

## Quantum tunneling in dissipative systems

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As a prelude to a discussion of tunneling in the presence of dissipation, we discuss the damped harmonic oscillator. We show that for a harmonic-oscillator potential, the Caldeira-Leggett Hamiltonian can be reduced to a sum of independent harmonic-oscillator Hamiltonians by a normal-mode transformation. We then discuss tunneling through a parabolic barrier and explain the apparently contradictory results in the literature. The decay of a metastable state is then discussed. We argue that much of the published work on tunneling in dissipative systems has assumed unphysical initial conditions. We calculate the tunneling out of a metastable state, on the assumption that the environment is initially at zero temperature, and find that quantum tunneling is enhanced by dissipation.

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### I. INTRODUCTION

In recent years there has been considerable interest in the tunneling of a particle through an energy barrier when dissipation is present. The problem was considered in detail by Caldeira and Leggett [1,2]. They considered tunneling of a particle in a potential of the form  $V(q) = \omega_0^2 q^2 / 2 - \beta q^3$ , although their conclusions were not limited to this particular form. They concluded that "the presence of dissipation always tends to suppress quantum tunneling" (Ref. [2], p. 423). (This statement must be interpreted in the context of their paper; it was not intended to be absolute.) Widom and Clark [3] considered tunneling through a parabolic potential barrier and found that dissipation enhanced tunneling. In an exchange of Comments [4,5] the authors could not reach agreement. Bruinsma and Bak [6] also considered tunneling through a barrier and found that at zero temperature the tunneling rate may be either increased or decreased by dissipation. Widom and Clark [7] investigated tunneling in a model ferroelectric capacitor with linear passable dissipation and found that dissipation does not impede macroscopic tunneling. In an adjacent paper Leggett [8] considered tunneling in the presence of an arbitrary dissipation mechanism and found that, normally, dissipation impedes tunneling, but he also found an anomalous case in which dissipation assists the tunneling process. Razavy [9] considered tunneling in a symmetric double-well potential and concluded that dissipation could inhibit or suppress tunneling. Fujikawa *et al.* [10] also considered tunneling in a double-well potential and found an enhancement of tunneling. It is not easy to reconcile these results since different authors attacked different problems by different methods. Caldeira and Leggett [1,2] calculated the decay rate for a particle in a metastable state using a field-theoretic technique (instanton technique). This technique is of quasiclassical accuracy in the sense that Planck's constant  $\hbar$  is considered to be small. Motivated by some skepticism which has been expressed concerning the instanton technique, Schmid [11] carried out a quasiclassical calculation by more generally accept-

ed techniques with results in agreement with Caldeira and Leggett.

In classical mechanics dissipation can be introduced through a phenomenological frictional force. In quantum mechanics this is not possible; one must begin with a Hamiltonian. What is commonly done is to couple the system of interest (a particle moving in a potential in the work discussed here) to an ensemble of harmonic oscillators. We shall call this ensemble "the environment." A Hamiltonian is written for the combined system of particle and oscillators. Energy and momentum can be exchanged between the particle and oscillators. With appropriately chosen initial conditions, the motion of the particle is damped. Since energy may be transferred from the oscillators to the particle as well as from the particle to the oscillators, it is possible to choose initial conditions so that the motion of the particle is undamped, or the damping is negative. These solutions are unphysical in the sense that they require a fine tuning of the environment (the ensemble of oscillators) that is unachievable. In this paper we shall argue that in much of the published work on tunneling in dissipative systems, unphysical initial conditions have been chosen, and that the results obtained are not relevant to the real world.

In Sec. II we present the Hamiltonian used in our calculations. This is a slight modification of the Hamiltonian used by Unruh and Zurek [12] and by Harris [13] to treat the damped harmonic oscillator. We show that by a canonical transformation it can be transformed to the Hamiltonian used by Caldeira and Leggett [1,2]. We show that Hamilton's equations have solutions in which the motion of the particle is either positively or negatively damped. Indeed, almost any motion of the particle can be obtained by proper choice of the initial conditions.

In Sec. III we discuss the case of the particle moving in a harmonic-oscillator potential. This problem can be solved exactly by a transformation to normal coordinates. This transformation has been made previously by van Kampen [14], Sollfrey and Goertzel [15], and Ullersma [16]. In the normal coordinate solution the motion of the particle is, on the average, undamped. The particle alter-

nately takes energy from and gives energy to the environment. This behavior is quite unlike that found by Harris [13]. In his solution the ensemble of oscillators was assumed to be initially in thermal equilibrium. As time increases, the particle approaches thermal equilibrium with the oscillators. If the initial temperature is zero, the energy of the particle decays until it reached the ground state. It is this solution rather than the normal coordinate solution that we believe to be physically realistic.

The transformation to normal coordinates works just as well when the parabolic potential well is inverted to give a potential barrier. We use this in Sec. III to calculate the transmission probability through a parabolic barrier, the problem treated by Widom and Clark [3]. The Hamiltonian used by Widom and Clark differed from that of Caldeira and Leggett by the omission of a renormalization term. Using the Widom-Clark Hamiltonian we find, as they did, that tunneling is enhanced by dissipation. Using the Caldeira-Leggett Hamiltonian we find that dissipation tends to suppress tunneling. Calculation of the classical motion of the particle reveals that at  $t = -\infty$  the particle has a negatively infinite energy. As it approaches the classical turning point it absorbs energy from the environment and reaches the turning point with a finite energy. Then, as it recedes from the turning point, it gives up energy to the environment, and its energy becomes negatively infinite again at  $t = +\infty$ . At all times the sum of particle, oscillators, and interaction energies is constant and finite. We think that no conclusions about tunneling in real systems should be drawn from this unphysical behavior.

In Sec. IV we discuss decay of a metastable state by tunneling. The initial state of the system is a superposition of states that interfere constructively in the region where the particle is initially confined. If the states that constitute the superposition are eigenstates of the Hamiltonian, then the expectation value of the particle's energy in each of these states is constant, indicating that there is no net transfer of energy from the particle to the environment. To prepare the system in one of these states would require an unattainable fine tuning of the environment. The assumption that the system is initially in a superposition of such states is unrealistic. We think that it is more realistic to assume that initially the particle is confined and the environment is in thermal equilibrium. In our calculation we take the temperature of the environment to be zero. The states that compose the superposition are then time-dependent states that decay toward the ground state. The effect of this decay is to shorten the lifetime of the particle in the metastable state.

Finally, in Sec. V we summarize our conclusions and comment on previous work on dissipative tunneling.

## II. MODEL

We consider a particle with coordinate  $q_0$  and momentum  $p_0$  moving in a potential  $V(q_0)$ . Its Hamiltonian is  $p_0^2/2m_0 + V(q_0)$ . It is coupled to a one-dimensional scalar field  $\Phi(x,t)$  confined between  $x = -L$  and  $+L$ . The field obeys the wave equation  $\ddot{\Phi} = v^2 \partial_x^2 \Phi$  where  $v$  is the wave velocity. When the field is written as a Fourier

series in  $x$  and the amplitudes  $Q_n$  are taken as coordinates, the Hamiltonian for the field has the form of a sum of harmonic-oscillator Hamiltonians. We adopt the form of the coupling assumed by Unruh and Zurek [12] and write the Hamiltonian for the coupled system of particle and field as

$$H = p_0^2/2m_0 + V(q_0) + \frac{1}{2} \sum_{n=1}^{\infty} [(P_n + \epsilon_n q_0/L^{1/2} \omega_n)^2/m_n + m_n \omega_n^2 Q_n^2] \quad (1)$$

where  $\omega_n = (n-1/2)\pi v/L$ . This Hamiltonian differs in some minor ways from that of Ref. [13] where the derivation can be found. We have assigned masses  $m_0$  and  $m_n$  to the particle and field oscillators and have assigned the coupling constants  $\epsilon_n$  differently to facilitate comparison with the Caldeira-Leggett Hamiltonian.

We make a canonical transformation from  $(Q_n, P_n)$  to  $(q_n, p_n)$  for  $n = 1, 2, 3, \dots$  using the generating function

$$F(q_n, Q_n) = - \sum_{n=1}^{\infty} m_n \omega_n q_n Q_n. \quad (2a)$$

The transformation equations are

$$P_n = - \frac{\partial F}{\partial Q_n} = m_n \omega_n q_n, \quad p_n = \frac{\partial F}{\partial q_n} = -m_n \omega_n Q_n. \quad (2b)$$

The transformed Hamiltonian is found to be

$$H = p_0^2/2m_0 + V(q_0) + \frac{1}{2} \sum_{n=1}^{\infty} [p_n^2/m_n + m_n \omega_n^2 q_n^2] + 1/L^{1/2} \sum_{n=1}^{\infty} \epsilon_n q_0 q_n + q_0^2/2L \sum_{n=1}^{\infty} \epsilon_n^2/m_n \omega_n^2. \quad (2c)$$

This is the Caldeira-Leggett Hamiltonian written in a different notation. The coupling constant  $C_n$  of Caldeira and Leggett is our coupling constant  $\epsilon_n/L^{1/2}$ . We have found it convenient to retain  $L$  in the formulas until such a time that we shall let  $L$  approach infinity and convert sums over  $n$  into integrals over  $\omega$  according to the prescription

$$\sum_{n=1}^{\infty} \rightarrow (L/\pi v) \int_0^{\infty} d\omega \quad \text{as } L \rightarrow \infty. \quad (3)$$

Leggett [8] has shown that a large class of Hamiltonians may be reduced to the form of Eq. (2c) by appropriate transformations. Before continuing it is convenient to simplify the equations by defining new variables so as to eliminate the masses from  $H$ . We define  $q'_n = m_n^{1/2} q_n$ ,  $p'_n = p_n/m_n^{1/2}$ , and  $\epsilon'_n = \epsilon_n/(m_0 m_n)^{1/2}$ . We make this change of variable in Eq. (2c) but drop the cumbersome primes and obtain

$$H = p_0^2/2 + V(q_0) + \frac{1}{2} \sum_{n=1}^{\infty} [p_n^2 + \omega_n^2 q_n^2] + 1/L^{1/2} \sum_{n=1}^{\infty} \epsilon_n q_0 q_n + q_0^2/2L \sum_{n=1}^{\infty} \epsilon_n^2/\omega_n^2. \quad (4)$$

This is the Hamiltonian that shall be used throughout this paper.

