Dissipative Quantum Tunneling in a Biased Double-Well System at Finite Temperatures

Matthew P. A. Fisher and Alan T. Dorsey
Physics Department, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 21 January 1985)

We study quantum tunneling in a biased double-well potential in the presence of Ohmic dissipation with a friction coefficient $\alpha > 1$. The tunneling rate out of the metastable well is calculated in real time as a function of the temperature T and bias energy ϵ. The $T=0$ result agrees with a droplet-model calculation in imaginary time. At low temperatures we find an enhancement to the $T=0$ rate varying as $(T/\epsilon)^2$.

PACS numbers: 05.30.−d, 71.25.Mg, 74.50.+r

Recently there has been much interest in understanding the effect of dissipation and finite temperature on quantum mechanical tunneling.[1-3] The case of Ohmic dissipation, which is relevant to the problem of macroscopic quantum tunneling[1] and other physical systems,[4] has received considerable attention. Most authors to date[1,2] have studied decay from a metastable well into a continuum and employed an *imaginary*-time approach to obtain the decay rate both at zero[1,2] and at nonzero temperature.[2] All of these calculations rely on associating the decay rate with the imaginary part of the system's free energy. Unfortunately, it has not been possible to check these results independently by a real-time calculation.[3] In this Letter we consider instead double-well systems in which the tunneling is from the metastable well into a bounded stable well slightly lower in energy. Besides being appropriate for many physical systems, this choice has the added advantage that we are then able to compute directly the system's *real*-time dynamics as it relaxes into the lower well. Doing so, we obtain the tunneling rate as a function of the friction coefficient α, the temperature T, and bias energy ϵ. In addition we carry out an imaginary-time calculation of the $T=0$ tunneling rate by applying the droplet-model technique[5] to the system's partition function. A comparison shows complete agreement with the real-time results, thus confirming the validity of our imaginary-time approach.

We are interested in a quantum coordinate q with a mass M which moves in a symmetric double-well potential with a small bias energy ϵ between the two minima at $\pm q_0/2$. The dissipation is introduced in the usual way[1] via a linear coupling of q to a bath of oscillators assumed to have an Ohmic spectrum with friction coefficient η. We assume that the barrier height between the two wells is much larger than the small undamped oscillation frequency, ω_0, in either well. Consequently, when $\epsilon=0$ the level splitting of the ground state in the absence of dissipation, Δ_0, satisfies[6] $\Delta_0 \ll \omega_0$. If in addition we assume that both the temperature and bias energy are much smaller than the smallest single-well frequency ω_b (equal to ω_0 for weak damping and $M\omega_0^2/\eta$ for strong damping), then it is possible to reduce the double-well problem to an effective but equivalent two-state system. This procedure will be discussed in detail elsewhere[7] and is described only briefly here.

Imagine dividing the bath of oscillators into two groups; those with frequencies larger or smaller than a cutoff frequency ω_c chosen to satisfy[8] $T, \epsilon \ll \omega_c \ll \omega_b$. The high-frequency oscillators will reduce the bare level splitting Δ_0, giving an effective or renormalized level splitting Δ. Since the remaining oscillators all have frequencies much less than ω_b it can be argued[7] that it is possible to truncate to a two-state system coupled to the low-frequency oscillators with a Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\hbar\Delta\sigma_x + \tfrac{1}{2}\epsilon\sigma_z + \sum_\alpha \tfrac{1}{2}(p_\alpha^2/m_\alpha + m_\alpha\omega_\alpha^2 x_\alpha^2) + \tfrac{1}{2}q_0\sigma_z\sum_\alpha C_\alpha x_\alpha \tag{1}$$

where σ_x and σ_z are Pauli matrices. The spectral density of the oscillators, defined by

$$J(\omega) = (\pi/2)\sum_\alpha (C_\alpha^2/m_\alpha\omega_\alpha)(\delta\omega - \omega_\alpha), \tag{2}$$

has an upper cutoff ω_c. For an Ohmic bath $J(\omega)$ is linear in ω, $J(\omega)=\eta\omega$. The renormalized level splitting in (1) also depends on the cutoff ω_c and to lowest order in ω_c/ω_b is given by[7]

$$\Delta(\omega_c) = g(\alpha, v_0)(\omega_c/\omega_0)^\alpha\Delta_0 \tag{3}$$

with g a function only of the dimensionless friction coefficient $\alpha \equiv \eta q_0^2/2\pi\hbar$ and the dimensionless "barrier height" $v_0 = M\omega_0^2 q_0^2/\hbar\omega_0$. The precise functional form of g depends on the detailed shape of the double well. However, in the large-α limit $g \sim (\omega_0/\omega_b)^\alpha \sim (\alpha/v_0)^\alpha$ independent of the shape of the double well. In this limit the undamped frequency ω_0 cancels in (3), leaving ω_c scaled by the overdamped frequency $M\omega_0^2/\eta$. The tunneling rate which we obtain from the two-state Hamiltonian (1) (see below) can then be expressed back in terms of the double-well parameters by use of (3) to eliminate $\Delta(\omega_c)$ in favor of Δ_0. The arbitrary frequency ω_c drops out of the resulting expression.

