Quantum decay in a dissipative system

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In view of recent interest in the problem of macroscopic quantum tunneling in systems involving the Josephson effect, we present an accurate numerical calculation of the tunneling rate of a system from a metastable well, at zero temperature, in the presence of dissipative coupling to the environment. Although we concentrate on a specific form of dissipation, as discussed by Caldeira and Leggett, we believe that such a numerical method can be extended to other forms of dissipation as well. Our method is based on the framework recently described by Caldeira and Leggett, and requires (a) a novel treatment of a nonlinear integro-differential equation and (b) an extension of the usual Fredholm scattering theory so as to be applicable to the present dissipative problem. We present explicit results for wide ranges of dissipation and estimate our error in the calculation of the exponent to be no larger than 0.1% and of the prefactor to be no larger than 2%.

I. INTRODUCTION

Considering the recent interest in the subject of macroscopic quantum tunneling and related quantum phenomena in systems involving the Josephson effect,¹⁻¹² we present a precise numerical calculation of the quantum decay rate from a metastable well in a dissipative system. Although the results presented here are for a specific model for the dissipative mechanism, we believe that the method discussed is of wider applicability, and may even be applicable in the discussions of deep inelastic collisions of heavy ions in nuclear physics.¹³ The technique we develop requires (a) a novel analytical treatment of a nonlinear integro-differential equation and (b) an extension of the Fredholm scattering theory so as to be applicable to the present dissipative problem. In view of the recent experimental interest $^{14-16}$ in the subject of macroscopic quantum tunneling it is important to know that the theorist can calculate the decay rate with great precision.

The underlying basis of the calculation was laid out by Langer¹⁷ some times ago and we stick to that framework. The extension of Langer's method to the dissipative case presents, at least superficially, no specific difficulty and has been expounded by Caldeira and Leggett² at great length. There are still some subtle points unresolved, but it appears that they are of little practical consequence. At zero temperature the decay rate from a metastable well can be conveniently expressed as

$$W(\alpha) = A(\alpha)e^{-B(\alpha)/\hbar}$$

Here α is a parameter which characterizes the dissipation such that $\alpha=0$ corresponds to the nondissipative case whereas $\alpha \to \infty$ corresponds to strong damping of the system undergoing tunneling. Caldeira and Leggett have obtained $B(\alpha)$ in the limit of both $\alpha \to 0$ and $\alpha \to \infty$. For intermediate α 's they have given variational estimates.¹⁸ We present exact numerical estimate of $B(\alpha)$ throughout the entire range and estimate our accuracy to be better

than 0.1%. $A(\alpha)$ for $\alpha=0$ is of course readily obtained from Langer's method; for $\alpha \rightarrow \infty$, $A(\alpha)$ has been calculated by Caldeira and Leggett and follows a $\alpha^{9/2}$ behavior. Although the present calculation verifies this $\frac{9}{2}$ power in this limit, the exact value of $A(\alpha)$ is off by a factor of 2. The general prescription¹⁷ of defining the prefactor as being proportional to a ratio of determinants is still correct for the dissipative problem to be discussed in the present paper. However, the method to calculate the ratio of the determinants as given by Caldeira and Leggett is generally incorrect as one can trivially verify by taking $\alpha \rightarrow 0$ in their formalism. It turns out that their method does become quite accurate in the limit of large α , a conclusion that we reach from our present work. As discussed here the correct treatment requires an extension of Fredholm scattering theory to the present problem. $A(\alpha)$ shows a sharp crossover behavior at $\alpha \sim 1$.

II. QUANTUM DECAY IN A DISSIPATIVE SYSTEM

Dissipation is taken into account by coupling the system variable q to an environment consisting of infinite number of degrees of freedom. This coupling can potentially take many different forms, but of particular interest is the case where the classical equation of motion of the system variable q contains a dissipative term linear in the time derivative of q. The applicability of this form of dissipation rests on the semiguantitative success of the phenomenological equation commonly known as the resistively shunted junction¹⁹ (RSJ) equation applicable to a large class of weak links involving superconductors. For a good oxide layer junction the assumption of linear dissipation may not be correct for very low temperatures and for frequencies below the gap frequency.²⁰ Nonetheless we believe that the numerical method described in this paper can, if required, be adapted to a large class of dissipative couplings. Here we shall concentrate exclusively on the case of linear dissipation. The system to keep in mind is a

radio frequency superconducting quantum interference device (SQUID); the relevant macroscopic variable q is the total magnetic flux through the superconducting ring. The Lagrangian that we use to discuss macroscopic quantum tunneling at zero temperature is that employed by Caldeira and Leggett:^{1,2}

$$\mathcal{L} = \frac{1}{2}M\dot{q}^{2} - V(q) + \sum_{\alpha} (\frac{1}{2}m_{\alpha}\dot{x}_{\alpha}^{2} - \frac{1}{2}m_{\alpha}x_{\alpha}^{2}\omega_{\alpha}^{2}) - q\sum_{\alpha} c_{\alpha}x_{\alpha} - \frac{1}{2}q^{2}\sum_{\alpha} \frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}^{2}}.$$
 (2.1)

