Quantum Tunneling Rates for Asymmetric Double-Well Systems with Ohmic Dissipation

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(Received 26 December 1984)

The dynamics of an asymmetric double-well system coupled to a heat bath is studied at low temperatures where transitions between the wells involve quantum tunneling. The time evolution of the occupation probabilities of the wells is calculated by means of instanton techniques. For a wide range of parameters incoherent relaxation is found at a rate whose dependence both on temperature and bias is nonanalytic, in general.

PACS numbers: 05.40.+j, 05.30.−d

A great variety of phenomena in physical and chemical sciences are caused by transitions between states that would be stable if there were no thermal and quantal fluctuations. Frequently, the basic physics of such systems can be described by the model of a Brownian particle of mass m moving in a multistable potential $V(q)$. The quantity of interest is then the rate for transitions between adjacent potential wells. At very low temperatures these transitions are caused by quantum mechanical tunneling. Recently, Caldeira and Leggett[1] have shown that tunneling rates are sensitively affected by dissipation leading to a strong suppression of the decay rate at $T=0$. Furthermore, for $T>0$, the temperature dependence of the rate changes drastically in the presence of dissipation.[2]

In this Letter we restrict attention to a slightly asymmetric double-well system where the depths of the potential minima at $\pm q_0/2$ differ by a small bias energy $\hbar\sigma$ (Fig. 1). The barrier between the two wells is assumed to be large so that the tunneling frequency Δ_0 of the undamped and unbiased system is much smaller than the frequency $\omega_0=[V''(\pm q_0/2)/m]^{1/2}$ of small oscillations in each well. The coupling of the tunneling coordinate to its environment gives rise to dissipation. Specifically, we consider an environmental coupling leading in the classical limit to the familiar equation of motion $m\ddot{q}+\eta\dot{q}+\partial V/\partial q=0$. This case of Ohmic dissipation presents many special features[3,4] and it arises, e.g., in the phenomenological description of Josephson systems. Thus our results should apply to the tunneling of the magnetic flux embraced by a SQUID ring,[5] a problem which has attracted a great deal of theoretical and experimental interest recently. Furthermore, for the range of parameters where the relaxation is exponential in time (see below), the results can also be used to describe the motion of particles in distorted periodic potentials with Ohmic dissipation.[6]

We examine the dynamics of a system which at time $t=0$ starts out, say, from the left-hand well. This may be the upper or lower well, according as σ is positive or negative. At later times the system is then found again in the left-hand well with probability $P_{--}(t)$ or it occupies the right-hand well with probability $P_{+-}(t)=1-P_{--}(t)$. The dynamics of tunneling transitions is characterized conveniently by $P(t)=P_{--}(t)-P_{+-}(t)$. In the absence of dissipation, this quantity shows oscillatory behavior $P(t)=\sigma^2/\Delta_b^2+(\Delta_0^2/\Delta_b^2)\cos(\Delta_b t)$ where $\Delta_b=(\Delta_0^2+\sigma^2)^{1/2}$ is the tunneling frequency of the undamped system with bias $\hbar\sigma$. For zero bias, the influence of Ohmic dissipation on $P(t)$ has been studied in detail by Chakravarty and Leggett.[4] In terms of the dimensionless dissipation coefficient

$$\alpha=\eta q_0^2/2\pi\hbar, \tag{1}$$

they find at zero temperature damped oscillations of $P(t)$ for $0<\alpha<\frac{1}{2}$ and incoherent relaxation for $\frac{1}{2}<\alpha<1$. For $\alpha>1$, tunneling transitions are suppressed completely at zero temperature[3] while for finite temperatures $P(t)$ relaxes exponentially at a rate proportional to $T^{2\alpha-1}$. Our calculation reproduces these predictions as special cases.

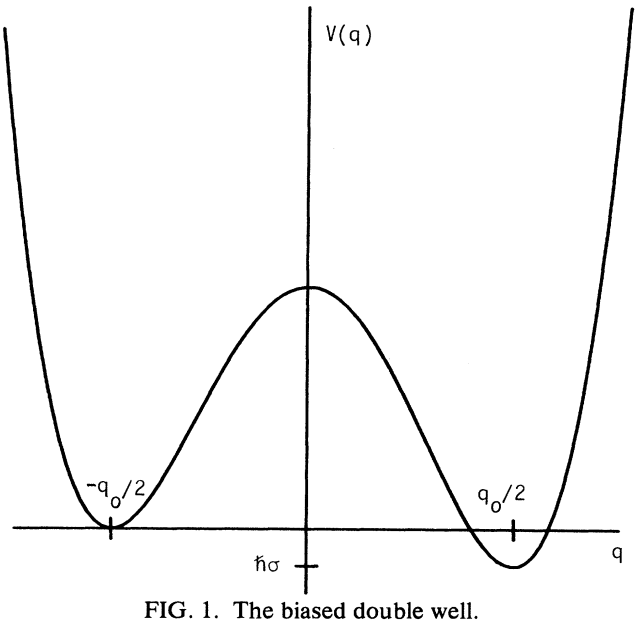

FIG. 1. The biased double well.

