(\beta\omega_*/2)}{\omega_* \sin(\beta\omega_B/2)} e^{-\beta V_0} \\ &+ \frac{1}{1 + e^{-2\pi[\omega_*/(2\omega_B) - V_0/\omega_B]}} \end{aligned} \quad (100)$$

is compared to the exact result in the case of $\omega_B = \omega_*$. This interpolation formula is a simple sum of the improved high and the improved low temperature limits.

We now present our understanding of the result of Caldeira and Leggett for the cubic potential $V(x)$ [Eq. (94)]. For this we extend our result of the IVHO to this class of potential by the formula

$$I(\infty, t) = \exp\left(-2 \int_{x_1}^{x_2} dx \sqrt{2[V(x) - E]}\right) \frac{1}{\omega_B} \frac{d}{dt} \ln|q_0(t)|, \quad (101)$$

where x_i are turning points for the energy $E = -V_0$ solution. We take as the reference curvature $\tilde{\omega} = \omega_B$. The trajectory function $q_0(t)$ is taken as the classical, zero energy solution, but we ignore the dynamical function since it is almost unity in the equilibrium circumstance of [9]. Thus we find for the tunneling probability to be compared

$$I(\infty, t) \approx |T(E)|^2 = \exp\left(-\frac{36}{5} \frac{V_0}{\omega_B}\right). \quad (102)$$

The authors of [9] write the tunneling probability in terms of the renormalized curvature ω_R and the friction η . For the Ohmic model of small friction, we get [using Eq. (86) with $\eta \ll \omega_R$]

$$|T(E)|^2 \approx e^{-2\pi V_0/\omega_R} e^{-\Delta B} \quad (103)$$

with

$$\Delta B \approx \frac{18}{5} \frac{\eta V_0}{\omega_R^2} = 3.6 \frac{\eta V_0}{\omega_R^2}. \quad (104)$$

If we had used the IVHO potential instead of the cubic form, we would have obtained a numerical factor slightly different from this value, $3.6 \rightarrow \pi \approx 3.14$. On the other hand, Caldeira and Leggett obtain, using a different method,

$$\Delta B_{\text{CL}} \approx \frac{162\zeta(3)}{\pi^3} \frac{\eta V_0}{\omega_R^2} \approx 6.28045 \frac{\eta V_0}{\omega_R^2}. \quad (105)$$

Thus our result gives a result numerically different by a factor of about 2 in the weak coupling limit.

On the other hand, in the large coupling limit $\eta \gg 2\omega_R$, these two are

$$\Delta B = \frac{36}{5} \frac{\eta V_0}{\omega_R^2}, \quad \Delta B_{\text{CL}} = 3\pi \frac{\eta V_0}{\omega_R^2}. \quad (106)$$

(Although our notation here suggests that this is a correction term to the main term of $e^{-2\pi V_0/\omega_R}$, it is actually a leading term for the case of $\eta \gg 2\omega_R$.) Our result is about 0.8 times the Caldeira-Leggett value.

In general, when one writes the deviation of the penetration factor from the case of no environment as $e^{-\Delta B}$, one has the form

$$\Delta B = \Phi \left(\frac{\eta}{2\omega_R} \right) \frac{\eta V_0}{\omega_R^2}. \quad (107)$$

Both in our case and in the case of Caldeira and Leggett the function $\Phi(\alpha)$ is slowly varying albeit numerically different, and the deviation factor is dominated by $\eta V_0/\omega_R^2$. This appears to be the most important dependence of the parameters, the numerical factor being a secondary effect.

In our interpretation of the result of Caldeira and Leggett it is crucial to use the pole curvature ω_B as our reference, and this choice is reasonable because it corresponds to an equilibrium in the zero temperature limit considered in [9]. With the dynamical function taken as $f(t) = 1$, this is the only way the friction (η) dependence can appear in our approach, namely, via the parameter ω_B in the initial density matrix. It is important that our inequality $\omega_B^2 < \omega_R^2$ implies the general result of a suppressed rate of tunneling in the medium, the main point stressed by Caldeira and Leggett. We also note that detailed comparison between our result and that of [9] is possible only by assuming the relation (86), specific to the Ohmic spectrum. For different models the difference between the two might be larger.

In the future we wish to examine further this discrepancy after we develop a formalism for more general potentials.