The variables x_{α} represent the environment degrees of freedom and c_{α} denotes the coupling between the system variable q and the environment. The justification of being able to treat the environment as a collection of harmonic oscillators for the purpose of calculating the zero temperature tunneling rate has been discussed in great detail by Caldeira and Leggett² and we refrain from duplicating their arguments. All information concerning the effect of the environment on the dynamics of the system variable, q, is contained in the spectral density of the environment $J(\omega)$ given by

$$J(\omega) = \frac{\pi}{2} \sum_{\alpha} \frac{c_{\alpha}^{2}}{m_{\alpha}\omega_{\alpha}} \delta(\omega - \omega_{\alpha}) . \qquad (2.2)$$

It can be shown that if $J(\omega) \rightarrow \eta \omega$ as $\omega \rightarrow 0$, q in the classical limit obeys the equation of motion which is exactly the RSJ equation mentioned earlier; this fixes our choice of $J(\omega)$. The counter term in the Lagrangian is necessary for the definition of the damping coefficient η to agree with the phenomenological (observable) definition as would be measured in the classical limit described by the RSJ equation. The classical equation of motion of q can be obtained from the above Lagrangian by eliminating the variables x_{α} and using a $J(\omega)$ which varies as $\eta \omega$ in the limit $\omega \rightarrow 0$ as mentioned before. The result is

$$M\ddot{q} + \eta \dot{q} = -\frac{dV(q)}{dq} . \qquad (2.3)$$

We assume that the potential energy V(q) has a single metastable minimum as shown in Fig. 1; the local



FIG. 1. Typical metastable potential well.

minimum is taken to be situated at q=0. More specifically, the potential relevant for tunneling in a SQUID can be well represented by a cubic²¹

$$V(q) = \frac{1}{2} M \omega_0^2 (q^2 - q^3/q_0) , \qquad (2.4)$$

where q_0 is the distance under the barrier, and ω_0 is the small oscillation frequency at the local minimum. This completes our definition of the problem and we now turn to the problem of calculation of the decay rate. We first write down the Feynman path integral describing the amplitude that the system begins at the local minimum and returns to the local minimum after a time T regardless of the final state of the environment. The environment degrees of freedom can be integrated out; the resulting amplitude contains only the system degree of freedom, i.e., q. The decay rate can be calculated quite conveniently if we rotate the amplitude to imaginary times $T = i\beta$. The rotation to the imaginary time maps the amplitude to an expression which is formally identical to the expression for the partition function given by

$$Z = \int \mathscr{D}q \, e^{-S_{\rm eff}[q]/\hbar} \,, \tag{2.5}$$

where $S_{\text{eff}}[q]$ is given by

$$S_{\text{eff}}[q] = \int_{0}^{\beta \hbar} d\tau [\frac{1}{2}M\dot{q}^{2} + V(q)] + \frac{\eta}{4\pi} \int_{-\infty}^{+\infty} d\tau \int_{0}^{\beta \hbar} d\tau' \frac{[q(\tau) - q(\tau')]^{2}}{(\tau - \tau')^{2}} .$$
(2.6)

One must, however, remember that $q(0) = q(\beta \hbar)$; the desired decay rate at zero temperature is given by $-\lim_{\beta\to\infty} \operatorname{Im}(\ln Z/\beta\hbar)$, a prescription due to Langer. A systematic accurate evaluation of the decay rate follows from the application of the method of steepest descent, also originally due to Langer. The approach needs improvement because V(q) does not have a lower bound and strictly speaking the "partition function" Z is undefined. However, one can argue that the ground-state energy $E_0 = -\lim_{\beta \to \infty} (\ln Z / \beta \hbar)$ will acquire an imaginary part if we begin with a bounded potential and then analytically continue in a variable which turns the potential into an unbounded one. This sounds reasonable except that the calculation does not quite proceed along these lines; one begins with a potential that is unbounded to begin with and then judiciously interprets the results when one gets into any trouble. In the nondissipative case it can be verified that this gives results in agreement with those obtained from WKB method. From an analysis of a Fokker-Planck equation it was also verified by Langer²² that the classical nucleation rate from a metastable phase obtained from the imaginary part of the partition function is the correct one if some care is taken in defining the prefactor. It therefore seems that the imaginary part of the partition function gives the correct decay rate whether we are calculating a classical nucleation rate or the quantum decay form a metastable well at zero temperature. (In this case the connection to the nucleation problem can be a bit misleading since the partition function Z is actually a result of the rotation to the imaginary time of a zero temperature transition amplitude. However, an imprecise analogy can indeed be constructed since one can always map a zero-dimensional quantum problem to a onedimensional classical statistical mechanical problem. The difficulty, however, is in defining the dynamics which causes the nucleation and which also determines the prefactor.) Along with Caldeira and Leggett we shall assume that this prescription remains unchanged even for the dissipative case as formulated above.