We restrict attention to the region where both k_BT and $\hbar|\sigma|$ are small compared to $\hbar\omega_0$. Then the double well behaves effectively like a biased two-state system, and the dynamics of $P(t)$ depends essentially on three dimensionless parameters: $k_BT/\hbar\omega_0$, σ/Δ_0, and α. Since $\Delta_0 \ll \omega_0$, all parameters may vary from 0 to values much larger than 1. The calculation of $P(t)$ is based on functional integral techniques which are convenient because they allow the inclusion of dissipation as a nonlocal term (influence functional) in the effective action.[7,8] In the functional integral expression for $P(t)$, tunneling transitions between the wells are related to the contribution of instanton (or "kink") trajectories connecting the ground states in the two wells. In the dissipative case the instanton interactions must be treated carefully. An appropriate method, which is an extension of the approach developed recently by Zinn-Justin[9] for undamped systems, will be presented here.

Let $w(q,0)$ be the probability distribution of the coordinate of the Brownian particle measured at $t=0$. Then the probability distribution $w(q,t)$ at time t may be written as a double functional integral[7,8]

$$w(q_f,t)=\int D[q]D[q']\exp(i\hbar^{-1}\{S[q]-S[q']\}+\hbar^{-1}\Phi[q,q])\,w(q_i,0), \tag{2}$$

where the integral is over all paths $q(\tau)$, $q'(\tau)$, $0\le\tau\le t$ with $q(0)=q'(0)=q_i$, $q(t)=q'(t)=q_f$, and where q_i is integrated over;

$$S[q]=\int_0^t d\tau\,\{\tfrac{1}{2}m\dot{q}^2-V(q)\} \tag{3}$$

is the action of an undamped particle, and $\Phi[q,q']$ is the Feynman-Vernon influence functional[7,8] describing the frictional influence of the environment. For Ohmic dissipation $\Phi[q,q']$ can be written as

$$\Phi[q,q']=\int_0^t d\tau\int_0^\tau ds\,\{\dot{q}(\tau)-\dot{q}'(\tau)\}\{Q(\tau-s)\dot{q}(s)-Q^*(\tau-s)\dot{q}'(s)\}, \tag{4}$$

where[10]

$$Q(\tau)=\frac{\eta}{\pi}\ln\left[\frac{\hbar\beta\omega_0}{\pi}\sinh\left(\frac{\pi\tau}{\hbar\beta}\right)\right]+\frac{1}{2}i\eta. \tag{5}$$

Now, let $w(q,0)$ be centered around $-q_0/2$ which is the case for an ensemble of systems initially in the left-hand well. Since the probability distribution $w(q,t)$ will be centered around $+q_0/2$ and $-q_0/2$, it is sufficient to consider the occupation probabilities $P_{+-}(t)=\int_0^\infty dq\,w(q,t)$, $P_{--}(t)=1-P_{+-}(t)$ of the two wells. For $k_BT\ll\hbar\omega_0$, $|\sigma|\ll\omega_0$, excitations in either well are negligible, and the contribution of the functional integral (2) to $P_{+-}(t)$ arises from multi-instanton paths which start at $-q_0/2$, traverse the potential barrier possibly several times, and end at $+q_0/2$.

The path probability of a multi-instanton trajectory can be decomposed into a product of various factors: a factor $i\Delta/2$ for every single instanton, an interaction factor for every pair of instantons, and a bias factor for every sojourn in the right-hand well. Because of the dissipative self-interaction of an instanton, Δ is diminished as compared to the tunneling frequency Δ_0 of an undamped system with zero bias. To determine the instanton-pair interaction factors and the bias factors we may approximate the paths by

$$\dot{q}(\tau)=\sum_{j=1}^{2n+1}(-1)^{j+1}q_0\delta(\tau-t_j),$$

$$\dot{q}'(s)=\sum_{k=1}^{2m+1}q_0\delta(s-t_k').$$

The flip times t_j and t_k' are the collective coordinates of the problem. $P_{+-}(t)$ is obtained by integration of the multi-instanton path probability over the region $0<t_1<\ldots<t_{2n+1}\le t$, $0\le t_1'<\ldots<t_{2m+1}'\le t$, and summing over all positive numbers n and m.