© 1985 The American Physical Society

We first consider the *real*-time dynamics for the Hamiltonian (1). We are interested in computing $P(t)=\langle\sigma_z(t)\rangle$ given that for $t<0$ σ_z is localized in the $+1$ state. We follow very closely the recent calculations by Chakravarty and Leggett[9] (CL), generalizing their results to include a nonzero bias. Consider the exact double path integral [over functions $\sigma_z(t)$ and $\sigma_z'(t)$] for $P(t)$, which results after averaging over an initial thermal distribution of oscillators at temperature T. As shown in CL, by the writing of the double path integral as a single path integral over four states ($\sigma_z=\pm1$, $\sigma_z'=\pm1$) and consideration of the transitions between the diagonal states ($\sigma_z=\sigma_z'$, referred to as sojourns) and the off-diagonal states ($\sigma_z=-\sigma_z'$, referred to as blips), $P(t)$ can be expressed as a power series in Δ^2. In the term of order Δ^{2n} there are $2n$ transitions at times t_i ($i=1,\ldots,2n$) with n blips (in the time intervals t_{2j-1} to t_{2j}) separated from one another by sojourns. We refer the reader to CL for details. Generalizing to nonzero ϵ we find

$$P(t)=\sum_{n=0}^{\infty}(-1)^n\Delta^{2n}\int_{t_{2n-1}}^{t}dt_{2n}\int_{t_{2n-2}}^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1\,F(t_1,t_2,\ldots,t_{2n}), \tag{4}$$

$$F=\exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{j=1}^{n}S_j\right]2^{-n}\sum_{\{\xi_j=\pm1\}}\exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{\substack{j,k=1\\ j>k}}\Lambda_{jk}\xi_j\xi_k\right]\prod_{k=0}^{n-1}\cos\left[\sum_{j=k+1}^{n}\xi_j\left(\frac{q_0^2}{\pi\hbar}X_{jk}-\frac{\epsilon}{\hbar}\Delta t_{2j}\delta_{k,0}\right)\right], \tag{5}$$

where $\Delta t_{2j}=t_{2j}-t_{2j-1}$ and t_0 equals $-\infty$ by definition. The functions S_j, Λ_{jk}, and X_{jk} are defined by

$$S_j\equiv P_{2j,2j-1}, \tag{6a}$$

$$\Lambda_{jk}\equiv P_{2k,2j-1}+P_{2k-1,2j}-P_{2k,2j}-P_{2k-1,2j-1}, \tag{6b}$$

$$X_{jk}\equiv R_{2j,2k+1}+R_{2j-1,2k}-R_{2j,2k}-R_{2j-1,2k+1}, \tag{6c}$$

where $R_{n,m}\equiv Q_1(t_n-t_m)$, $P_{n,m}\equiv Q_2(t_n-t_m)$, and the functions Q_1 and Q_2 are

$$Q_1(t)\equiv\int_0^{\infty}d\omega\,\omega^{-2}J(\omega)\sin\omega t, \tag{7a}$$

$$Q_2(t)=\int_0^{\infty}d\omega\,\omega^{-2}J(\omega)(1-\cos\omega t)\coth(\tfrac{1}{2}\beta\hbar\omega). \tag{7b}$$

The ϵ dependence enters only through the last term in (5).

If $Q_2(t)$ grows large with time the first term in (5), $A(t)\equiv\exp\{-q_0^2Q_2(t)/\pi\hbar\}$, suppresses configurations with wide blips. This enables us to put a rough upper bound on the average blip length $\langle t\rangle$ of

$$\langle t\rangle\lesssim\int_0^{\infty}dt\,tA(t)/\int_0^{\infty}dt\,A(t). \tag{8}$$

If the average blip length is small compared to the typical time scale of a blip and its neighboring sojourn [which is expected to be the time scale of $P(t)$; i.e., the tunneling time], Eq. (5) can be simplified considerably. One can ignore all interblip interactions ($\Lambda_{jk}=0$) and all but the nearest-neighbor phase factors $X_{j+1,j}\simeq Q_1(\Delta t_{2j})$. Within this "dilute blip" approximation $P(t)$ can be determined explicitly. The tunneling time Γ^{-1} which emerges from the calculation must satisfy $\Gamma^{-1}\gg\langle t\rangle$ in order that this procedure be self-consistent.