III. CALCULATION OF THE EXPONENT

The steepest-descent method to calculate the imaginary part of $\ln Z$ requires that we solve the following Euler-Lagrange equation² of motion (we let $\beta\hbar \rightarrow \infty$):

$$M\ddot{q} = \frac{\partial V}{\partial q} + \frac{\eta}{\pi} \int_{-\infty}^{+\infty} d\tau' \frac{q(\tau) - q(\tau')}{(\tau - \tau')^2} .$$
(3.1)

It is to be understood that the boundary condition is $q_c(\infty) = q_c(-\infty) = 0$. The solution $q_c(\tau)$ when substituted in the expression for S_{eff} gives the exponent *B*. For the sake of convenience we introduce the following dimensionless variables:

$$u = \omega_0 \tau ,$$

$$Z(u) = q(u)/q_0 ,$$

$$\alpha = \eta/2M\omega_0 ,$$

$$\mathscr{S}[z] = S_{\text{eff}}[q(\tau)]/\frac{1}{2}M\omega_0 q_0^2 ,$$

$$b[\alpha] = B/\frac{1}{2}M\omega_0 q_0^2 .$$

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We therefore have to evaluate the following expression to obtain the exponent B:

$$\mathscr{S}[z] = \int_{-\infty}^{+\infty} du \left[\left(\frac{dz}{du} \right)^2 + z^2 - z^3 \right] + \frac{\alpha}{\pi} \int_{-\infty}^{+\infty} du \int_{-\infty}^{+\infty} du' \left[\frac{z(u) - z(u')}{u - u'} \right]^2, \quad (3.2)$$

where z is the solution of the following nonlinear integrodifferential equation:

$$\frac{d^2z}{du^2} = z - \frac{3}{2}z^2 + \frac{2\alpha}{\pi} \int_{-\infty}^{+\infty} \frac{z(u) - z(u')}{(u - u')^2} .$$
(3.3)

When $\alpha = 0$ this equation can be solved exactly and the result is

$$z(u) = \operatorname{sech}^2(u/2)$$
. (3.4)

An analytical solution can also be obtained in the limit $\alpha \rightarrow \infty$ and the result is²

$$z(u) = \frac{4}{3} \left[1 + \left(\frac{u}{2\alpha} \right)^2 \right]^{-1}$$
 (3.5)

For intermediate values of α , so far it has not been possible to obtain an analytical solution of this equation; we now describe a numerical method valid for all values of α . Introducing the Fourier transform

$$z(\omega) = \frac{1}{\sqrt{2}\pi} \int_{-\infty}^{+\infty} z(u) e^{i\omega u} du , \qquad (3.6)$$

we can convert the nonlinear integro-differential equation into a nonlinear integral equation given by

$$z(\omega) = \frac{1}{1 + 2\alpha |\omega| + \omega^2} \left[\frac{3}{2\sqrt{2}\pi} \right]$$
$$\times \int_{-\infty}^{+\infty} d\omega' z(\omega - \omega') z(\omega') . \tag{3.7}$$

A direct iteration technique to solve this equation would fail for reasons to be discussed below. The algorithm that we have devised relies on the following interesting features of the equation.

(1) The scaling property. By introducing a parameter λ one can rewrite the equation as

$$z(\omega) = \frac{1}{1+2\alpha |\omega| + \omega^2} \lambda \int_{-\infty}^{+\infty} d\omega' z(\omega - \omega') z(\omega') . \quad (3.8)$$

It is thus apparent that if $(\lambda_0, z_0(\omega))$ satisfies the equation then so would $(\lambda_1, z_1(\omega))$ provided the λ 's and q's are scaled in the following way:

$$\lambda_1 = \lambda_0 / \xi ,$$

$$z_1(\omega) = z_0(\omega) \xi .$$

This means that if we can find one solution $(\lambda_1, z_1(\omega))$ for an arbitrary parameter λ_1 , we can obtain the solution for a particular λ_0 by simply rescaling $z_1(\omega)$ by a factor $\xi = \lambda_0/\lambda_1$.