Either Hamilton's equations for the classical variables or the Heisenberg equations for the quantum-mechanical operators yield the equations of motion

$$\ddot{q}_n + \omega_n^2 q_n = -\epsilon_n q_0 / L^{1/2} \quad \text{for } n=1,2,3,\dots, \quad (5a)$$

$$\ddot{q}_0 + \frac{\partial V}{\partial q_0} = - \sum_{n=1}^{\infty} [\epsilon_n q_n / L^{1/2} + \epsilon_n^2 q_0 / L \omega_n^2]. \quad (5b)$$

We may solve Eq. (5a) as an initial value problem and substitute the results into Eq. (5b) to obtain

$$\begin{aligned} \ddot{q}_0 + \frac{\partial V}{\partial q_0} + \frac{d}{dt} \int_0^t dt' G(t-t') q_0(t') \\ = -1/L^{1/2} \sum_{n=1}^{\infty} \epsilon_n \{ q_n(0) \cos(\omega_n t) \\ + (1/\omega_n) p_n(0) \sin(\omega_n t) \} \end{aligned} \quad (6a)$$

where

$$G(t-t') = (4v/L) \sum_{n=1}^{\infty} \gamma_n \cos[\omega_n(t-t')] \quad (6b)$$

and  $\gamma_n = \epsilon_n^2 / 4v\omega_n^2$ .

The third term on the left-hand side of Eq. (6a) is a (generally nonlocal) damping term. It takes a particularly simple form if  $\gamma_n = \gamma = \text{const}$  for then  $G(t-t') = 4\gamma\delta(t-t')$  and Eq. (6a) has the form

$$\begin{aligned} \ddot{q}_0 + 2\gamma \frac{d}{dt} \theta(t) q_0(t) + \frac{\partial V}{\partial q_0} \\ = -1/L^{1/2} \sum_{n=-1}^{\infty} \epsilon_n \{ q_n(0) \cos \omega_n t \\ + (1/\omega_n) p_n(0) \sin \omega_n t \} \end{aligned} \quad (6c)$$

where  $\theta(t) = +1$  for  $t > 0$  and  $-1$  for  $t < 0$ . If  $q_0$  and  $q_n$  are interpreted as classical variables, we may choose the initial conditions  $q_n(0) = p_n(0) = 0$ . Then, Eq. (6) describes a particle moving in a potential  $V(q_0)$  subject to a damping force  $-2\gamma q$  for  $t > 0$  and a negative damping force  $+2\gamma \dot{q}$  for  $t < 0$ . (There is nothing special about the time  $t=0$ ; we could equally well have chosen an arbitrary time  $t_0$ .) The presence of negatively damped solutions does not seem to have been commented on in previous work with which I am familiar. Clearly, such solutions must exist for Hamilton's equations are invariant under time reversal. If  $q_0$  and  $q_n$  are interpreted as quantum-mechanical operators, then we cannot choose  $q_n(0)$  and  $p_n(0)$  to vanish, but we can choose their expectation values  $\langle q_n(0) \rangle$  and  $\langle p_n(0) \rangle$  to vanish.

It is clear from inspection of Eq (6a) that almost any motion of a classical particle can be obtained by the appropriate choice of  $q_n(0)$  and  $p_n(0)$ . Suppose we choose some sufficiently well-behaved function  $q_0(t)$  defined on the interval  $-T < t < T$  where  $T = L/v$ . We substitute it into the left-hand side of Eq. (6a) and denote the left-hand side by  $F(t)$ , which is now a known function. We recognize the resulting equation as a Fourier series for  $F(t)$  with  $\epsilon_n q_n(0)/L^{1/2}$  and  $\epsilon_n p_n(0)/L^{1/2}$  as the Fourier coefficients. These coefficients can be calculated by the usual formulas.  $L$ , and hence  $T$ , can be made arbitrarily

large. The only restriction on the choice of  $q_0(t)$  is that it must be possible to represent  $F(t)$  by a Fourier series. For such a solution to be realized, the initial coordinates and momenta of the infinite number of field oscillators must be carefully chosen. This requires an impossibly difficult fine tuning of the environment.

### III. NORMAL COORDINATES AND THE DAMPED HARMONIC OSCILLATOR

In this section we choose  $V$  to be the harmonic-oscillator potential  $V(q_0) = \omega_0^2 q_0^2 / 2$ . We assume a solution

$$q_n(t) = a_n \cos(\Omega t + \delta) \quad (7a)$$

for  $n=0,1,2,3,\dots$  where the  $a_n$ 's are constants and  $\Omega$  is a frequency still to be determined. Substituting this into Eq. (5a) we find

$$a_n = \frac{\epsilon_n a_0}{L^{1/2}(\Omega^2 - \omega_n^2)} \quad (7b)$$

for  $n=1,2,3,\dots$ . Substituting this into Eq. (5b) and canceling  $a_0$  from both sides gives

$$\Omega^2 = \omega_0^2 + (4v/L)\Omega^2 \sum_{n=1}^{\infty} \frac{\gamma_n}{(\Omega^2 - \omega_n^2)}, \quad (7c)$$

which may also be written as

$$\Omega = \omega_0 + (4v/L) \frac{\Omega^2}{(\Omega + \omega_0)} \sum_{n=1}^{\infty} \frac{\gamma_n}{(\Omega^2 - \omega_n^2)}. \quad (7d)$$

This equation gives the possible values of  $\Omega$ . It can be solved graphically by plotting the left- and right-hand sides of the equation against  $\Omega$  and finding the intersections [17]. We shall label the solutions  $\Omega_\alpha$  and choose their order so that  $\Omega_\alpha$  approaches  $\omega_\alpha$  as the coupling constants  $\gamma_n$  approach zero. We shall label the corresponding values of  $a_n$  as  $a_{n\alpha}$ . The Hamiltonian of Eq. (4) may be written as

$$H = \frac{1}{2} \sum_{n=0}^{\infty} p_n^2 + \frac{1}{2} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} v_{nm} q_n q_m \quad (8a)$$

where  $v_{nm} = v_{mn}$ ,  $v_{nn} = \omega_n^2$ ,  $V_{0n} = \epsilon_n / \sqrt{L}$  for  $n=1,2,3$ ,

$$v_{00} = \omega_0^2 + 1/L \sum_{n=1}^{\infty} \epsilon_n^2 / \omega_n^2, \quad (8b)$$

and others are equal to zero. We normalize the  $a_{n\alpha}$ 's by choosing

$$a_{0\alpha} = \left[ 1 + 1/L \sum_{n=1}^{\infty} \frac{\epsilon_n^2}{(\Omega_\alpha^2 - \omega_n^2)^2} \right]^{-1/2}. \quad (9a)$$

It is easily shown that

$$\sum_{n=0}^{\infty} a_{n\alpha} a_{n\beta} = \delta_{\alpha\beta}, \quad (9b)$$

$$\sum_{m=0}^{\infty} v_{nm} a_{m\alpha} = \Omega_\alpha^2 a_{n\alpha}. \quad (9c)$$

We define normal coordinates  $Q_\alpha$  and momenta  $P_\alpha = \dot{Q}_\alpha$  by

$$q_n(t) = \sum_{\alpha=0}^{\infty} a_{n\alpha} Q_\alpha(t). \quad (10a)$$

Substituting into Eq. (8) and using Eqs. (9a) and (9b) we obtain

$$H = \frac{1}{2} \sum_{\alpha=0}^{\infty} (P_\alpha^2 + \Omega_\alpha^2 Q_\alpha^2). \quad (10b)$$

This is the Hamiltonian for a collection of independent oscillators. The classical particle, which in the absence of interaction with the environment oscillated with frequency  $\omega_0$ , has been replaced by an oscillator with the frequency  $\Omega_0$  whose motion is not damped. For a harmonic-oscillator potential the expectation values obey the same equations of motion as the classical variables, so the same remark may be made about  $\langle q_0(t) \rangle$ . Let us suppose that  $Q_\alpha = 0$  for  $\alpha \neq 0$  and  $Q_0 = A_0 \cos(\Omega_0 t)$ . The calculation of the energy of the particle, the energy of the field, and the interaction energy gives

$$E_p = \frac{1}{2} (p_0^2 + \omega_0^2 q_0^2) = \frac{1}{2} a_{00}^2 A_0^2 \Omega_0^2 \left\{ 1 - \frac{(\Omega_0^2 - \omega_0^2) \cos^2 \Omega_0 t}{\Omega_0^2} \right\}, \quad (11a)$$

$$E_f = \frac{1}{2} \sum_{n=1}^{\infty} [p_n^2 + \omega_n^2 q_n^2] = A_0^2 a_{00}^2 \Omega_0^2 \sum_{n=1}^{\infty} \frac{\epsilon_n^2}{2L(\Omega_0^2 - \omega_n^2)^2} \times \left\{ 1 - \frac{(\Omega_0^2 - \omega_n^2) \cos^2 \Omega_0 t}{\Omega_0^2} \right\}, \quad (11b)$$

$$E_i = \sum_{n=1}^{\infty} (\epsilon_n q_0 q_n / \sqrt{L} + \epsilon_n^2 q_0^2 / 2L \omega_n^2) = A_0^2 a_{00}^2 \cos^2(\Omega_0 t) \sum_{n=1}^{\infty} \frac{\epsilon_n^2 (\Omega_0^2 + \omega_n^2)}{2L \omega_n^2 (\Omega_0^2 - \omega_n^2)}. \quad (11c)$$

The energy of the particle oscillates as energy is alternately transferred from the particle to the environment and back to the particle. The field energy and interaction energy also oscillate in such a way that the sum of particle, field, and interaction energies is the constant  $A_0^2 \Omega_0^2 / 2$ .

To achieve such an undamped state the initial values of the field coordinates must be adjusted to the values

$$q_n(0) = \frac{\epsilon_n q_0(0)}{L^{1/2} (\Omega_0^2 - \omega_n^2)}. \quad (12)$$

Such an initial state is not attainable in practice. For example, consider a pendulum mounted in a container of gas. In principle one could write a Hamiltonian for the interacting system of pendulum and gas molecules. There must be solutions of the equations of motion in which the pendulum executes damped, negatively

damped, or undamped motion, but in practice only damped motion is observed, because the experimenter has very little control over the initial positions and velocities of the gas molecules. A more reasonable assumption about the environment is that it is in thermal equilibrium at some temperature (which may be zero).