The second application of our general formula is the problem of time evolution for the same potential as above. For this we consider the temperature range of $\omega_* \ll T \ll V_0$ such that the average energy eigenstate (of $\bar{E} \approx T$) may be treated semiclassically. We thus regard a particle in the n th energy level ($n \gg 1$) of the left harmonic oscillator as moving almost classically with a periodic motion of frequency ω_* . Each time this particle hits against the right barrier, it has a prescribed probability (72) of tunneling into the far right region. Starting at time $t=0$, one counts the k th encounter with the barrier at time $t = 2\pi k/\omega_*$ until the final time t_f such that there are roughly $t_f \omega_*/2\pi$ times of possibility of barrier penetration. We find it reasonable to use a reset time for each encounter for the time t of Eq. (72). Summing up all these possibilities, one gets the total tunneling probability

$$\Gamma_n(t_f) = |T(E_n)|^2 \frac{t_f \omega_*}{2\pi} \bar{f}, \quad (108)$$

where \bar{f} is some sort of representative value for the dynamical factor for each encounter, perhaps some average of $f(t)$ [Eq. (73)] over one period of oscillation under the harmonic well, like

$$\bar{f} = \frac{1}{t_*} \int_0^{t_*} dt f(t), \quad t_* = \frac{\omega_*}{2\pi}. \quad (109)$$

Another choice for \bar{f} is the dynamical function at some particular value of time during one period of oscillation, for instance, at the classical turning point.

For $\omega_B \gg \omega_*$, $\bar{f} \approx 1$, and

$$\Gamma_n(t) \approx |T(E_n)|^2 \frac{t \omega_*}{2\pi}. \quad (110)$$

Thus, the total probability is proportional to time t , and one may define the tunneling rate per unit time,

$$\frac{\Gamma_n(t)}{t} = \frac{\omega_*}{2\pi} |T(E)|^2. \quad (111)$$

This is nothing but the classic Kramers formula [7].

On the other hand, for $\omega_B \approx \omega_*$ there may be a large deviation from the quantum mechanical formula. We plot in Fig. 11 some examples of the factor \bar{f} [Eq. (109)] as a function of the average time t_* . In most cases studied, \bar{f} is some fraction of unity, typically larger than 0.5.

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APPENDIX A: INTEGRAL TRANSFORM OF THE WIGNER FUNCTION

After some algebra, we obtain

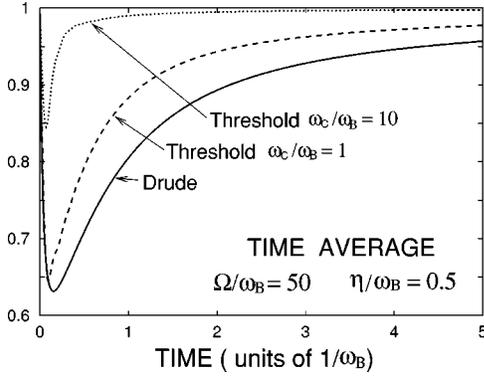


FIG. 11. Time averaged dynamical factor $f(t)$ for a few models.

$$f_W^{(R)}(x,p) = \frac{1}{2\pi\sqrt{I_1 I_2 - I_3^2}} \int_{-\infty}^{\infty} dx_i \int_{-\infty}^{\infty} dp_i f_W^{(i)}(x_i, p_i) \times \exp \left[-\frac{1}{2(I_1 I_2 - I_3^2)} [I_1(p - p_{cl})^2 + I_2(x - x_{cl})^2 - 2I_3(x - x_{cl})(p - p_{cl})] \right], \quad (\text{A1})$$

$$x_{cl} = \dot{g}x_i + gp_i, \quad p_{cl} = \ddot{g}x_i + \dot{g}p_i. \quad (\text{A2})$$

The definitions of I_i are given in the text, Eqs. (51)–(53). The time dependent functions $x_{cl}(t)$ and $p_{cl}(t)$, are homogeneous solutions to the Langevin equation (43) with $F_Q = 0$.

One may view the mapping from $f_W^{(i)}$ to $f_W^{(R)}$ as a kind of fluid flow. Compared to the classical mapping given in Sec. II, the quantum solution (A1) in a thermal medium is not deterministic with a broadening given by the coefficient matrix

$$(I) = \begin{pmatrix} I_1 & I_3 \\ I_3 & I_2 \end{pmatrix}. \quad (\text{A3})$$

Moreover, the initial distribution $f_W^{(i)}$ itself is broadened by quantum mechanical effects. The peak point of the distribution is at $(x_{cl}(t), p_{cl}(t))$. One might imagine that the mapping $(x_i, p_i) \rightarrow (x_{cl}(t), p_{cl}(t))$ is not invertible due to dissipative effects from the environment. This is not true; the mapping is actually invertible and

$$x_i = \frac{\dot{g}x_{cl} - gp_{cl}}{\dot{g}^2 - g\ddot{g}}, \quad p_i = \frac{-\ddot{g}x_{cl} + \dot{g}p_{cl}}{\dot{g}^2 - g\ddot{g}}, \quad (\text{A4})$$

with $\dot{g}^2 - g\ddot{g} \neq 0$.