Following Chakravarty and Leggett,[4] we rewrite this result in the form of the contribution of a *single* functional integral by embedding the flip times t_j,t_k' into a single interval $[0,t]$. This transformation is straightforward but tedious, and it leads for $P(t)=1-2P_{+-}(t)$ to the formula

$$P(t)=\sum_{n=0}^{\infty}(-1)^n\Delta^{2n}\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1\,F_{2n}(t_1,\ldots,t_{2n}), \tag{6}$$

where

$$F_{2n}=\exp\left(-\sum_{j=1}^{n}S_j\right)\cos(\pi\alpha)^{n-1}2^{-n}\sum_{\{\zeta_j=\pm1\}}\cos\left(\zeta_1\pi\alpha-\sigma\sum_{j=1}^{n}\zeta_j\tau_j\right)\exp\left(\sum_{\substack{j,k=1\\k>j}}^{n}\Lambda_{jk}\zeta_j\zeta_k\right), \tag{7}$$

and where $\tau_j=t_{2j}-t_{2j-1}$. The functions S_j and Λ_{jk} are given by[11]

$$S_j=S(\tau_j), \tag{8}$$

$$\Lambda_{jk}=S(t_{2k}-t_{2j-1})+S(t_{2k-1}-t_{2j})-S(t_{2k}-t_{2j})-S(t_{2k-1}-t_{2j-1}), \tag{9}$$

where $S(\tau)=2\alpha\ln[\pi^{-1}\hbar\beta\omega_0\sinh(\pi\tau/\hbar\beta)]$.

In (7) the $2n$ instantons are arranged in pairs of neighboring instantons which flip at times t_{2j-1} and t_{2j}. These pairs may be looked upon as "bounces" of length τ_j. For each bounce, (7) contains a factor of the form $w(\tau)=\exp[-S(\tau)]\cos(\sigma\tau-\phi)$, where the phase ϕ depends on the other bounces. Hence, very long bounces are suppressed. At zero temperature, where the bounce length is largest, it can be estimated as[12] $\tau\simeq 2\alpha/|\sigma|$. It will be shown below self-consistently that for a wide range of parameters the relaxation rate Γ is small compared with τ^{-1}. On this assumption the bounces form a "dilute gas," and the exponential factor under the summation sign may be set equal to unity. In this approximation[13] we then find

$$F_{2n}=\exp\left(-\sum_{j=1}^{n}S_j\right)\cos(\pi\alpha-\sigma\tau_1)\prod_{j=2}^{n}\cos(\pi\alpha)\cos(\sigma\tau_j), \tag{10}$$

and (6) can now be summed explicitly by means of an appropriate extension of Zinn-Justin's method[9] to yield

$$P(t)=-\frac{1}{2\pi i}\int_{-i\infty-\epsilon}^{i\infty-\epsilon}\frac{d\lambda}{\lambda}e^{-\lambda t}\frac{\lambda+i\sin(\pi\alpha)[J_+(\lambda)-J_-(\lambda)]}{\lambda+\cos(\pi\alpha)[J_+(\lambda)+J_-(\lambda)]}, \tag{11}$$

where

$$J_\pm(\lambda)=-\frac{\Delta^2}{2\omega_0}\left(\frac{\hbar\beta\omega_0}{2\pi}\right)^{1-2\alpha}\Gamma(1-2\alpha)\frac{\Gamma(\alpha-\hbar\beta(\lambda\pm i\sigma)/2\pi)}{\Gamma(1-\alpha-\hbar\beta(\lambda\pm i\sigma)/2\pi)}. \tag{12}$$

This is the central result of our work.

Let us first study the high-temperature approximation of (11) which is obtained by substituting $J_\pm(0)$ for $J_\pm(\lambda)$. Then the integrand in (11) has two poles at $\lambda=0$ and $\lambda=\Gamma$ where

$$\Gamma=\frac{1}{2}\frac{\Delta^2}{\omega_0}\left(\frac{\hbar\beta\omega_0}{2\pi}\right)^{1-2\alpha}\cosh(\hbar\beta\sigma/2)\frac{|\Gamma(\alpha+i\hbar\beta\sigma/2\pi)|^2}{\Gamma(2\alpha)}. \tag{13}$$

Closing the integration contour in the right-hand half-plane we find

$$P(t)=-\tanh(\hbar\beta\sigma/2)+[1+\tanh(\hbar\beta\sigma/2)]\exp(-\Gamma t). \tag{14}$$

This result describes incoherent relaxation to equilibrium with the tunneling rate Γ. The expression (13) for the rate can be substantiated from an "imaginary-time" calculation[10] based on the methods of Refs. 1 and 2.