The Hamiltonian of Eq. (10b) has the energy eigenvalues

$$E = \sum_{\alpha=0}^{\infty} \hbar \Omega_\alpha (N_\alpha + \frac{1}{2}) \quad (13a)$$

and the eigenvectors

$$|E\rangle = |N_0\rangle |N_1\rangle |N_2\rangle \cdots = |\mathbf{N}\rangle \quad (13b)$$

where

$$\frac{1}{2} (P_\alpha^2 + \Omega_\alpha^2 Q_\alpha^2) |N_\alpha\rangle = \hbar \omega_n (N_\alpha + \frac{1}{2}) |N_\alpha\rangle \quad (13c)$$

and the  $N_\alpha$ 's are integers. The expectation value of the particles' energy can be calculated for this state with the results

$$\langle E_p \rangle = \langle \frac{1}{2} (p_0^2 + \omega_0^2 q_0^2) \rangle = \sum_{\alpha=1}^{\infty} a_{0\alpha}^2 \hbar \Omega_\alpha (N_\alpha + \frac{1}{2}) \left[ 1 - \frac{(\Omega_\alpha^2 - \omega_0^2)}{2\Omega_0^2} \right]. \quad (13d)$$

If  $N_\alpha = 0$  for all  $\alpha$  except  $\alpha = 0$ , we can compare this with the classical  $E_p$  of Eq. (11a). The term with  $\alpha = 0$  in Eq. (13c) is like that of Eq. (11a) with  $A_0^2 \Omega_0^2 / 2$  replaced by  $\hbar \Omega_0 (N_0 + \frac{1}{2})$  and  $\cos^2 \Omega_0 t$  replaced by its average value of  $\frac{1}{2}$ . The terms with  $\alpha > 0$  represent the contributions of the zero-point vibrations of the field oscillators to the energy of the particle.

A quite different result is obtained if it is assumed that initially the environment is in thermal equilibrium at a temperature  $\beta^{-1}$ . We have treated this problem in some detail elsewhere [13] and shall briefly review some of the results here. The calculation is based on Eq. (6c) for  $t > 0$  and  $V(q_0) = \omega_0^2 / 2$ . This is the Heisenberg equation of motion for the operator  $q_0$ . It can be solved exactly for  $q_0(t)$  in terms of the initial values of all of the operators  $q_n(0)$  and  $p_n(0)$ . Then the expectation values  $\langle q_n(t) \rangle$ ,  $\langle p_n(t) \rangle$ ,  $\langle q_n^2(t) \rangle$ , and  $\langle p_n^2(t) \rangle$  can be calculated in terms of initial expectation values. Here the angular brackets denote both a quantum-mechanical average and an average over a thermal ensemble. For the field oscillators we shall assume the initial conditions

$$\langle q_n(0) \rangle = \langle p_n(0) \rangle = 0, \quad (14a)$$

$$\langle q_n(0) q_{n'}(0) \rangle = \langle p_n(0) p_{n'}(0) \rangle = 0 \text{ for } n \neq n', \quad (14b)$$

$$\langle q_n(0) p_{n'}(0) + p_{n'}(0) q_n(0) \rangle = 0 \text{ for all } n \text{ and } n', \quad (14c)$$

$$\omega_n^2 \langle q_n^2(0) \rangle = \langle p_n^2(0) \rangle = (\hbar \omega_n / 2) \coth(\hbar \omega_n \beta / 2). \quad (14d)$$

We shall quote the results for the case of weak damping ( $\gamma \ll \omega_0$ ) and the initial conditions  $\langle q_0(0) \rangle = \langle p_0(0) \rangle = \langle q_0(0) p_0(0) + p_0(0) q_0(0) \rangle = 0$ . (A more extensive discussion may be found in Ref. [13].) The expectation value

of the particles energy is

$$\begin{aligned} & \langle \frac{1}{2}[p_0^2(t) + \omega_0^2 q_0^2(t)] \rangle \\ &= \langle \frac{1}{2}[p_0^2(0) + \omega_0^2 q_0^2(0)] \rangle \exp(-2\gamma t) \\ &+ (\hbar\omega_0/2) \coth(\hbar\omega_0\beta/2) [1 - \exp(-2\gamma t)]. \end{aligned} \quad (15)$$

The initial energy decays and the particle approaches thermal equilibrium with the environment in a time of the order of  $1/2\gamma$ . If the temperature of the environment is zero, the final energy of the particle is  $\hbar\omega_0/2$ , the zero-point energy.

It is worth noting that the same conclusion would be reached by applying time-dependent perturbation theory with the terms containing  $q_0 q_n$  in Eq. (4) as the perturbation. It is useful to introduce the annihilation operators for field quanta

$$C_n = (\omega_n/2\hbar)^{1/2} q_n + i p_n / (2\hbar\omega_n)^{1/2} \quad (16a)$$

and their adjoints  $C_n^\dagger$ , the corresponding creation operators. In terms of these operators, the Hamiltonian of Eq. (4) becomes

$$\begin{aligned} H &= p_0^2/2 + V(q_0) + \sum_{n=1}^{\infty} \hbar\omega_n C_n^\dagger C_n \\ &+ q_0/L^{1/2} \sum_{n=1}^{\infty} \epsilon_n (\hbar/2\omega_n)^{1/2} (C_n + C_n^\dagger) \\ &+ (q_0^2/L) \sum_{n=1}^{\infty} \epsilon_n^2 / \omega_n^2. \end{aligned} \quad (16b)$$

We will write this as  $H = H_0 + H_1 + H_2$  where  $H_0$  is the sum of the particle and field Hamiltonians,  $H_1$  is the sum of terms containing  $\epsilon_n$ , and  $H_2$  is the sum of the terms containing  $\epsilon_n^2$ . Assuming  $\gamma_n = \epsilon_n^2 / 4v\omega_n^2 = \gamma = \text{const}$  and using the Fermi golden rule we calculate the transition probability per unit time from an initial eigenstate of  $H_0$  in which the particle is in the state  $|\Psi_i\rangle$  and all of the field oscillators are in their ground states to a final eigenstate in which the particles is in the state  $|\Psi_f\rangle$  and one of the field oscillators is in its first excited state. We find

$$T(i \rightarrow f) = (4\gamma/\hbar) |\langle \Psi_f | q_0 | \Psi_i \rangle|^2 \omega_{if} \quad (17)$$

where  $\omega_{if} = (E_i - E_f)/\hbar$  and  $E_i$  and  $E_f$  are particle energies. If  $V(q_0)$  is the harmonic-oscillator potential, the matrix element vanishes except for neighboring states. Taking the initial state to have the energy  $E = \hbar\omega_0(N_0 + \frac{1}{2})$  and the final state to have the energy  $\hbar\omega_0(N_0 - 1 + \frac{1}{2})$ , the matrix element is found to be  $\hbar N_0 / 2\omega_0$ . This gives  $T(i \rightarrow f) = 2\gamma N_0$ . The energy lost by the particle in this transition is  $\hbar\omega_0$ . Replacing the jumps between discrete levels by a continuous change, we may write the rate of change of the energy as

$$\frac{dE}{dt} = -(2\gamma N_0) \hbar\omega_0 = -2\gamma(E - \hbar\omega_0/2). \quad (18a)$$

The solution of this equation is

$$E(t) = E(0) \exp(-2\gamma t) + (\hbar\omega_0/2) [1 - \exp(-2\gamma t)]. \quad (18b)$$

It is of some interest to see how accurately the energy eigenvalues of Eq. (13a) can be calculated from perturbation theory. We have treated the terms containing  $\epsilon_n^2$  in Eq. (4) as perturbations and used second-order time-independent perturbation theory. The results can be put in the form of Eq. (13a) with the frequencies  $\Omega_\alpha$  given by

$$\Omega_0 \simeq \omega_0 + (2v/L) \sum_{n=1}^{\infty} \frac{\gamma_n \omega_0}{\omega_0^2 - \omega_n^2}, \quad (19a)$$

$$\Omega_\alpha \simeq \omega_n - (2v/L) \frac{\gamma_n \omega_n}{\omega_0^2 - \omega_n^2}. \quad (19b)$$

These formulas agree to order  $\epsilon_n^2$  with the exact formulas of Eq. (7d).

#### IV. TUNNELING THROUGH A PARABOLIC BARRIER

We take the potential in Eq. (4) to be  $V(q_0) = -\omega_0^2 q_0^2 / 2$ ; now the parabolic well of the preceding section has become a parabolic barrier. Classically, a particle incident on the barrier would be reflected if its energy is negative and transmitted if its energy is positive. The quantum-mechanical transmission probability for a particle of energy  $E$  is

$$P(E, \omega_0) = [1 + \exp(-2\pi E / \hbar\omega_0)]^{-1}. \quad (20)$$

This expression is rigorous and well known [18,19].

The transformation to normal coordinates goes through as in the preceding section and gives the Hamiltonian

$$H = \frac{1}{2}(P_0^2 - \Omega_0^2 Q_0^2) + \frac{1}{2} \sum_{\alpha=1}^{\infty} (P_\alpha^2 + \Omega_\alpha^2 Q_\alpha^2). \quad (21)$$

The frequency of interest  $\Omega_0$  is found by assuming a solution

$$q_n = a_n \cosh \Omega_0 t \quad (22a)$$

for all  $n$ . Substituting into Eq. (5a) gives

$$a_n = -\frac{\epsilon_n a_0}{L^{1/2}(\Omega_0^2 + \omega_n^2)}, \quad n = 1, 2, 3, \dots \quad (22b)$$

Using this in Eq. (5b) and canceling  $a_0$  from both sides gives

$$\Omega_0^2 = \omega_0^2 - (4v\Omega_0^2/L) \sum_{n=1}^{\infty} \frac{\gamma_n}{(\Omega_0^2 + \omega_n^2)}, \quad (22c)$$

which is to be solved for  $\Omega_0$ . We shall label the solution  $\Omega_0(\text{CL})$  since it was obtained using the Caldeira-Leggett Hamiltonian. Clearly,  $\Omega_0(\text{CL}) < \omega_0$ .

Widom and Clark used the Hamiltonian of Eq. (4), but with the last term omitted. This leads to

$$\Omega_0^2 = \omega_0^2 + (4v/L) \sum_{n=1}^{\infty} \frac{\gamma_n \omega_n^2}{(\Omega_0^2 + \omega_n^2)}. \quad (23)$$

We shall label the solution  $\Omega_0(\text{WC})$ . Clearly,  $\Omega_0(\text{WC}) > \omega_0$ . Taking the limit as  $L \rightarrow \infty$  and using Eq. (3) gives

$$\Omega_0^2(\text{CL}) = \omega_0^2 - (4\Omega_0^2/\pi) \int_0^\infty d\omega \frac{\gamma(\omega)}{\Omega_0^2 + \omega^2}, \quad (24a)$$

$$\Omega_0^2(\text{WC}) = \omega_0^2 + (4/\pi) \int_0^\infty d\omega \frac{\gamma(\omega)\omega^2}{\Omega_0^2 + \omega^2}. \quad (24b)$$

Equation (24b) agrees with the expression found by Widom and Clark using an analyticity dispersion relation for the friction coefficient  $\gamma(\omega)$ .