For the case of an Ohmic spectrum $Q_2(t)$ grows logarithmically with time giving (at $T=0$) a blip suppression factor $A(t)=(1+\omega_c^2t^2)^{-\alpha}$. For $\alpha>1$, (8) then provides an upper bound on $\langle t\rangle$ proportional to ω_c^{-1}. However, no such bound exists when $\alpha<1$, suggesting that the dilute-blip approximation may be unreliable within this regime.[10] We thus restrict attention to the case $\alpha>1$.

Within the dilute-blip approximation, F in (5) becomes a simple product of terms depending on Δt_{2j}. The Laplace transform of $P(t)$ is then a geometric series which can be summed. For $T,\epsilon,\Delta\ll\omega_c$ we find upon Laplace inversion the desired result[11] for the real-time dynamics when $\alpha>1$:

$$P(t)=-\tanh(\tfrac{1}{2}\beta\epsilon)+[1+\tanh(\tfrac{1}{2}\beta\epsilon)]\exp(-\Gamma t), \tag{9}$$

$$\Gamma=\frac{\Delta^2}{2\omega_c}\left(\frac{2\pi T}{\hbar\omega_c}\right)^{2\alpha-1}\frac{\cosh(\frac{1}{2}\beta\epsilon)}{\Gamma(2\alpha)}|\Gamma(\alpha+i\beta\epsilon/2\pi)|^2. \tag{10}$$

Equation (9) describes exponential incoherent relaxation with a rate Γ. Since we are considering a biased double-well potential (in contrast to tunneling into the continuum) it is also possible that the system can exhibit underdamped coherent oscillations.[9,12] For $\alpha>1$ these oscillations are suppressed. As $\epsilon\to0$ the tunneling rate Γ reduces to the $\epsilon=0$ result, Eq. (14) in CL.

We now examine the self-consistency of the above procedure. From (10) we deduce that $\langle t\rangle\Gamma=O(\Delta^2/\omega_c^2)\ll1$ irrespective of how large T, ϵ, and Δ are relative to one another. Thus the dilute-blip approximation is self-consistent.

Before using (3) to express (10) back in terms of

the original double-well parameters, we rederive the $T=0$ tunneling rate using an *imaginary*-time approach.[13] Consider the partition function for the Hamiltonian (1) expressed as a path integral over functions $\sigma_z(\tau)=\pm 1$, $\{x_\alpha(\tau)\}$, with the imaginary time τ running from 0 to β. After the performing of the oscillator path integrals and the scaling of all times by ω_c, $\tau \to \tau' = \omega_c \tau$, the partition function is given by

$$Z \sim \sum_{n=0}^{\infty}\left(\frac{\Delta}{2\omega_c}\right)^{2n}\int_{\tau_{2n-1}}^{\beta\omega_c} d\tau_{2n-1}\cdots\int_0^{\tau_2} d\tau_1 \exp(-S), \tag{11}$$

with the action

$$S=\frac{\epsilon}{2\omega_c}\int_0^{\beta\omega_c} d\tau\, \sigma_z(\tau)+\frac{\alpha}{8}\int_0^{\beta\omega_c} d\tau \int_{-\infty}^{\infty} d\tau' \frac{[\sigma_z(\tau)-\sigma_z(\tau')]^2}{(1+|\tau-\tau'|)^2}. \tag{12}$$

Here $\tau_1, \ldots, \tau_{2n}$ denote the times that $\sigma_z(\tau)$ jumps from one state $(+,-)$ to the other $(-,+)$. This partition function is equivalent to that of a one-dimensional inverse square Ising model in an external field ϵ, and for $\alpha>1$ is spontaneously magnetized.[14] Away from the critical region near $\alpha=1$ [of width $(\Delta/\omega_c)^2$] and in the limit $\Delta/\omega_c \ll 1$ the bulk phases are effectively frozen with negligible internal fluctuations. It is in precisely such a limit that a droplet calculation is expected to be valid.