(2) A relevant dangerous direction at the fixed point. Suppose that $(\lambda_0, z_0(\omega))$ satisfies the equation. Now let $f_0(\omega) = \xi z_0(\omega)$. For ξ not equal to 1, f_0 is a vector in the right direction but wrong amplitude. For a fixed λ_0 successive iterations lead to the following:

$$f_1(\omega) = f_0(\omega)\xi^2,$$

$$f_2(\omega) = f_0(\omega)\xi^4,$$

$$\vdots$$

$$f_n(\omega) = f_0(\omega)\xi^{2^n}.$$



FIG. 2. Flow diagram of the iteration process.

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FIG. 3. $z(\omega)$ as a function of ω for two different values of α .

It is obvious that f_n tends to infinity or 0 depending on whether ξ is greater than 1 or less than 1; we have found at least one relevant dangerous direction at the fixed point.

We now explain how we can make use of the properties mentioned above to generate an efficient algorithm to solve Eq. (3.8). Suppose that $(1, f_0)$ is one solution of Eq. (3.8) then it is clear from the scaling properties that any point on the curve $\lambda \xi = 1$ (see Fig. 2) represents a valid solution given by the pair $(\lambda, \xi f_0)$. The dangerous directions correspond to the directions flowing to infinity or zero. However, we can eliminate these dangerous directions by adjusting λ to bring the point P_1 on to the curve as shown by the dashed lines. This means that when ξ increases λ should be decreased and vice versa. We therefore design an iteration procedure which is as follows:

(1) Start with an initial $z_0(\omega)$.

(2) Calculate $z_1(\omega) = O(\lambda_0, z_0(\omega))$, where O is the operation defined by the right-hand side of the Eq. (3.8).

(3) Calculate $\lambda_1 = \lambda_0 \xi^{-2}$, where $\xi = z_1(\omega = 0)/z_0(\omega = 0)$.



FIG. 4. z(u=0) as a function of α .



FIG. 5. Exponent $b(\alpha)$ as a function of α . The inset is a blowup of the small α region.

(4) Find $z_2(\omega) = O(\lambda_1, z_1(\omega))$.

(5) Repeat steps (2)-(4) until the successive difference satisfies a preset convergence criterion.

When step (5) is completed we will have a pair $(\lambda_n, z_n(\omega))$ which satisfies Eq. (3.8). From the scaling property we simply need to scale $z_n(\omega)$ to get the solution for $\lambda = \frac{3}{2}(2\pi)^{-1/2}$. Such a procedure seems to converge usually within tens of iterations. At this point we do not know if there are other dangerous directions or not, but the stability of the iteration procedure with respect to the initial choice of $z_0(\omega)$ seems to indicate that there are not.

Some representative $z(\omega)$'s are shown in Fig. 3. As α increases from 0, $z(\omega)$ changes from $\sqrt{8/\pi}(\pi\omega/\sinh\pi\omega)$ to a dependence $\sim e^{-\omega}$. In Fig. 4 we show z(u=0) as a function of α . The curve approaches $\frac{4}{3}$ in the limit $\alpha \rightarrow \infty$; this is in agreement with the limiting value calculated by Caldeira and Leggett. In Fig. 5 we show $b(\alpha)$ as a function of α . The straight line is the large α asymptote

TABLE I. Data for the exponent and the prefactor of the decay rate as a function of α .

α	$b(\alpha)$	$[b(\alpha)k(\alpha)]^{1/2}$
0.0	1.067	8.094
0.01	1.085	8.395
0.05	1.161	9.695
0.10	1.258	11.562
0.50	2.110	41.175
1.00	3.302	15.233×10^{1}
1.50	4.576	45.947×10 ¹
2.00	5.893	11.516×10^{2}
2.50	7.234	25.102×10^{2}
3.00	8.591	49.218×10^{2}
3.50	9.957	88.915×10^{2}
4.00	11.330	15.054×10^{3}
10.0	27.972	70.981×10^{4}

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calculated by the above authors. The limiting values as $\alpha \rightarrow 0$ or as $\alpha \rightarrow \infty$ are also in agreement with the results calculated by these authors. They have shown that

$$b(\alpha) = b(0) + 1.86\alpha + O(\alpha^2), \quad \alpha \to 0$$

$$b(\alpha) = \frac{8\pi\alpha}{9} + \frac{2\pi}{9} \frac{1}{\alpha} + O\left[\frac{1}{\alpha^2}\right], \quad \alpha \to \infty$$

Table I contains some sample numerical results. By using various different integration grids and cutoffs we estimate that the numerical error in $b(\alpha)$ is not larger than 0.1%.