We see that

$$\Omega_0(\text{CL}) < \omega_0 < \Omega_0(\text{WC}). \quad (25a)$$

From Eq. (18) it follows that

$$P(E, \Omega_0(\text{CL})) < P(E, \omega_0) < P(E, \Omega_0(\text{WC})) \quad (25b)$$

when  $E$  is negative. Whether one concludes that dissipation enhances the tunneling probability as claimed by Widom and Clark or decreases it as claimed by Caldeira and Leggett depends on which Hamiltonian is used in the calculation.

Widom and Clark attributed this difference in the results to a divergent renormalization used by Caldeira and Leggett. We note that the last term in Eq. (4) is divergent if one assumes  $\gamma_n = \epsilon_n^2/4v\omega_n^2 = \gamma = \text{const.}$  To investigate this question further it is enlightening to calculate the energy of the particle, the energy of the field, and the interaction energy separately. First, we note that when  $\gamma(\omega) = \gamma = \text{const.}$ , the integral in Eq. (24a) can be done to yield the quadratic equation

$$\Omega_0^2 + 2\gamma|\Omega_0| - \omega_0^2 = 0 \quad (26a)$$

with the solution

$$|\Omega_0| = -\gamma + (\omega_0^2 + \gamma^2)^{1/2} \quad (26b)$$

and  $\Omega_0 = \pm|\Omega_0|$ . Using Eqs. (22a) and (22b) we calculate

$$E_p = \frac{1}{2}(p_0^2 - \omega_0^2 q_0^2) \\ = -\frac{1}{2}a_0^2\Omega_0^2\{(2\gamma/|\Omega_0|)\cosh^2\Omega_0 t + 1\}, \quad (27a)$$

$$E_f = \frac{1}{2} \sum_{n=1}^{\infty} (p_n^2 + \omega_n^2 q_n^2) \\ = \frac{1}{2}a_0^2(4\gamma/\pi) \int_0^\infty d\omega \left\{ \frac{\omega^2 \cosh^2\Omega_0 t}{(\Omega_0 + \omega^2)} - \frac{\omega^2 \Omega_0^2}{(\Omega_0^2 + \omega^2)^2} \right\}, \quad (27b)$$

$$E_i = (1/L^{1/2}) \sum_{n=1}^{\infty} \epsilon_n q_0 q_n + (q_0^2/2L) \sum_{n=1}^{\infty} \epsilon_n^2/\omega_n^2 \\ = \frac{1}{2}a_0^2(4\gamma/\pi) \int_0^\infty d\omega \frac{(\Omega_0^2 - \omega^2)\cosh^2\Omega_0 t}{(\Omega_0^2 + \omega^2)}. \quad (27c)$$

Both  $E_f$  and  $E_i$  are seen to contain divergent integrals, but when they are added together the divergences cancel. One can assume that  $\gamma(\omega)$  vanishes above some arbitrarily large but finite value of  $\omega$ ; then after the cancellation occurs, we let the cutoff value approach infinity. This seems unobjectionable. If the last term in  $E_i$  were omitted as it was in the work of Widom and Clark, the cancel-

lation would not occur. Canceling the divergent terms and carrying out the integrals gives

$$E_f + E_i = \frac{1}{2}a_0^2\Omega_0^2(\gamma/|\Omega_0|)(2\cosh^2\Omega_0 t - 1). \quad (28a)$$

The total energy is

$$E = E_p + E_f + E_i = \frac{1}{2}a_0^2\Omega_0^2(1 + \gamma/|\Omega_0|). \quad (28b)$$

At  $t = -\infty$  the particle has an energy of  $E_p = -\infty$ , and  $E_f + E_i = +\infty$ . As the particle approaches the turning point at  $q_0 = a_0$ , its energy increases, and  $E_f + E_i$  decreases; energy is being transferred from the field to the particle. After being reflected at the turning point,  $E_p$  decreases and  $E_f + E_i$  increases as energy is transferred from the particle to the field. This behavior requires a fine tuning of the initial values of the field coordinates  $q_n(0)$  and momenta  $p_n(0)$  that could never be attained. This strange combination of negatively damped and positively damped motion of the particle is quite unphysical. In our view no conclusions about real systems should be drawn from these calculations.

We have also considered positive-energy solutions of the form  $q_n = a_n \sinh \Omega t$  for  $n = 0, 1, 2, 3, \dots$ . In these solutions the particle passes over the top of the barrier at time  $t = 0$ .  $\Omega$  is again given by Eq. (22c). We find the energies

$$E_p = \frac{1}{2}a_0^2\Omega_0^2\{1 - (2\gamma/\Omega_0)\sinh^2\Omega_0 t\}, \quad (29a)$$

$$E_f + E_i = \frac{1}{2}a_0^2\Omega_0^2\{\gamma/\Omega_0 - (2\gamma/\Omega_0)\sinh^2\Omega_0 t\}. \quad (29b)$$

Once again divergent terms have canceled when  $E_f$  and  $E_i$  are added. The velocity of the particle as it passes over the top of the barrier is  $v_0(0) = a_0\Omega_0$ . The case of a free particle is also of interest. If we set  $\omega_0 = 0$  in Eq. (22c), we find  $\Omega_0 = 0$  is a solution. We let  $\Omega_0 \rightarrow 0$  and  $a_0 \rightarrow \infty$  in such a way that  $\Omega_0 a_0 = v_0 = \text{const.}$  Then  $q_0 = v_0 t$ ,  $E_p = v_0^2/2$ , and  $E_f + E_i \rightarrow (v_0^2/2)(\gamma/\Omega_0) \rightarrow \infty$ . The particle moves with a constant velocity, but the energy in the field and the interaction is infinite. This is clearly unphysical.

## V. DECAY OF A METASTABLE STATE

For the purposes of this section it is useful to consider a potential that is sufficiently simple to discuss in some detail. Let

$$V(q_0) = \begin{cases} \infty & \text{for } q_0 < 0 \\ 0 & \text{for } 0 < q_0 < a \\ V_1 & \text{for } a < q_0 < b \\ 0 & \text{for } b < q_0 < c \\ \infty & \text{for } c < q_0 \end{cases} \quad (30)$$

where  $V_1$  is constant. A classical particle with  $E < V_1$  could be confined in the region  $0 < q_0 < a$ , but a quantum-mechanical particle could tunnel through the barrier and emerge in the region  $b < q_0 < c$ . The Schrödinger equation for a particle in this potential is easily solved for  $\Psi(E, q_0)$ , the energy eigenfunctions of

the operator  $\frac{1}{2}(p_0^2 + \omega_0^2 q_0^2)$ . Details of the solution have been relegated to the Appendix. A computer program has been written to calculate the eigenvalues, the eigenfunctions, and the transition probabilities from any state to any other state.

We shall consider three special cases that depend on the assumed values  $c$  and  $G = (b - a)[2(V_1 - E)/\hbar^2]^{1/2}$ . The first case considered is that of  $c - b = a$ ; then the well is symmetric about the point  $q_0 = c/2$ , and the particle tunnels back and forth between the two potential wells. In the second case,  $(c - b) \gg a$  and  $a \gg c \exp(-G)$ . In this case the stationary states can be divided into two groups. In one group the particle is primarily confined to the narrow potential well and in the other group it is primarily confined in the wide potential well. The case of most interest is the final case  $c = \infty$ . Here the states form a continuum and a metastable state is formed by a superposition of these continuum states.

#### A. $c = b = a$

The potential is symmetric about the point  $q_0 = c/2$ . The eigenfunctions of the particles Hamiltonian are either symmetric or antisymmetric about this point. If  $\exp(-G) \ll 1$ , the eigenvalues occur in closely spaced pairs with the one corresponding to the symmetric eigenfunction being lower than that corresponding to the antisymmetric wave function. Let us suppose that initially the particle is initially in a state which is a linear combination of such a pair  $\Psi_s + \Psi_a$ , where the subscripts denote symmetric and antisymmetric states. If we suppose that the wave functions interfere constructively in the region  $0 < q_0 < a$  and destructively in the region  $b < q_0 < c$ , then initially  $\langle q_0 \rangle \simeq a/2$ . In the absence of interaction with the environment, the probability density for later times is

$$|\Psi(q_0, t)|^2 = |\Psi_s|^2 + |\Psi_a|^2 + 2|\Psi_s||\Psi_a| \cos \omega_{as} t \quad (31)$$

where  $\omega_{as} = (E_a - E_s)/\hbar$ . The expectation value  $\langle q_0(t) \rangle$  oscillates back and forth between the regions  $0 < q_0 < a$  and  $b < q_0 < c$  with the frequency  $\omega_{sa}$ . For very closely spaced levels, the frequency of oscillation may be calculated to be approximately

$$\omega_{as} = \frac{8(2E)^{1/2}}{a + 1/\kappa} (E/V_1)^{1/2} (1 - E/V_1)^{1/2} \exp(-G) \quad (32)$$

where  $E = (E_s + E_a)/2$  and this value of  $E$  is to be used in  $\kappa$  and  $G$ . The derivation is given in the Appendix. As a crude classical picture, we may think of the particle bouncing back and forth with velocity  $(2E)^{1/2}$  over a distance  $a + 1/\kappa \simeq a$ ; at each encounter with the potential barrier it has a probability amplitude proportional to  $\exp(-G)$  of penetrating the barrier. The rate at which tunneling occurs depends on the energy difference and would vanish if the states were degenerate.

Now we ask how tunneling is affected by interaction with the environment. In the case of the harmonic oscillator we found the energy levels were shifted from  $\hbar\omega_0(N + \frac{1}{2})$  to  $\hbar\Omega_0(N + \frac{1}{2})$ . If we were sufficiently clever to find exact solutions as we did in the case of the para-

bolic potential, we would expect a similar energy shift. Whether the tunneling rate is increased or decreased by the interaction would depend on whether the energy difference between the closely lying symmetric and antisymmetric states is increased or decreased. The shift in energies due to interaction could be calculated by perturbation theory. This was done by Fujikawa *et al.* [10] for a different form of potential. In our view calculations of tunneling rates based on exact eigenvalues and eigenfunctions or approximations to them are physically irrelevant. Since these are stationary states there must be no net transfer of energy from the particle to the environment as should occur in a truly dissipative system. The construction of such stationary states requires an unattainable fine tuning of the environment.