Consider then a single droplet configuration of the path, $\sigma_z(\tau)$, equal to $+1$ everywhere except a region of length τ equal to -1. The dimensionless droplet energy $U(\tau)$, obtained from the action S, is given by

$$U(\tau)=2\alpha\ln(1+\tau)-(\epsilon/\omega_c)\tau. \tag{13}$$

This function has a maximum at $\tau_0=2\alpha(\epsilon/\omega_c)^{-1}-1$ which corresponds to the "critical droplet." One naively expects the decay rate into the stable phase to be proportional to $\exp[-U(\tau_0)]$. This is in fact the case; however, to obtain the correct prefactor we follow the procedure developed by Langer.[5] Since the interaction between droplets falls off as τ^{-2} the partition function (in the metastable phase) can be well approximated by an ideal gas of such droplets,

$$Z(\beta) \sim \sum_{n=0}^{\infty}\frac{(\beta\omega_c)^n}{n!}(\Delta/2\omega_c)^{2n}\left(\int_0^{\beta\omega_0} d\tau\, e^{-U(\tau)}\right)^n. \tag{14}$$

This procedure is valid since the typical separation between droplets (i.e., the tunneling time which emerges below) is much larger than the critical radius τ_0. After exponentiating (14) and taking $\beta\to\infty$ we find the ground-state energy to be

$$E_0=-\frac{\Delta^2}{4\omega_c}\int_0^{\infty} d\tau\, e^{-U(\tau)}. \tag{15}$$

This integral is formally divergent and a standard analytic continuation must be used. The procedure[5,6] is to carry the integration contour along the real axis to the saddle point at τ_0, at which point it is deformed into the complex plane down the direction of steepest descent. This introduces an imaginary part in E_0. Associating a tunneling rate with $2\,\mathrm{Im}E_0/\hbar$ gives complete agreement[15] with the $T=0$ real-time result which follows from (10).

Although the imaginary-time calculation (using the system's partition function) gives the correct decay rate, it is by no means obvious that this is a general feature of all decay problems. In particular, for *classical* systems the dynamics is not specified by the partition function and a given "imaginary-time" calculation is not necessarily appropriate for the dynamics of interest. For the *quantum* system considered here, however, agreement between the two methods is somewhat less surprising, since the partition function retains some of the noncommuting aspects of the dynamical variables. Such agreement is an interesting new result and lends credence to the imaginary-time approach (at least when quantum coherence effects are unimportant).

We finally express the tunneling rate back in terms of the original double-well parameters by inserting the effective level splitting $\Delta(\omega_c)$ (3) into the two-state results (10). The result is

$$\Gamma=g^2(\alpha,v_0)\frac{\Delta_0^2}{2\omega_0}\left(\frac{2\pi T}{\hbar\omega_0}\right)^{2\alpha-1}\frac{\cosh(\frac{1}{2}\beta\epsilon)}{\Gamma(2\alpha)}|\Gamma(\alpha+i\beta\epsilon/2\pi)|^2. \tag{16}$$

Notice that as required the arbitrary cutoff frequency ω_c has dropped out of the calculation.[16] For $\alpha>1$, $\Delta_0 \ll \omega_0$, and $\epsilon, T \ll \omega_b$, (16) is what we believe to be the exact leading tunneling rate for a system in a biased double well, coupled to an Ohmic spectrum of oscillators. For $T \ll \epsilon$ an asymptotic expansion of the Γ function gives

$$\Gamma=\Gamma(T=0)\{1+\pi^2\times\tfrac{1}{3}[\alpha(2\alpha-1)(2\alpha-2)](T/\epsilon)^2+O((T/\epsilon^4)\}, \tag{17}$$

$$\Gamma(T=0)=g^2(\alpha,v_0)\frac{\pi}{2}\frac{\Delta_0^2}{\omega_0}\frac{(\epsilon/\hbar\omega_0)^{2\alpha-1}}{\Gamma(2\alpha)}. \tag{18}$$

For larger α, we have $g \sim (\alpha/v_0)^\alpha$, which cancels the leading large-α behavior of the gamma function in (18). Hence in this limit the $T=0$ tunneling rate is suppressed exponentially in α. Caldeira and Leggett[1] also found an exponential dependence on α for the decay rate from a metastable well into the continuum. However, since (18) only applies to a bounded double well a precise comparison between these results is not possible.