IV. CALCULATION OF THE PREFACTOR

The prefactor of the decay rate is obtained from the quadratic fluctuations around the steepest-descent solution given in Sec. III. The prefactor A is given by

$$A = (B/2\pi\hbar)^{1/2}K^{1/2}, \qquad (4.1)$$

where

$$K = \left| \frac{\det(\omega_0^2 + H_0)}{\det'(\omega_0^2 + H_0 + V)} \right| .$$
(4.2)

The operator H_0 is defined by the following equation:

$$H_0\psi(t) = -\frac{d^2\psi}{dt^2} + \frac{\eta}{\pi M} \int_{-\infty}^{+\infty} dt' \frac{\psi(t) - \psi(t')}{(t - t')^2} , \quad (4.3)$$

and the potential V is given by

$$V = -3q_c(t)/M . \tag{4.4}$$

Here $q_c(t)$ is the steepest-descent solution obtained in Sec. III. The symbol det' in Eq. (3.2) means that the 0 eigenvalue is to be omitted; H_0 can be easily shown to be Hermitian. We again introduce a set of dimensionless variables as defined in the earlier section. We therefore write

$$A = \omega_0 \left[\frac{M \omega_0 q_0^2}{4\pi \hbar} \right]^{1/2} [b(\alpha)k]^{1/2}, \qquad (4.5)$$

where

$$k = \left| \frac{\det(1+h_0)}{\det'(1+h_0+v)} \right| \,. \tag{4.6}$$

The operator h_0 is given by

$$h_0\psi(u) = -\frac{d^2\psi}{du^2} + \frac{2\alpha}{\pi} \int_{-\infty}^{+\infty} du' \frac{\psi(u) - \psi(u')}{(u - u')^2} , \quad (4.7)$$

and the potential v is

$$v = -3z_c(u) . (4.8)$$

As mentioned earlier b and $z_c(u)$ are known from the preceding section. For $\alpha = 0$ the prefactor can be calculated in many different ways (see, for example, the paper by Langer, Ref. 17). However, for α not equal to 0 we have to extend the usual Fredholm scattering theory²³ so as to be applicable to the present problem. Before we do that we shall now show how one must define phase shift for

the present problem.

We start by considering a simple one-dimensional potential scattering problem (nondissipative case). We therefore have

$$H\psi \equiv -\frac{d^2\psi}{du^2} + V\psi , \qquad (4.9)$$

and

$$v(u) = 0, |u| > T.$$
 (4.10)

Let us further assume that v(u)=v(-u). Then the Hamiltonian and the parity operator can be simultaneously diagonalized to give even- and odd-parity standing-wave solutions

$$\Psi^{+} = \begin{cases} \cos(\omega u + \delta_{+}), & u > T \\ \cos(\omega u - \delta_{+}), & u < -T \end{cases}$$
(4.11)

and

$$\Psi^{-} = \begin{cases} \sin(\omega u + \delta_{-}), & u > T \\ \sin(\omega u - \delta_{-}), & u < -T \end{cases}$$
(4.12)

If necessary it is easy to construct a representation in terms of incoming and outgoing waves from Eqs. (4.11) and (4.12). For example, if we consider a wave incident from the left giving rise to a reflected and a transmitted wave, we get

$$\Psi_{\rightarrow}(u) = \begin{cases} Se^{i\omega u}, & u > T \\ e^{i\omega u} + Re^{-i\omega u}, & u < -T \end{cases}$$
(4.13)

where

$$S = 1 + \sum_{\sigma = +, -} i e^{i\delta_{\sigma}} \sin \delta_{\sigma}$$
(4.14)

and

$$R = i \sum_{\sigma = +, -} \sigma e^{i\delta_{\sigma}} \sin \delta_{\sigma} .$$
(4.15)

For the dissipative case, h_0 as given by Eq. (4.7) has eigenstates given by the following expressions:

$$\Psi_n^+(u) = \frac{1}{\sqrt{R}} \cos(\omega_{0n}^+ u) \equiv |\omega_{0n}^+\rangle$$
(4.16)

and

$$\Psi_n^{-}(u) = \frac{1}{\sqrt{R}} \sin(\omega_{0n} u) \equiv |\omega_{0n}| \rangle , \qquad (4.17)$$

which are also the eigenstates of parity. The length of the box in which the wave functions are normalized is 2R. Defining ω_{0n}^+ and ω_{0n}^- in the following way,

$$\omega_{0n}^{+} = \frac{(2n-1)\pi}{2R} \tag{4.18}$$

and

$$\omega_{0n}^{-} = \frac{n\pi}{R} , \qquad (4.19)$$

the energy eigenvalues are given by

$$E_{0n}^{\sigma} = (\omega_{0n}^{\sigma})^2 + 2\alpha \omega_{0n}^{\sigma} , \qquad (4.20)$$

where the integers n take the values $1, 2, 3, \ldots$, and σ is either + or -.