Except for the different shape of the potential this is not different in principle from a particle moving in a harmonic-oscillator potential. The lowest state is symmetric and the first excited state antisymmetric. If the state is a linear combination of these two states with appropriately chosen coefficients,  $\langle q_0(t) \rangle$  will oscillate back and forth across  $q_0 = 0$  with the frequency  $\omega_0$  if there is no interaction with the environment. If exact eigenvalues and eigenfunctions are used, the frequency will be  $\Omega_0$  where  $\Omega_0$  is found by solving Eq. (7d). A quite different result is obtained if initially the environment is at zero temperature. Equation (15) tells us that the particle decays to its ground state in a time of order  $1/2\gamma$ . In the language of perturbation theory, we would say that there was a transition from the state  $a_s\Psi_s + a_a\Psi_s$  to the state  $\Psi_s$  with emission of a quantum of energy into the environment. We expect similar conclusions for any form of potential. Interaction with a zero-temperature environment both shifts the energy levels and causes the particle to decay to its ground state.

We can use perturbation theory to calculate the transition probability per unit time from the state  $\Psi_s + \Psi_a$  to the state  $\Psi_s$  where  $\Psi_s$  and  $\Psi_a$  are the two lowest states in the potential of Eq. (30). We estimate  $\langle \Psi_a | q_0 | \Psi_s \rangle \simeq a$ . Then using Eq. (17) we find  $T(i \rightarrow f) = 4\gamma a^2 \omega_{as} / \hbar$ . Ultimately, the particle decays to its ground state. The ground state is symmetric and the particle is equally likely to be in either potential well.

It is helpful to consider the analogy with a more realistic physical system. Consider a hydrogen atom interacting with an electromagnetic field [20]. Both field and atom may be confined in a large box. (The system described by the Caldeira-Leggett Hamiltonian may be regarded as toy model of this more realistic system.) If we were sufficiently clever, we could find eigenvalues and eigenfunctions for the interacting system. Some of these would correspond to excited states of the atom which do not decay because energy emitted into the field is balanced by energy absorbed from the field in analogy with the harmonic oscillator of Sec. III. These are not observed in nature. To prepare the system in such a state would require an unattainable control over the initial state of the field. If there were no photons present in the initial state, the effect of the interaction would be to shift the unperturbed energy levels of the atom (the Lamb shift) and also to cause the atom to decay to its ground

state. In the absence of the interaction, the  $2s$  and  $2p$  states of the atom are degenerate. Consider a linear combination of the states with quantum numbers  $n, l, m = 2, 0, 0$  and  $2, 1, 0$ . A linear combination  $a_{2s}\Psi_{200} + a_{2p}\Psi_{211}$  with suitably chosen coefficients would have a probability density that is large along the  $+z$  axis and small along the  $-z$  axis. In the absence of interaction this is a stationary state; there is no "tunneling" from the  $+z$  axis to the  $-z$  axis. When the interaction is turned on, the degeneracy is removed and the expectation value  $\langle z(t) \rangle$  oscillates with a frequency of about 1057 MHz. Also the atom makes a transition to the ground state with the emission of a photon.

### B. $c - b \gg a$ and $a \gg c \exp(-G)$

For the purposes of this paragraph we neglect the interaction of the particle with the environment. For orientation let us assume that  $V_1 \gg E$  for all energies of interest. Then the energies can be divided into two groups: those with energies  $E_n \simeq n^2 \hbar^2 \pi^2 / a^2$  for  $n = 1, 2, 3, \dots$  and those with energies  $E_m \simeq m^2 \hbar^2 \pi^2 / (c - b)^2$  for  $m = 1, 2, 3, \dots$ . The spacing between members of the second group will be much smaller than that between members of the first group since  $c - b \gg a$ . For  $\exp(-G) \ll 1$ , members of the first group have  $f_+(k) \simeq 0$ ; their wave functions oscillate in the region  $0 < q_0 < a$ , fall off exponentially in the region  $a < q_0 < b$ , and then oscillate in the region  $b < q_0 < c$  with an amplitude reduced by a factor  $\exp(-G)$ . The probability of finding the particle in a state belonging to the first group in the region  $0 < q_0 < a$  is approximately  $|A|^2 a / 2$ , and the probability of finding it in the region  $b < q_0 < c$  is approximately  $|A|^2 (c/2) \exp(-G)$ . If  $a \gg c \exp(-G)$  as assumed, we may say that the particle is approximately confined in the region  $0 < q_0 < a$ . Similar considerations show that when the particle is in a state belonging to the second group it is approximately confined in the region  $b < q_0 < c$ . In anticipation of the work of the next subsection, we shall say that members of the first and second groups are "approximately confined states" and "approximately unconfined states," respectively. These qualitative arguments have been verified by calculation. For instance, we have made calculations for the case  $b = a$ ,  $c = 8a$ , and  $2a^2 V_1 / \hbar^2 = 100$ . The two lowest approximately confined states had  $k = 2.85234/a$  and  $k = 5.67921/a$ . The probabilities for finding the particle in the region  $0 < q_0 < a$  were 0.9913 and 0.9650, respectively. There were five approximately unconfined states below the lowest approximately confined state.

Now we ask how these results are changed when the interaction with the environment is turned on. Suppose we were sufficiently clever to find exact energy eigenvalues and eigenfunctions of the Caldeira-Leggett Hamiltonian for this potential as we did for the harmonic-oscillator potential. These are stationary states so the expectation value of the particle's energy does not change with time, indicating no net transfer of energy between particle and environment. We expect that in some of these states the particle is approximately confined. Since these are stationary states it will remain approximately

confined; there is no tunneling from the region  $0 < q_0 < a$  to the region  $b < q_0 < c$ . As we have argued before, these stationary states are unphysical. To prepare the system in one of these stationary states requires an unattainable control over the initial state of the environment.

A very different result emerges if the initial state of the system is one in which the particle is approximately confined and each of the field oscillators is in its ground state. This is not a stationary state, so it evolves with time. Experience leads us to expect that the system evolves toward a final state in which the particle is in its ground state and its initial energy is dispersed among the many degrees of freedom of the environment. (This is what we found in the exactly solvable damped harmonic-oscillator problem.) Since the ground state is an approximately unconfined state, the particle escapes confinement. Dissipation has not impeded escape, but has made it possible when it would not otherwise occur.

Suppose the particle was in one of the higher-lying approximately confined states. Perturbation theory would lead us to expect it to preferentially jump to a lower-lying approximately confined state, since the matrix element of  $q_0$  between approximately confined and approximately unconfined states is reduced by a factor of about  $\exp(-G)$ . Once it has reached the lowest-lying approximately confined state, the only option is for a jump to an approximately unconfined state of lower energy. These expectations have been verified by our calculations. The transition probability per unit time for the transition from the approximately confined state with  $k = 5.67921/a$  to the lowest approximately confined state with  $k = 2.85234/a$  was  $12.284\gamma$ , while for the transition to the nearest unconfined state with  $k = 5.65923/a$  was  $0.00738\gamma$ . The transition probability per unit time for the transition from the state with  $k = 2.85234/a$  to the nearest approximately unconfined state with  $k = 2.57459/a$  was  $0.62940\gamma$ . This is higher than the transition rate to any of the other four lower-lying states.

### C. $c \rightarrow \infty$

We now let the potential barrier at  $q_0 = c$  recede to infinity. The previously discrete eigenvalues of the particle Hamiltonian move closer together until they form a continuum. The formerly approximately confined states are replaced by bands of states whose eigenfunctions are large in the region  $0 < q_0 < a$  and small in the region  $b < q_0 < \infty$ . The designation "approximately confined" is now inappropriate since the probability of finding the particle in the region  $0 < q_0 < a$  is essentially zero since  $c = \infty$ . All stationary states represent unconfined particles.

If  $V_1$  is sufficiently large or  $b - a$  is sufficiently large, then  $\Delta E$ , the width of a band of states whose eigenfunctions are large in the region  $0 < q_0 < a$ , will be very small. One can construct a particle wave function  $\Psi_0(q_0)$  by superposition of wave functions  $\Psi(E, q_0)$  with  $E$  lying in one of these bands in such a way that there is constructive interference in the region  $0 < q_0 < a$  and destructive interference elsewhere. Such a wave function can be written as



$$\Psi_0(q_0) = \int_0^\infty dE \Psi(E, q_0) \langle \Psi(E) | \Psi_0 \rangle \quad (33a)$$

where

$$\langle \Psi(E) | \Psi_0 \rangle = \int_0^\infty dq_0 \Psi^*(E, q_0) \Psi_0(q_0). \quad (33b)$$

This constitutes a metastable state or virtual bound state. It is not an eigenstate of  $p^2/2 + V(q_0)$  but rather a superposition of such states. Even in the absence of dissipation the metastable state decays by phase mixing. We shall first discuss the decay in the absence of interaction with the environment.

We solve the time-dependent Schrödinger equation subject to the initial condition  $\Psi(q_0, t=0) = \Psi_0(q_0)$  and obtain

$$\Psi(q_0, t) = \int_0^\infty dE \Psi(E, q_0) \langle \Psi(E) | \Psi_0 \rangle \exp(-iEt/\hbar). \quad (34)$$

The probability amplitude that the system is still in its initial state at time  $t$  is

$$\begin{aligned} K(t) &= \langle \Psi_0 | \Psi(t) \rangle \\ &= \int_0^\infty dE |\langle \Psi(E) | \Psi_0 \rangle|^2 \exp(-iEt/\hbar). \end{aligned} \quad (35a)$$

To represent a virtual bound state,  $\Psi_0(q_0)$  must be large in the region  $0 < q_0 < a$  and small elsewhere. Then  $|\langle \Psi(E) | \Psi_0 \rangle|^2$  will be strongly peaked about a value  $E_n$  near the center of one or another of the bands where  $\Psi(E, q_0)$  is large in this region. We shall approximate this sharply peaked function by the Lorentzian function

$$|\langle \Psi(E) | \Psi_0 \rangle|^2 = \frac{\hbar \Gamma_n / \pi}{(E - E_n)^2 + \hbar^2 \Gamma_n^2} \quad (35b)$$

where  $\hbar \Gamma_n$  is the width of the peak. Assuming the peak to be very narrow, we can extend the lower limit of the integral to  $-\infty$  and evaluate the integral by the residue theorem to obtain

$$K(t) = \exp(-iE_n t / \hbar - \Gamma_n t). \quad (35c)$$

The probability of finding the system in the same state (the  $n$ th virtual state) at time  $t$  that it was in initially is  $|K(t)|^2 = \exp(-2\Gamma_n t)$ . The lifetime of the state  $1/2\Gamma_n$  is inversely proportional to the width of the band. It is as if the virtual state had an energy  $E_n - i\hbar\Gamma_n$ , but, of course, this is not the eigenvalue of any Hermitian operator. We shall refer to this mechanism of decay as phase mixing. [We shall parenthetically remark that approximating the peak by a Lorentzian function is not always a good approximation. For large times  $\exp(-iEt/\hbar)$  oscillates rapidly with  $E$ , and the results are sensitive to the shape of the peak. Nonexponential decays for large times are well known. In our work we restrict ourselves to times for which exponential decay is a good approximation.]