At low temperatures (17) gives a tunneling enhancement[17] which varies as $(T/\epsilon)^2$. It is instructive to contrast this with a prediction based entirely on equilibrium considerations. Consider the equilibrium density matrix, $\rho_{\rm eq}(q)$, for a coordinate q in a harmonic-oscillator potential coupled to a bath. It has been suggested that the tail of $\rho_{\rm eq}$ can perhaps be associated with the tunneling rate out of a metastable well, $\Gamma \sim \rho_{\rm eq}(q_0)$. For an Ohmic bath this predicts a low-temperature enhancement varying as $v_0(T/\omega_0)^2$. Although this term is also proportional to T^2 it is down by order $(\epsilon/\omega_0)^2$ relative to our result (17). Such terms were ignored from the start of our calculation since truncating to the two-state system forced us to work in the limit $\epsilon, T << \omega_b \leq \omega_0$. Consequently it is not possible for us to determine whether a term of the form $v_0(T/\omega_0)^2$ would actually be present if higher-order corrections were included. We can only conclude that (17) is expected to give the correct low-temperature enhancement to *leading* order in $\epsilon, T << \omega_b$.

It is a pleasure to acknowledge stimulating discussions with W. Zwerger, S. Chakravarty, A. Garg, and in particular A. J. Leggett. After this work was completed we received a preprint of similar work by H. Grabert and U. Weiss (preceding Letter). One of us (M.P.A.F.) expresses gratitude for an AT&T Bell Laboratories scholarship. This research was supported in part by the MacArthur Professorship endowed by the John D. and Catherine T. MacArthur Foundation at the University of Illinois under Grant No. 0-6-40129.

[1]A. O. Caldeira and A. J. Leggett, Ann. Phys. (N.Y.) **149**, 374 (1983), and **153**, 445(E) (1984).

[2]A. I. Larkin and Yu. N. Ovchinnikov, Pis'ma Zh. Eksp. Teor. Fiz. **37**, 322 (1983) [JETP Lett. **37**, 382 (1983)]; H. Grabert, U. Weiss, and P. Hanggi, Phys. Rev. Lett. **52**, 2193 (1984); U. Weiss, P. Riseborough, P. Hanggi, and H. Grabert, Phys. Lett **104A**, 10, 492(E) (1984); H. Grabert and U. Weiss, Z. Phys. B **56**, 171 (1984).

[3]See W. Zwerger, Phys. Rev. A **31**, 1745 (1985), for a recent attempt at calculating the decay rate into the continuum using a real-time formulation.

[4]F. Guinea, Phys. Rev. Lett. **53**, 1268 (1984).

[5]J. S. Langer, Ann. Phys. (N.Y.) **41**, 108 (1967).

[6]S. Coleman, in *The Whys of Subnuclear Physics,* edited by A. Zichichi (Plenum, New York, 1979).

[7]A. T. Dorsey, M. P. A. Fisher, M. Wartak, and A. J. Leggett, to be published.

[8]For $\alpha < 1$ we must also satisfy $\Delta_0 << \omega_c$.

[9]S. Chakravarty and A. J. Leggett, Phys. Rev. Lett. **53**, 5 (1984).

[10]If the temperature or bias energy is much larger than $\Delta_r \equiv \Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$ then the dilute-blip approximation can be justified for all $0 < \alpha < 1$.

[11]Equations (9) and (10) also hold for $\alpha < 1$ when T or ϵ is much larger than Δ_r. See Ref. 10.

[12]For a complete discussion of the double-well problem for general spectral densities, which will focus on the conditions necessary for coherent or incoherent behavior, see S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and A. J. Leggett, to be published.

[13]This calculation is similar to one found in Weiss *et al.* (Ref. 2). We emphasize, however, that these authors considered tunneling into the continuum, in contrast to the double-well system which we study here.

[14]S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982); A. J. Bray and M. A. Moore, Phys. Rev. Lett. **49**, 1545 (1982); V. Hakim, A. Muramatsu, and F. Guinea, Phys. Rev. B **30**, 464 (1984).

[15]For the non-Ohmic spectra, $J(\omega) \sim \omega^3$, J. P. Sethna also found agreement between a real- and imaginary-time calculation of the tunneling rate: Doctoral thesis, Princeton University, 1981 (unpublished).

[16]This is no longer true if we work to higher order in ϵ/ω_c, T/ω_c, or ω_c/ω_b, indicating that the reduction scheme to the two-state system is only valid to leading order in $\epsilon, T << \omega_b$.

[17]For a non-Ohmic spectra, $J \sim \omega^s$ with $s < 1$, we find a finite temperature enhancement varying as T^{1+s}. For $s > 1$ the situation is more complicated since coherent oscillations are present (at small T and ϵ) in the double-well system. See Ref. 12 for details.