When $v \neq 0$, the Hamiltonian in the dissipative case is $h_0 + v$. The following arguments show that the concept of phase shift still remains meaningful. If we assume that $\Psi(u) \sim e^{i\omega u}$ when $u \rightarrow \infty$, the error comes from two separate sources: (a) the error from $v\psi$ and (b) the error from the nonlocal term. Both of these errors vanish as $u \rightarrow \infty$, the first because $v \Psi \rightarrow 0$ as $u \rightarrow \infty$ and the second because the error coming from the nonlocal term vanishes as 1/u as $u \to \infty$. Since parity is still a good quantum number for $h_0 + v$, we can construct, once again, even- and odd-parity standing waves just as in the nondissipative case. Now the spectrum will be given by

$$E_n^{\sigma} = (\omega_n^{\sigma})^2 + 2\alpha \omega_n^{\sigma} , \qquad (4.21)$$

where

$$\omega_n^+ = \frac{(2n-1)\pi}{2R} - \frac{\delta_n^+}{R}$$
(4.22)

and

$$\omega_{\overline{n}} = \frac{n\pi}{R} - \frac{\delta_{\overline{n}}}{R} \,. \tag{4.23}$$

Now define

 $r \sigma$

$$\Delta E_{0n}^{\sigma} = E_{0n+1}^{\sigma} - E_{0n}^{\sigma}$$
$$= \frac{2\pi}{R} (\omega_{0n}^{\sigma} + \alpha)$$
(4.24)

and

$$\begin{aligned} \partial E_n^{\sigma} &= E_n^{\sigma} - E_{0n}^{\sigma} \\ &= -\frac{2\delta_n^{\sigma}}{R} (\omega_{0n}^{\sigma} + \alpha) . \end{aligned}$$

$$\tag{4.25}$$

We therefore have

$$\frac{\delta E_n^{\sigma}}{\Delta E_{0n}^{\sigma}} = -\frac{1}{\pi} \delta_n^{\sigma} , \qquad (4.26)$$

and k can now be calculated in terms of the phase shifts defined above, and we have the following:

$$k^{-1} = \frac{\operatorname{der}(1+h_{0}+1)}{\operatorname{det}(1+h_{0})}$$

$$= \prod_{\text{bound states}} (1+E_{b}) \exp\left[\sum_{n,\sigma} \ln\left[1+\frac{\delta E_{n}^{\sigma}}{1+E_{0n}^{\sigma}}\right]\right]$$

$$= \prod_{\text{bound states}} (1+E_{b}) \exp\left[\sum_{n,\sigma} \left[\frac{\delta E_{n}^{\sigma}}{\Delta E_{0n}^{\sigma}}\right] \left[\frac{1}{1+E_{0n}^{\sigma}}\right] \Delta E_{0n}^{\sigma}\right] + O\left[\frac{1}{R}\right]$$

$$= \prod_{\text{bound states}} (1+E_{b}) \exp\left[-\frac{1}{\pi} \int_{0}^{\infty} dE' \frac{\delta^{+}(E') + \delta'(E')}{(1+E')}\right].$$
(4.27)

Clearly the final equation is of the same form as for the nondissipative cases. An expansion of the Fredholm determinant gives the tangent of the phase shift as follows:

$$\tan\delta^{\sigma}(E) = -\pi \left[\sigma \langle E \mid V \mid E \rangle_{\sigma} + \int_{0}^{\infty} \frac{dE_{1}}{E - E_{1}} \sigma \langle E \mid V \mid E_{1} \rangle_{\sigma \sigma} \langle E_{1} \mid V \mid E \rangle_{\sigma} + \cdots \right].$$
(4.28)

However, one must remember that

 $det'(1+h_0+V)$

$$\langle u | E_{0n} \rangle_{\sigma} = \frac{\langle u | \omega_{0n}^{\sigma} \rangle}{\sqrt{\Delta E_{0n}^{\sigma}}}$$

$$= \left[\frac{1}{2\pi(\omega_{0n}^{\sigma} + \alpha)} \right]^{1/2} \times \begin{cases} \cos(\omega_{0n}^{+} u) \\ \sin(\omega_{0n}^{-} u) \end{cases}.$$
(4.29)