We have calculated  $\Gamma_n$  for the potential of Eq. (30) with the result

$$\Gamma_n = \frac{4(2E_n)^{1/2}(E_n/V_1)(1-E_n/V_1)\exp(-2G_n)}{a+1/\kappa} \quad (36)$$

where  $\kappa_n^2 = 2(V_1 - E_n)/\hbar^2$  and  $G_n = \kappa_n(b-a)$ . The derivation is given in the Appendix. This has a simple interpretation. The frequency with which the particle bounces back and forth is approximately  $(2E_n)^{1/2}/(a+1/\kappa_n)$ . The remaining factor is (to within a numerical factor) the transmission factor for a rectangular barrier [21]. For a potential of different shape,  $\Gamma_n$  must have the form

$$\Gamma_n = A(E_n) \exp(-2G_n) \quad (37a)$$

where  $A(E_n)$  will depend on the shape of the potential and  $G_n$  for the rectangular barrier should be replaced by

$$G_n = \int dq_0 \{2[V(q_0) - E_n]/\hbar^2\}^{1/2} \quad (37b)$$

where the limits of the integral are the classical turning points.

We believe that this way of calculating the rate of decay in the absence of dissipation is well known. It is presented here as a prelude to the dissipative case to which we now turn.

We write the Caldeira-Leggett Hamiltonian of Eq. (4) as  $H = H_0 + H_i$  where  $H_0$  is the sum of the particle and field Hamiltonians and  $H_i$  is the interaction Hamiltonian. Let  $H_0 |E\rangle = E |E\rangle$ . The eigenvectors  $|E\rangle$  are given by

$$|E\rangle = |e\rangle \prod_{n=1}^{\infty} |N_n\rangle = |e\rangle |N\rangle \quad (38)$$

where  $|e\rangle$  is an eigenvector of  $p_0^2/2 + V(q_0)$  with eigenvalue  $e$ , and  $|N_n\rangle$  is an eigenvector of  $(p_n + \omega_n^2 q_n^2)/2$  with eigenvalue  $\hbar\omega_n(N_n + \frac{1}{2})$ . [Note the change in notation between Eq. (13b) and Eq. (38).]

If the state of the system of particle and field at time  $t=0$  is  $|i\rangle$ , then its state at time  $t$  is  $\exp(-iHt/\hbar)|i\rangle$ . The probability amplitude for finding it in state  $|f\rangle$  at time  $t$  is  $K(f; i; t) = \langle f | \exp(-iHt/\hbar) | i \rangle$ . In calculating rates of decay we shall be interested in  $K(i; i; t)$ , the probability amplitude that the system is in the same state at time  $t$  that it was in initially.

To investigate the decay of a virtual state we shall take the initial state to be one in which the particle is in the virtual state  $|\Psi_0\rangle$  and the  $n$ th field oscillators is in a state  $|N_n\rangle$ . That is,  $|i\rangle = |\Psi_0\rangle |N\rangle$ . We choose  $\Psi_0(w_0) = \langle q_0 | \Psi_0 \rangle$  to be given by Eq. (33a), but with our change in notation  $E$  is replaced by  $e$ . The probability amplitude that the system has not decayed at time  $t$  is

$$\begin{aligned} K(i; i; t) &= K(\Psi_0, N; \Psi_0, N; t) \\ &= \langle N | \langle \Psi_0 | \exp(-iHt/\hbar) | \Psi_0 \rangle | N \rangle. \end{aligned} \quad (39)$$

We shall abbreviate this as  $K(t)$ .

Denoting the eigenvectors of  $H_0$  as  $|E'\rangle = |e'\rangle |N'\rangle$  we can write the unit operator as

$$1 = \sum_{E'} |E'\rangle \langle E'| \quad (40a)$$

where

$$\sum_{E'} = \sum_{e'} \sum_{N_1} \cdots \sum_{N_n} \cdots = \sum_{e'} \sum_{N'} \quad (40b)$$

For the present we are keeping  $c$  finite so that the eigenvalues  $e'$  are discrete. At the appropriate point in the calculation we shall let  $c \rightarrow \infty$  and replace the sum over  $e'$  by an integral.

The unit operator is inserted on each side of the exponential in Eq. (39) to obtain

$$\begin{aligned} K(t) &= \sum_{E'} \sum_{E''} \langle \mathbf{N} | \langle \Psi_0 | E' \rangle \langle E' | \exp(-iHt/\hbar) | E'' \rangle \\ &\quad \times \langle E'' | \mathbf{N} \rangle | \Psi_0 \rangle \\ &= \sum_{e'} \sum_{e''} \langle \Psi_0 | e' \rangle \langle \mathbf{N} | \langle e' | \exp(-iHt/\hbar) | e'' \rangle | \mathbf{N} \rangle \\ &\quad \times \langle e'' | \Psi_0 \rangle \end{aligned} \quad (41)$$

where we have used  $\langle \mathbf{N} | E' \rangle = 0$  unless  $\mathbf{N} = \mathbf{N}'$ . We shall write

$$\begin{aligned} \exp(-iHt/\hbar) &= \exp(-iH_0t/\hbar) \\ &\quad \times T \exp \left[ (-i/\hbar) \int_0^t dt' H_i(t') \right] \end{aligned} \quad (42a)$$

where

$$\begin{aligned} T \exp \left[ (-i/\hbar) \int_0^t dt' H_i(t') \right] \\ &= \sum_{n=0}^{\infty} (1/n!) (-i/\hbar)^n \\ &\quad \times \int_0^t dt_1 \cdots \int_0^t dt_n T \{ H_i(t_1) \cdots H_i(t_n) \}, \end{aligned} \quad (42b)$$

$$H_i(t) = \exp(iH_0t/\hbar) H_i \exp(-iH_0t/\hbar), \quad (42c)$$

and  $T$  is the chronological operator. We now examine the central bracket in Eq. (41). That is

$$\begin{aligned} \langle \mathbf{N} | \langle e' | \exp(-iHt/\hbar) | e'' \rangle | \mathbf{N} \rangle \\ &= \exp(-ie't/\hbar) \exp[-iE(\mathbf{N})t/\hbar] F(e', e'', \mathbf{N}, t) \end{aligned} \quad (43a)$$

where

$$\begin{aligned} F(e', e'', \mathbf{N}, t) \\ &= \langle \mathbf{N} | \langle e' | T \exp \left[ -i/\hbar \int_0^t dt' H_i(t') \right] | e'' \rangle | \mathbf{N} \rangle. \end{aligned} \quad (43b)$$

For  $t=0$ , this is  $\delta(e', e'')$ . Also for large times this must vanish for  $e' \neq e''$  because of the conservation of energy. Only for short times when the energy uncertainty relation  $\Delta e \Delta t \geq \hbar/4$  is important will it be nonzero for  $e' \neq e''$ . We shall only consider times longer than this and write  $F(e', e'', \mathbf{N}, t) = \delta(e', e'') F(e', e', \mathbf{N}, t)$ . We use this in Eq. (41); let  $c \rightarrow \infty$  so that the sum over  $e'$  is replaced by an integral and obtain

$$\begin{aligned} K(t) &= \exp[-iE(\mathbf{N})t/\hbar] \\ &\quad \times \int_0^{\infty} de |\langle \Psi_0 | e \rangle|^2 \exp(-iet/\hbar) F(e, e, \mathbf{N}, t). \end{aligned} \quad (44)$$

We have dropped the prime on  $e'$ . In the following we shall also discard the phase factor  $\exp[-iE(\mathbf{N})t/\hbar]$  as it plays no role in the tunneling rate. What remains may be compared to Eq. (35a). Aside from differences in notation, they differ by the factor  $F(e, e, \mathbf{N}, t)$  in the integrand of Eq. (44). This factor is the probability amplitude that the system will be in the state  $|e\rangle | \mathbf{N} \rangle$  at time  $t$  if it is known to be in that state initially. The modulus of  $F(e, e, \mathbf{N}, t)$  cannot exceed unity since it is the expectation value of a unitary operator. We expect the modulus to decrease with increasing time since  $H_i$  operating on  $|e\rangle | \mathbf{N} \rangle$  converts it into a linear combination of states, most of which are orthogonal to  $|e\rangle | \mathbf{N} \rangle$ . We shall assume an exponential decay for the state  $|e\rangle | \mathbf{N} \rangle$  with decay constant  $\Gamma(e, \mathbf{N})$  and a phase shift of  $\Delta e(e, \mathbf{N})$  and write

$$F(e, e, \mathbf{N}, t) = \exp[-i\Delta e(e, \mathbf{N})t/\hbar - \Gamma(e, \mathbf{N})t]. \quad (45)$$

Using this in Eq. (44) gives

$$\begin{aligned} K(t) &= \int_0^{\infty} de |\langle \Psi_0 | e \rangle|^2 \\ &\quad \times \exp[-iet/\hbar - i\Delta e(e, \mathbf{N})t/\hbar - \Gamma(e, \mathbf{N})t]. \end{aligned} \quad (46)$$

Equation (46) should be compared with Eq. (35). The physical interpretation of the difference of these two results is quite clear. In the absence of interaction with the environment,  $\Psi(q_0, t)$  is a superposition of stationary states. The modulus of  $K(t)$  decays by phase mixing since each of these states oscillates with a different frequency. When the particle interacts with its environment, there is an additional factor of  $F(e, e, \mathbf{N}, t)$  in the integrand. The interaction causes the probability for the system to remain in its initial state to decrease with time as energy is interchanged between particle and field. The interaction also shifts the energy of the particle from  $e$  to  $e + \Delta e(e, \mathbf{N})$ . We may define a new energy variable  $E = e + \Delta e(e, \mathbf{N})$  and rewrite Eq. (46) as

$$K(t) = \int_0^{\infty} dE \left[ \frac{de}{dE} \right] |\langle \Psi_0 | E \rangle|^2 \exp[-iEt/\hbar - \Gamma(E, \mathbf{N})t]. \quad (47a)$$

We now assume that  $(de/dE) |\langle \Psi_0 | E \rangle|^2$  is a sharply peaked Lorentzian function about  $E_n$  with width  $\hbar\Gamma_n$  and assume that  $\Gamma(E, \mathbf{N})$  is slowly varying functions of  $E$ , we may carry out the integral in Eq. (46) and obtain

$$K(t) = \exp\{-iE_n t/\hbar - [\Gamma_n + \Gamma(E, \mathbf{N})]t\}. \quad (47b)$$

There are two effects of the interaction on  $K(t)$ . First, the interaction has shifted the energy of each of the states that constitute  $|\Psi_0\rangle$ . This may make  $|\langle \Psi_0 | E \rangle|^2$  more or less sharply peaked than  $|\langle \Psi_0 | e \rangle|^2$ . The change in the width of the peak changes  $\Gamma_n$ . The second effect is the decay toward the ground state which is accounted by  $\Gamma(E, \mathbf{N})$ . It is this second effect that may properly be called an effect of dissipation.