APPENDIX B: FOKKER-PLANCK EQUATION

One may derive the master equation for the reduced density matrix as described in Ref. [20]. Our formula for the Wigner function (A1) is considered as an explicit and con-

venient solution to this type of master equation. From the master equation one can derive a Fokker-Planck equation for the Wigner function:

$$\begin{aligned} \frac{\partial f_W^{(R)}}{\partial t} = & -p \frac{\partial f_W^{(R)}}{\partial x} + \Omega^2(t)x \frac{\partial f_W^{(R)}}{\partial p} \\ & + C(t) \frac{\partial}{\partial p} (p f_W^{(R)}) - 2D_{pp}(t) \frac{\partial^2 f_W^{(R)}}{\partial p^2} \\ & + 2D_{xp}(t) \frac{\partial^2 f_W^{(R)}}{\partial x \partial p}, \end{aligned} \quad (\text{B1})$$

$$\Omega^2(t) = -\frac{\ddot{g}^2 - \dot{g}\ddot{g}}{g\ddot{g} - \dot{g}^2} = \frac{\dot{g}}{g} \frac{d}{dt} \ln \left[\frac{g}{\dot{g}} \left(\ddot{g} - \frac{\dot{g}^2}{g} \right) \right], \quad (\text{B2})$$

$$C(t) = -\frac{g\ddot{g} - \dot{g}\ddot{g}}{g\ddot{g} - \dot{g}^2}, \quad (\text{B3})$$

$$D_{pp}(t) = \frac{1}{2} \left(\frac{g\ddot{g} - \dot{g}\ddot{g}}{g\ddot{g} - \dot{g}^2} U + \frac{\dot{g}}{2g} \frac{g^2\ddot{g} - 2g\dot{g}\ddot{g} + \dot{g}^3}{g\ddot{g} - \dot{g}^2} W - \frac{\dot{U}}{2} - \dot{g}\dot{W} \right), \quad (\text{B4})$$

$$D_{xp}(t) = U - g\dot{W} + \frac{g^2\ddot{g} - 2g\dot{g}\ddot{g} + \dot{g}^3}{g\ddot{g} - \dot{g}^2} W, \quad (\text{B5})$$

where the coefficient functions $\Omega^2(t)$, $C(t)$, $D_{pp}(t)$, and $D_{xp}(t)$ are local functions of time and are written in terms of $g(t)$, U , V , and W .

The quantities that appear in this equation are well understood by writing a set of moment equations of low orders:

$$\frac{d\langle x \rangle}{dt} = \langle p \rangle, \quad \frac{d\langle p \rangle}{dt} = -\Omega^2(t)\langle x \rangle - C(t)\langle p \rangle, \quad (\text{B6})$$

$$\frac{d\langle x^2 \rangle}{dt} = 2\langle xp \rangle, \quad (\text{B7})$$

$$\frac{d\langle p^2 \rangle}{dt} = -2\Omega^2(t)\langle xp \rangle - 2C(t)\langle p^2 \rangle - 4D_{pp}(t), \quad (\text{B8})$$

$$\frac{d\langle xp \rangle}{dt} = \langle p^2 \rangle - \Omega^2(t)\langle x^2 \rangle - C(t)\langle xp \rangle + 2D_{xp}(t). \quad (\text{B9})$$

For instance, the quantity $\Omega^2(t)$ here is a time dependent curvature parameter modified from the original ω_0^2 to that in a thermal medium, while $C(t)$ is a time dependent friction. In similar fashion one understands D_{pp} and D_{xp} as fluctuations. The physical behaviors of the harmonic oscillator system under a thermal environment are all determined by these four quantities, which are functions of the local time t .

Limiting values relevant to large times $t \gg 1/\omega_B$ are

$$\Omega^2(t) \approx -\omega_B^2, \quad C(t) \approx 0, \quad (\text{B10})$$

$$D_{pp}(t) \approx -\frac{\omega_B}{4} \dot{g} W \approx \frac{\omega_B^3}{4} \int_{\omega_c}^{\infty} d\omega \cosh\left(\frac{\beta\omega}{2}\right) H(\omega), \quad (\text{B11})$$

$$D_{xp}(t) \approx U - \dot{g} W \approx \int_{\omega_c}^{\infty} d\omega \cosh\left(\frac{\beta\omega}{2}\right) \left(\omega^2 + \frac{5}{4}\omega_B^2\right) H(\omega). \quad (\text{B12})$$

APPENDIX C: PARAMETERS IN SPECIFIC ENVIRONMENT MODELS

We give the various parameters in the four specific models of the environment given in Sec. III C. These parameters are used to calculate $g(t)$ according to

$$g(t) = \frac{N}{\omega_B} \sinh(\omega_B t) + 2 \int_{\omega_c}^{\infty} d\omega H(\omega) \sin(\omega t), \quad (\text{C1})$$

$$H(\omega) = \frac{r(\omega)}{[\omega^2 + \omega_R^2 - \Pi(\omega)]^2 + \pi^2 r(\omega)^2}, \quad (\text{C2})$$

$$\omega_R^2 = \omega_B^2 + C(\omega_B). \quad (\text{C3})$$

The parameters are given as follows.