Note the presence of α in the above equation. Although the above series converges for large ω (or α), for $\omega \rightarrow 0$ and small α its convergence is quite poor. For small ω we calculate the ratios of the eigenvalues numerically; $|\omega_{0n}^{\sigma}\rangle$ are chosen as the basis to represent $h_0 + v$ as a 291×291 matrix. The choice of the size of the matrix reflects a compromise between the computing time and the accuracy gained in making the matrix larger. Figures 6 and 7

show $(1+E_{0n})/(1+E_n)$ as a function of ω_n for $\alpha=0$ and $\alpha = 1$, respectively. Although ω_n 's are discrete we have drawn smooth lines through them. The solid line is the result of changing the integral in Eq. (4.27) into a discrete using approximation sum and the $\delta^{\sigma}(E)$ $\sim -\pi_{\sigma} \langle E | V | E \rangle_{\sigma}$. Note that the discrete sum that results depends on the grid size. Both grid sizes (Figs. 6 and 7) were chosen to be 0.03. The dashed line is the result of the numerical diagonalization of the matrices using the same grid size mentioned above. It turns out that the ratios $(1+E_{0n}^{\sigma})/(1+E_n^{\sigma})$ are almost the same, on the scale of the figures, for $\sigma = +$ or $\sigma = -$. We therefore do not distinguish between them in the plot. As expected when ω or α is large the approximate expression for the phase shift given above does quite well. At this point it is important to note the following: The approximate form



FIG. 6. Ratio of the eigenvalues of h_0 and h_0+v as a function of ω_n . Dashed line corresponds to the numerical diagonalization of the matrices and solid line corresponds to a simple approximation given in the text. The parameter α is equal to 0.

 $\delta^{\sigma}(E) \sim -\pi_{\sigma} \langle E \mid V \mid E \rangle_{\sigma}$ is used only for high energies. It certainly would be more accurate to use $\delta^{\sigma}(E) \sim \tan^{-1}(\pi_{\sigma} \langle E \mid V \mid E \rangle_{\sigma})$; however, this is not necessary since for low energies we use the exact numerical results obtained from diagonalizing the matrix, as mentioned above. On the other hand, the use of arctan would make the ratio $(1+E_n^0)/(1+E_n)$ finite instead of infinity at zero energy for the case $\alpha = 0$. Thus it is because of the approximation $\arctan(x) \sim x$ that the Born approximation curve is seen to blow up at zero energy. There is an important difference between the present one-dimensional case and the usual three-dimensional case²³ where $\langle r \mid E \rangle_l = (2km/\pi\hbar^2)^{1/2}j_l(kr)$ and therefore for potentials with support we find that $_l \langle E \mid V \mid E \rangle_l \sim k^{2l+1}$ for small k. In the present case note that [see Eq. (4.29)] $\langle u \mid E_{0n} \rangle_{\sigma} \sim (\omega_{0n}^{\sigma})^{-1/2}$ leading to a different behavior as



FIG. 7. Same as in Fig. 6 except that the parameter α is 1.



FIG. 8. Log-log plot of the prefactor as a function of α .

we have just discussed. The bound-state eigenvalues are easily distinguished from the continuum; not only are they well separated from the continuum but their wave functions have the characteristic signature of normalizability. For $\alpha = 0$ the three bound-state eigenvalues obtained numerically were $E_b = -1.25, 0.0, 0.75$ in excellent agreement with the exact analytical results. For $\alpha = 10$, we again found three bound-state eigenvalues given by $E_b = -1.615, 0.0, 0.618$, once again in excellent agreement with the exact analytical results obtained by Caldeira and Leggett³ in this limit. In this large damping limit the analytical results are given by $E_b = -(\sqrt{5}+1)/2$, 0, $(\sqrt{5}-1)/2$. As far as we know there are no more than three bound states for $0 < \alpha < 10$.

To calculate K we therefore multiply the ratios of the numerical eigenvalues up to a cutoff frequency ω_c and then use the Fredholm theory to integrate the phase shift for $\omega > \omega_c$ using the approximation $\delta^{\sigma} = -\pi_{\sigma} \langle E | V | E \rangle_{\sigma}$. We have chosen ω_c such that it is not too small in order to have a good fit with the approximation mentioned above, and not too large in order to avoid the effect of finite matrix size. For $\alpha = 0$, $\omega_c = 3.93$, this method gives $k^{1/2} = 7.84$ instead of the analytical result $(60)^{1/2}$; the error is clearly less than 1.5%. For large α this procedure should be even better since the asymptotic fit is considerably more accurate. In Fig. 8 we show $\frac{1}{2}\log_{10}(kb)$ vs $\log_{10}(\alpha)$; some sample data are also presented in Table I. The curve suggests a crossover from small α to large α at $\alpha \sim 1$. The slope of the straight line which goes through $\alpha = 4$ and $\alpha = 10$ (Fig. 8) is 4.2. However, the curve is concave upward; this means that the asymptotic slope is greater than 4.2. In fact the slope of 4.5 is expected for large α , since $b \sim \alpha$, and $k \sim \alpha^8$. The fact that b is proportional to α follows from the calculations in Sec. III, and the fact that k is proportional to α^8 follows from the replacement of the phase shift δ^{σ} in Eq. (4.27) by $-\pi_{\sigma}\langle E | V | E \rangle_{\sigma}.$