It should be clear from the derivation that the qualitative conclusion that dissipation enhances decay is not

dependent on the use of perturbation theory or on the form assumed in Eq. (45). We emphasize this point because an earlier, unpublished version of this work that reached the same conclusion was criticized for the use of perturbation theory.

It should be noted that this qualitative conclusion is independent of  $|\mathbf{N}\rangle$ , the initial state of the environment. Any interaction that removes the particles energy from the energy band that constitutes the virtual state, whether it is emission of quanta into the environment or absorption of quanta from the environment, will contribute to the decay of the virtual state. Of course,  $\Gamma(e, \mathbf{N})$  depends on  $|\mathbf{N}\rangle$ . Generally, the state  $|i\rangle = |\Psi_0\rangle|\mathbf{N}\rangle$  is not a physically reasonable initial state. It implies that each field oscillator is in one of its energy eigenstates, which is beyond experimental control. A physically reasonable initial state is one in which the environment is in thermal equilibrium. If the temperature is zero, then each oscillator is in its ground state. We consider the state  $|\Psi_0\rangle|0\rangle$  to be a physically reasonable initial state.

If the interaction is sufficiently weak, perturbation theory should be applicable. We have assumed that the initial state of the environment is  $|0\rangle$  (that is,  $N_n = 0$  for all  $n$ ) and used first-order perturbation theory to calculate  $\Gamma(e_1, \mathbf{0})$  where  $e_1$  is the lowest energy of a virtual state. We find

$$\Gamma(e_1, \mathbf{0}) = (\gamma T_b / 2) \Gamma_1 \ln(e_1 / \hbar \Gamma_1) \quad (48)$$

where  $T_b = 2(a + 1/\kappa_1) / (2e_1)^{1/2}$  is the bounce time, that is, the time for the particle to bounce back and forth over a distance  $(a + 1/\kappa_1)$  with the velocity  $(2e_1)^{1/2}$ . The derivation is given in the Appendix. We have not taken into account the shift of the energy levels from  $e$  to  $E$  in this calculation. The effect of the decay of the particles energy toward its ground state is to replace  $\Gamma_1$  by  $\Gamma_1 [1 + (2\gamma T_b / 2) \ln(e_1 / \hbar \Gamma_1)]$ .

## VI. SUMMARY AND DISCUSSION

In Sec. II we showed that the Unruh-Zurek and Caldeira-Leggett Hamiltonians were related by a canonical transformation. We also showed that Hamilton's equation of motion exhibited not only damping but negative damping as well. Indeed, with an appropriate choice of the initial conditions of the environment, almost any motion can be obtained. This is not surprising since the system has an infinite number of degrees of freedom. In most real physical systems one has little control over the preparation of the environment and only damped motion is observed.

The Caldeira-Leggett Hamiltonian is sufficiently simple that exact solutions can be obtained for the harmonic-oscillator potential  $V = \omega_0^2 q_0^2 / 2$  or the parabolic barrier  $V = -\omega_0^2 q_0^2 / 2$ . Either the classical equations of motion for  $q_0$  and  $p_0$  or the Heisenberg equations for the corresponding operators can be solved exactly. This was done in a previous publication [13] with the assumption that the environment was in thermal equilibrium, and it was found that the particle came into thermal equilibrium with its environment. If the temperature was zero, the parti-

cles energy decayed to the ground-state energy. In Sec. II we transformed the Caldeira-Leggett Hamiltonian to a sum of harmonic-oscillator Hamiltonians by a normal coordinate transformation. In a normal mode of the system there is no net damping of the particles motion. Energy is alternately transferred from the particle to the environment and from the environment to the particle. Exact eigenvalues and eigenstates of the transformed Hamiltonian are easily obtained. In an exact eigenstate, the expectation value of the particle's energy is constant, indicating no net damping. We point out that to prepare the system in such an eigenstate would require a precise adjustment of the initial values of the coordinates and momenta of the field oscillators. We argue that such control over the environment is not attainable. A more reasonable assumption is that environment is in thermal equilibrium; this leads to damping.

In Sec. IV we discuss tunneling through a parabolic barrier. We make a normal coordinate transformation as in the preceding section. Using the Widom-Clark Hamiltonian we obtain results in agreement with Widom and Clark [3]; tunneling probability is enhanced by the interaction with the environment. Using the Caldeira-Leggett Hamiltonian we find that the tunneling probability is decreased. We think this resolves the disagreement that led to an exchange of comments [4,5]. However, these solutions are very unphysical. There is no net damping. A classical particle that approaches the barrier has a negatively infinite energy when it is at an infinite distance from the origin. It gains energy from the environment until the classical turning point is reached, and then returns the energy to the environment as it recedes. The quantum-mechanical expectation of the particles energy is negatively infinite and that of the environment and interaction is positively infinite.

Tunneling through a barrier was also discussed by Bruinsma and Bak [6]. Their barrier was of arbitrary shape. The problem of the exchange of energy between particle and environment as the particle approached and receded was avoided by assuming the coupling was switched off when the particle was not inside the barrier. The environment was assumed to be in thermal equilibrium. We consider this a physically reasonable treatment of the problem.

We begin Sec. V with a discussion of a particle in a symmetric double-well potential. In the absence of interaction with the environment, a particle that was initially in one of the wells would tunnel back and forth between them with a frequency proportional to the energy differences between closely spaced symmetric and antisymmetric states. We argue that if exact eigenstates of the system could be found and the system was initially in a superposition of exact eigenstates, the same thing would happen, but with the frequency modified by a shift in the energy levels due to the interaction. We think it is more reasonable to assume that initially the environment was in thermal equilibrium at zero temperature. Then the system would evolve toward its lowest energy state. In this lowest state the particle would have equal probabilities of being in either well. This problem was treated by Razavy [9] using the Caldeira-Leggett Hamiltonian

without the renormalization term. Razavy found a critical damping strength such that for damping in excess critical, tunneling could not occur. Nothing of this sort emerges from our work. It seems to imply that above the critical damping strength, the symmetric and antisymmetric states are degenerate, so that the tunneling frequency is zero. We note that Razavy assumed that initially the field oscillators were all in their ground states, so that  $\langle q_n(0) \rangle = \langle p_n(0) \rangle = 0$  for  $n = 1, 2, 3, \dots$ . However, expectation values of higher powers of these operators played no role in his calculations. He was led to an effective Hamiltonian that contained no field operators. The coordinate and momentum operators in this Hamiltonian did not obey the usual commutation relations. He remarked that there is no simple way of obtaining a wave equation from this Hamiltonian. It is not clear to the present writer that this is a valid approach to a problem in quantum mechanics.

Next we discussed tunneling in an asymmetric well with the parameters chosen so that in a stationary state the particle would have a large probability of being in one well and a small probability of being in the other. This should be the case whether the stationary states were eigenstates of the Hamiltonian of the entire system or the particle's Hamiltonian alone. If the state is an eigenstate of the Hamiltonian of the entire system, the expectation value of the particles energy is constant, indicating no net transfer of energy between particle and field. If the environment is initially in thermal equilibrium at zero temperature, the particle could tunnel from the small well to the large well with emission of energy into the environment. This provides a mechanism of tunneling that could not occur in the absence of dissipation.

Finally, we consider the tunneling of a particle from a metastable state. We assume that initially each of the field oscillators is in one of its energy eigenstates and the particle is in a superposition of states that interfere constructively in the region of confinement and destructively outside of this region. The energies of the particle states that constitute this superposition lie in a narrow band. In the absence of coupling of the particle to the environment, the metastable state would decay by phase mixing. Each state of the superposition has a different energy, so as time increases constructive interference is replaced by destructive interference. The rate of decay is inversely proportional to the width of the energy band. Interaction with the environment has two effects. First, the energy levels are shifted, so the width of the band may be changed. Second, the initial state was not a stationary state, so the state evolves toward thermal equilibrium at zero temperature. The particle's energy evolves toward its lowest-energy level, and this state of lowest energy is an unconfined state. Thus there are two mechanisms of tunneling out of the metastable state, phase mixing, and energy decay. It is only the second of these that can properly be called dissipative tunneling. We have used perturbation theory to calculate the second of these for the confining potential of Eq. (30) and found the result of Eq. (48). It was assumed that the temperature of the environment was zero.

We believe that the reason our results differ from those

of Caldeira and Leggett [1,2] and Schmid [11] is because of our different choices of initial conditions for the environment. It seems clear from Eq. (4.9) of Ref. [2] that the states in the equation are energy eigenstates of the total Hamiltonian  $H_0 + H_i$ . These are stationary states, so the expectation value of the particle's energy in any one of these states is constant indicating no net energy exchange between particle and environment. Our initial state was  $|\Psi_0\rangle|N\rangle$ , an eigenstate of  $H_0$ . This is not a stationary state. If  $|N\rangle = |0\rangle$ , then the environment is initially at zero temperature. As a result, only one of the effects of the interaction is taken into account in the calculation of Caldeira and Leggett, namely, the change in the decay rate due to the shift of energy levels. The evolution toward lower energies as the particle loses energy as the environment is omitted. It is this latter mode of decay that we would call dissipative tunneling. Although it might seem that a superposition of eigenstates of  $H_0 + H_i$  is preferable to a superposition of eigenstates of  $H_0$ , we believe that this is not the case. In the case of the harmonic oscillator and the parabolic barrier, exact eigenstates of  $H_0 + H_i$  can be found, and their unphysical nature is apparent.