(1) Ohmic model

$$N = \left(1 + \frac{\eta}{2\omega_B}\right)^{-1}, \quad C(\omega_B) = \eta\omega_B, \quad \Pi(\omega) = 0, \quad (\text{C4})$$

$$g(t) = \frac{N}{2\omega_B} (e^{\omega_B t} - e^{-(\omega+\eta)t}). \quad (\text{C5})$$

(2) Drude model

$$N = \left(1 + \frac{\eta}{2\omega_B} \frac{\Omega^2}{(\omega_B + \Omega)^2}\right)^{-1}, \quad (\text{C6})$$

$$C(\omega_B) = \frac{\eta\omega_B\Omega}{\omega_B + \Omega}, \quad \Pi(\omega) = \frac{\eta\omega^2\Omega}{\omega^2 + \Omega^2}, \quad (\text{C7})$$

$$g(t) = \frac{N}{\omega_B} \sinh(\omega_B t) + \frac{\eta\Omega^2}{(\alpha_+^2 - \omega_B^2)(\alpha_-^2 - \omega_B^2)(\alpha_+^2 - \alpha_-^2)} \\ \times [(\alpha_+^2 - \alpha_-^2)e^{-\omega_B t} + (\alpha_-^2 - \omega_B^2)e^{-\alpha_+ t} \\ + (\omega_B^2 - \alpha_+^2)e^{-\alpha_- t}], \quad (\text{C8})$$

$$\alpha_{\pm} = \frac{\omega_B + \Omega}{2} \pm \sqrt{\frac{(\omega_B - \Omega)^2}{4} - \frac{\eta\Omega^2}{\omega_B + \Omega}}. \quad (\text{C9})$$

(3) Threshold model

$$N = \left(1 - \frac{\eta}{\pi} \frac{\Omega - \omega_c}{\Omega^2 + \omega_B^2} + \frac{\eta}{\pi\omega_B} \arctan \frac{\Omega}{\omega_B} - \frac{\eta}{\pi\omega_B} \arctan \frac{\omega_c}{\omega_B}\right)^{-1}, \quad (\text{C10})$$

$$C(\omega_B) = \frac{2\eta\omega_B}{\pi} \left(\arctan \frac{\Omega}{\omega_B} - \arctan \frac{\omega_c}{\omega_B}\right) \\ + \frac{\eta\omega_c}{\pi} \left\{ \ln\left(1 + \frac{\omega_B^2}{\Omega^2}\right) - \ln\left(1 + \frac{\omega_B^2}{\omega_c^2}\right) \right\}, \quad (\text{C11})$$

$$\Pi(\omega) = \frac{\eta(\omega - \omega_c)}{2\pi} \ln\left(\frac{\omega}{\omega_c} - 1\right) - \frac{\eta(\omega + \omega_c)}{2\pi} \ln\left(\frac{\omega}{\omega_c} + 1\right) \\ - \frac{\eta(\omega - \omega_c)}{2\pi} \ln\left(\frac{\omega}{\Omega} - 1\right) + \frac{\eta(\omega + \omega_c)}{2\pi} \ln\left(\frac{\omega}{\Omega} + 1\right). \quad (\text{C12})$$

(4) Super-Ohmic model

$$N = \left(1 - \frac{\eta}{\pi} \frac{\Omega^2}{\Omega^2 + \omega_B^2} + \frac{\eta}{\pi} \ln \frac{\Omega^2 + \omega_B^2}{\omega_B^2}\right)^{-1}, \quad (\text{C13})$$

$$C(\omega_B) = \frac{\eta\omega_B^2}{\pi} \ln \frac{\Omega^2 + \omega_B^2}{\omega_B^2}, \quad \Pi(\omega) = -\frac{\eta\omega^2}{\pi} \ln \frac{\Omega^2 - \omega^2}{\omega^2}. \quad (\text{C14})$$

In calculation of $g(t)$ for the Ohmic model one needs a frequency cutoff in intermediate steps of integration, but the final result does not depend on this cutoff factor. For the model having a threshold and for the super-Ohmic model we cannot get analytic forms of the basic function $g(t)$.

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