To study the range of validity of (13) and (14), we first examine the limit $\sigma=0$ where (13) reduces to

$$\Gamma=\frac{\sqrt{\pi}}{2}\frac{\Delta^2}{\omega_0}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\left(\frac{\pi k_BT}{\hbar\omega_0}\right)^{2\alpha-1}. \tag{15}$$

Hence, for $\alpha>1$, $\hbar\beta\Gamma/2\pi$ is of order $\Delta^2/\omega_0^2\ll 1$ for all temperatures, and the high-temperature approximation is valid down to $T=0$. On the other hand, in the limit $T=0$, we obtain

$$\Gamma=\frac{\pi}{2}\frac{\Delta^2}{\omega_0}\frac{1}{\Gamma(2\alpha)}\left(\frac{|\sigma|}{\omega_0}\right)^{2\alpha-1}. \tag{16}$$

Consequently, even for very small $|\sigma|$, $2\alpha\Gamma/|\sigma|$ is always of order Δ^2/ω_0^2 in the region $\alpha>1$, so that the dilute bounce-gas approximation holds. This indicates, as can be shown more precisely, that in the region $\alpha>1$ the results (13) and (14) hold for *all* $\hbar|\sigma|$ and k_BT small compared with $\hbar\omega_0$. The limiting formulas (15) and (16) for the tunneling rate Γ have previously been derived by Chakravarty and Leggett[4] and by Weiss *et al.*,[12] respectively. Note that at zero temperature $P(t)=2\exp(-\Gamma t)-1$ if the particle starts out from the upper well ($\sigma>0$) and $P(t)\equiv 1$ if it starts from the lower well ($\sigma<0$). Thus, at $T=0$ and for $\alpha>1$ there are only transitions from the upper to the lower well.

At zero temperature the functions $J_\pm(\lambda)$ read

$$J_\pm(\lambda)=-\tfrac{1}{2}\Delta^2\omega_0^{-2\alpha}\Gamma(1-2\alpha)(-\lambda\mp i\sigma)^{2\alpha-1}. \tag{17}$$

Hence, in the presence of a bias, $\hbar\beta\Gamma/2\pi$ need not necessarily be small to be permitted to disregard the λ dependence of $J_\pm(\lambda)$; rather, a small $\Gamma/|\sigma|$ is sufficient. As a consequence of this fact one finds that (13), (14), and (16) also hold in the region $\frac{1}{2}<\alpha<1$ for all temperatures provided that the bias is not too small. The minimal bias required vanishes for large enough temperatures and is largest at $T=0$ where

$$|\sigma|\gg\omega_0\left(\frac{\pi\alpha\Delta^2}{\Gamma(2\alpha)\omega_0^2}\right)^{1/2(1-\alpha)} \tag{18}$$

should hold. For very small $|\sigma|$ the relaxation of $P(t)$ is nonexponential at zero temperature.[4]

In the region of parameters not covered by the high-temperature approximation (14), the formula (11) cannot be evaluated in closed form, except for the case $T=0$ and $\sigma=0$ where we find for $\alpha<1$ by virtue of (17)

$$P(t)=E_{2(1-\alpha)}(-y^{2(1-\alpha)}), \tag{19}$$

where $E_\nu(z)$ is the Mittag-Leffler function,[14] and where

$$y=\Delta_{\text{eff}}t\equiv[\cos(\pi\alpha)\Gamma(1-2\alpha)]^{1/2(1-\alpha)}(\Delta_0/\omega_0)^{\alpha/(1-\alpha)}\Delta_0 t. \tag{20}$$

The results of Chakravarty and Leggett[4] are now readily obtained from the known properties of the Mittag-Leffler function.[14] For $\alpha<\frac{1}{2}$ the function (19) has a damped oscillatory part and an incoherent part with a power-law decay. For $\frac{1}{2}<\alpha<1$ the function decays montonically.

It should be noted that the dilute bounce-gas approximation made to derive (19) is not strictly valid for $\alpha<1$, $T=0$, $\sigma=0$. However, the deviation $\Delta P(t)$ of $P(t)$ from (19) is very small.[4] This suggests that (11) gives a very reasonable approximation for $P(t)$ in the whole range of parameters.

The most likely system for an experimental test of these predictions is a SQUID,[5] in which the flux through the ring plays the role of the coordinate. The bias may be controlled by means of an external flux and $P(t)$ can be determined from the observation of fluxoid quantum transitions.

At the time of writing of this Letter we learned from M. Fisher and A. Dorsey (following Letter) that they have obtained results similar to the ones discussed here.

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[10]This expression is the limit as $\omega_c t\rightarrow\infty$ of the expressions given in Eqs. (12) and (13) of Ref. 4.

[11]As compared to Ref. 4 we have absorbed a factor $q_0^2/\pi\hbar$ into the definitions of S_j and Λ_{jk}. Further, it should be noted that all except the nearest-neighbor phase factors X_{jk} defined in Eq. (6c) of Ref. 4 vanish for strictly Ohmic dissipation, i.e., in the limit $\omega_c t\rightarrow\infty$ of Eq. (12) in Ref. 4.

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