It is not surprising that the quasiclassical calculation of Schmid [11] and the instanton calculation of Caldeira and Leggett [1,2] agree. It indicates that the calculations were done correctly in both cases. Schmid also used stationary states in his calculation. We do not question the accuracy of the calculations but the choice of initial conditions.

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#### APPENDIX

The solutions of the Schrödinger equation for the potential of Eq. (30) may be written as

$$\Psi(E, q_0) = \begin{cases} \Psi_1(E, q_0) & \text{for } 0 < q_0 < a \\ \Psi_2(E, q_0) & \text{for } a < q_0 < b \\ \Psi_3(E, q_0) & \text{for } b < q_0 < c \end{cases} \quad (\text{A1})$$

where

$$\Psi_1 = A \sin k q_0, \quad (\text{A2a})$$

$$\Psi_2 = A \{ f_+ \exp[\kappa(q_0 - a)] + f_- \exp[-\kappa(q_0 - a)] \}, \quad (\text{A2b})$$

$$\Psi_3 = A \{ S_+ \cos k(q_0 - b) + S_- \sin[k(q_0 - b)] \}, \quad (\text{A2c})$$

where  $k^2 = 2E/\hbar^2$ ,  $\kappa^2 = 2(V_1 - E)/\hbar^2$ , and  $A(E)$  is a normalization constant. These wave functions apply when  $E < V_1$ . By requiring that  $\Psi(q_0)$  and its first derivative be continuous at  $q_0 = a$  and  $b$ , and  $\Psi = 0$  at  $q_0 = c$  we find

$$f_+(k) = \frac{1}{2} [\sin ka + (k/\kappa) \cos ka], \quad (\text{A3a})$$

$$f_-(k) = \frac{1}{2}[\sin ka - (k/\kappa)\cos ka], \quad (\text{A3b})$$

$$S_+(k) = f_+ \exp(+G) + f_- \exp(-G), \quad (\text{A3c})$$

$$S_-(k) = (\kappa/k)[f_+ \exp(+G) - f_- \exp(-G)], \quad (\text{A3d})$$

$$\tan[k(c-b)] = -(S_+/S_-), \quad (\text{A3e})$$

where  $G = \kappa(b-a)$ . The energy eigenvalues are found from the solution of Eq. (A3e).

The derivation of Eq. (32) proceeds as follows. For the symmetric wave function we must have  $\Psi_2(E_s, a) = \Psi_2(E_s, b)$ . It follows from Eq. (A2b) that  $f_-(k_s) = f_+(k_s)\exp G_s$ . Then from Eqs. (A3a) we find

$$\tan k_s a = -\frac{k_s[1 + \exp(-G_s)]}{\kappa_s[1 - \exp(-G_s)]}. \quad (\text{A4a})$$

For the antisymmetric wave function we must have  $\Psi_2(E_a, a) = -\Psi_2(E_a, b)$  from which it follows that  $f_-(k_a) = -f_+(k_a)\exp G_a$  and

$$\tan k_a a = -\frac{k_a[1 - \exp(-G_a)]}{\kappa_a[1 + \exp(-G_a)]}. \quad (\text{A4b})$$

We write  $k_s = k - \xi$ ,  $k_a = k + \xi$ , and assume  $\xi \ll k$ . We take the difference of Eqs. (A4a) and (A4b), expand all quantities in  $\xi/k$  neglecting powers higher than the first; also we neglect powers of  $\exp(-G)$  higher than the first. Solving for  $\xi$  gives

$$\xi = \frac{4(E/V_1)^{1/2}(1-E/V_1)^{1/2}\exp(-G)}{a+1/\kappa}. \quad (\text{A4c})$$

Then from  $\omega_{as} = \hbar(k_a^2 - k_s^2) = 2\hbar k \xi$ , Eq. (32) follows.

The derivation of Eq. (36) proceeds as follows. We choose  $\Psi_0(q_0)$  to be

$$\Psi_0(q_0) = \begin{cases} C \sin(k_n q_0) & \text{for } 0 < a \\ C \sin(k_n a) \exp[-\kappa_n(q_0 - a)] & \text{for } a < q_0 \end{cases} \quad (\text{A5a})$$

where the normalization constant is  $C = [2/(a+1/\kappa_n)]^{1/2}$ . Requiring continuity of the derivative of  $\Psi_0$  at  $q_0 = a$  gives

$$\tan k_n a = -k_n/\kappa_n. \quad (\text{A5b})$$

This is equivalent to  $f_+(k_n) = 0$  where  $f_+(k)$  is given by Eq. (A3a).

The normalization factor  $A(E)$  in Eq. (A2) in the  $c \rightarrow \infty$  limit is

$$A(E) = \left[ \frac{2}{c[S_+^2(E) + S_-^2(E)]} \right]^{1/2}. \quad (\text{A6a})$$

From inspection of  $S_+$  and  $S_-$  it is apparent that  $A(E)$  is strongly peaked about  $E_n = \hbar^2 k_n^2/2$ . To a good approximation

$$\begin{aligned} \langle \Psi(E) | \Psi_0 \rangle &\simeq [A(E)/C] \langle \Psi_0 | \Psi_0 \rangle \\ &= A(E) \sqrt{(a+1/\kappa_n)/2}. \end{aligned} \quad (\text{A6b})$$

We shall expand  $S_+^2(E) + S_-^2(E) = F(E)$  about  $E_n$  to

obtain

$$\begin{aligned} F(E) &\simeq F(E_n) + F'(E_n)(E - E_n) + \frac{1}{2}F''(E_n)(E - E_n)^2 \\ &\simeq \frac{1}{2}F''(E_n)\{(E - E_n - \Delta_n)^2 + \hbar^2\Gamma_n^2\} \end{aligned} \quad (\text{A6c})$$

where

$$\Delta_n = -F'(E_n)/F''(E_n), \quad (\text{A6d})$$

$$\hbar^2\Gamma_n^2 = 2F(E_n)/F''(E_n) - F^2(E_n)/F''^2(E_n). \quad (\text{A6e})$$

In doing the expansions only the highest powers of  $\exp(-G_n)$  are retained. After a straightforward but tedious calculation, Eq. (A6e) yields Eq. (36).

The derivation of Eq. (48) proceeds as follows. According to Eq. (17), the transition probability per unit time for a transition from an initial state of energy  $e_i$  to a final state of energy  $e_f$  is given by

$$T(e_i \rightarrow e_f) = (4\gamma/\hbar^2) |\langle e_f | q_0 | e_i \rangle|^2 (e_i - e_f). \quad (\text{A7a})$$

The virtual state of lowest energy  $|\Psi_1\rangle$  is a coherent superposition of energy states  $|e\rangle$ . In the calculation of transition probabilities one must first sum probability amplitudes before squaring. The effect is to replace the matrix element of  $q_0$  by  $\langle \Psi_1 | q_0 | e_f \rangle$ . Then the transition rate from  $|\Psi_0\rangle$  to  $|e\rangle$  is

$$T(\Psi_0 \rightarrow e) = (4\gamma/\hbar^2) |\langle \Psi_1 | q_0 | e \rangle|^2 (e_1 - e). \quad (\text{A7b})$$

To calculate  $\Gamma(e_1, \mathbf{0})$ , the transition rate out of the lowest virtual state, we must sum over all lower energy states, that is

$$\begin{aligned} \Gamma(e_1, \mathbf{0}) &= \sum_{e=0}^{e_1} T(\Psi_1 \rightarrow e) \\ &\rightarrow (c/\pi\hbar) \int_0^{e_1} de T(\Psi_1 \rightarrow e) / (2e)^{1/2}. \end{aligned} \quad (\text{A7c})$$

In the last step we have taken the limit  $c \rightarrow \infty$  and replaced the sum by an integral.

It is now useful to extract the normalization factors from the wave functions and write  $\Psi_1(q_0) = C\Phi_1(q_0)$  and  $\Psi(e, q_0) = A(e)\Phi(e, q_0)$ . Equation (7c) becomes

$$\begin{aligned} \Gamma(e_1, \mathbf{0}) &= [16\gamma/\pi\hbar^2(a+1/\kappa_1)] \\ &\times \int_0^{e_1} de \frac{F^2(e_1, e)(e_1 - e)}{(2e)^{1/2}[S_+^2(e) + S_-^2(e)]} \end{aligned} \quad (\text{A8a})$$

where

$$F(e_1, e) = \int_0^\infty dq_0 q_0 \Phi_1(q_0) \Phi(e, q_0). \quad (\text{A8b})$$

We recall that  $[S_+^2(e) + S_-^2(e)]^{-1/2}$  is sharply peaked about  $e_1$ . We use Eq. (A6c), absorb  $\Delta_1$  into  $e_1$ , and obtain

$$\begin{aligned} \Gamma(e_1, \mathbf{0}) &= [32\gamma/\pi\hbar^3(a+1/\kappa_1)F''(e_1)] \\ &\times \int_0^{e_1} de \frac{F^2(e_1, e)(e_1 - e)}{(2e)^{1/2}[(e_1 - e)^2 + \hbar^2\Gamma_1^2]}. \end{aligned} \quad (\text{A8c})$$

The function  $(e_1 - e)/[(e_1 - e)^2 + \hbar^2 \Gamma_1^2]$  is sharply peaked about the value  $e_1 - \hbar \Gamma_1 \simeq e_1$ . The function  $F^2(e_1, e)$  is a function of  $e$  that varies slowly between its values of zero at  $e = 0$  and  $\frac{1}{4}(a + 1/\kappa_1)^2$  at  $e = e_1$ . We may replace  $e$  by  $e_1$  in  $F^2$  and  $(2e)^{1/2}$  and remove them from the integral. The remaining integral can be done to yield

$$\Gamma(e_1, 0) = (16\gamma/\pi\hbar^3) \frac{F^2(e_1, e_1)}{F''(e_1)(2e_1)^{1/2}} \times \ln[(e_1^2 + \hbar^2 \Gamma_1^2)/\hbar^2 \Gamma_1^2]. \quad (\text{A8d})$$

After some algebra and with the assumption that  $\hbar \Gamma_1 \ll e_1$  and  $k_1(a + 1/\kappa_1) \simeq \pi$ , Eq. (48) is obtained.

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