V. CONCLUSION

We have presented an accurate calculation of the decay rate from a metastable well in the presence of dissipative coupling to the environment at zero temperature. Although we have concentrated on a particular form of dissipation, which is currently under discussion for systems involving the Josephson effect, we believe that such a numerical method can be readily extended to other forms of dissipation provided that the environment degrees of freedom can be explicitly integrated out to produce an effective action involving the system variable alone. In fact the effective action derived by Ambegaokar et al.⁴ to discuss the problem of oxide layer junction would be simpler to handle than the dissipative model discussed here. The simplicity is due to the fact that the nonlocal kernel in the effective action derived by Ambegaokar et al. is shortranged, exponentially decaying, as opposed to the powerlaw decay in the present model. The equation equivalent to our (3.1) that can be derived from the action obtained by Ambegaokar et al. will be numerically quite well behaved. The reason why we were able to solve the present problem effectively is because of the two interesting properties of Eq. (3.1) discussed in Sec. III. A similar generalization of the Fredholm scattering theory to other forms of dissipation should be straightforward, and would be required to calculate the prefactor, unless some other

way is found to calculate the ratio of the determinants. In the future we plan to look into these problems. Lastly we must emphasize that given the rapidly growing interest in the subject of macroscopic quantum tunneling in systems involving the Josephson effect, it is important to know that the tunneling rate can be calculated in an accurate and conceptually straightforward fashion whether or not the current experiments are able to probe the finer details.

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- ¹A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. <u>46</u>, 211 (1981).
- ²A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) <u>149</u>, 374 (1983).
- ³A. J. Leggett, Prog. Theor. Phys. Suppl. <u>69</u>, 80 (1980).
- ⁴V. Ambegaokar, U. Eckern, and G. Schön, Phys. Rev. Lett. <u>48</u>, 1745 (1982).
- ⁵S. Chakravarty, Phys. Rev. Lett. <u>49</u>, 681 (1982).
- ⁶S. Chakravarty and S. Kivelson, Phys. Rev. Lett. <u>50</u>, 1811 (1983); <u>51</u>, 1109(E) (1983).
- ⁷A. J. Bray and M. A. Moore, Phys. Rev. Lett. <u>49</u>, 1546 (1982).
- ⁸K. K. Likharev, Physica <u>108B&C</u>, 1079 (1981).
- ⁹W. Zwerger, Z. Phys. B <u>47</u>, 129 (1982).
- ¹⁰J. Kurkijarvi, Phys. Lett. <u>88A</u>, 241 (1982).
- ¹¹A. Schmid, J. Low Temp. Phys. <u>49</u>, 609 (1982).
- ¹²M. Büttiker and R. Landauer, Phys. Rev. Lett. <u>49</u>, 1739 (1982).
- ¹³K. Mohring and U. Smilansky, Nucl. Phys. A <u>338</u>, 227 (1980).
- ¹⁴R. F. Voss and R. A. Webb, Phys. Rev. Lett. <u>47</u>, 265 (1981);
 Phys. Rev. B <u>24</u>, 7447 (1981); Physica <u>108B</u>, 1307 (1981).
- ¹⁵L. D. Jackel et al., Phys. Rev. Lett. <u>47</u>, 265 (1981).
- ¹⁶D. B. Schwartz, J. E. Lukens, and C. N. Archie, Bull. Am.

Phys. Soc. 28, n. 3, 569 (1983).

- ¹⁷J. S. Langer, Ann. Phys. <u>41</u>, 108 (1967). See also the later work by C. G. Callan and S. Coleman, Phys. Rev. D <u>16</u>, 1762 (1977).
- ¹⁸The variational estimates obtained by Caldeira and Leggett are in excellent agreement with the exact numerical results obtained in this paper. These estimates are never off by more than 1.5%, and are often much better than that. The comparison mentioned here is for $b(\alpha)$ and not for $B(\alpha)$, as defined in the text. We thank Tony Leggett and A. O. Caldeira for sharing with us their unpublished results.
- ¹⁹A. Barone and G. Paterno, *Physics and Applications of the Josephson Effect* (Wiley Interscience, New York, 1982).
- ²⁰This follows from the work of Ambegaokar *et al.* (Ref. 4).
- ²¹See A. J. Leggett, in Proceedings of the Sixth International Conference on Noise in Physical Systems, Gaithersburg, Maryland (1981), National Bureau of Standards (U.S.) Special Publication No. 614, (U.S. G.P.O., Washington, D.C., 1982), p. 355, for a particularly clear discussion.
- ²²J. S. Langer, Ann. Phys. (N.Y.) <u>54</u>, 258 (1969).
- ²³K. Gottfried, Quantum Mechanics (Benjamin, New York, 1966), Vol. I.