Quantum Tunneling at Low Temperatures: Results for Weak Damping

E. Freidkin and P.S. Riseborough
Department of Physics, Polytechnic Institute of New York, Brooklyn, New York, USA

P. Hänggi
Lehrstuhl für Theoretische Physik, Universität Augsburg, Federal Republic of Germany

We investigate the rate at which a particle decays out of a metastable potential well by quantum tunneling. We calculate the leading corrections to the exponent and the prefactor of the rate, due to coupling to the heat bath and finite temperatures. Since the results are essentially equivalent to those employing the transition state assumption, namely maintaining thermal equilibrium, we argue for the lower on the damping strength above which these results should be valid. These results are in good accord with recently reported experiments.

I. Introduction

The decay of a metastable state of a system to other states is a problem of considerable physical interest. Most of the conventional theories of decay invoke the notion that decay only occurs once spontaneous fluctuations of sufficiently large amplitude have appeared. The theories imply that once these fluctuations have occurred, the system will continuously evolve in time until a new state is reached. If these fluctuations are thermal in origin, they result in the familiar Arrhenius law of thermally activated decay [1].

At low temperatures, the Arrhenius factor does become extremely small, and other possible mechanisms of decay might be important in this temperature regime. Bailin and Love [2], have investigated the possibility that quantum tunnelling may be responsible for the decay of metastable states in superfluid ^{3}He. Caldeira and Leggett [3] have extended this notion to describe the decay of other macroscopic states by quantum tunnelling.

Most of the recent investigations of decay by quantum tunnelling use Feynman's functional integral formulation of quantum mechanics, as applied by Langer [4] and Coleman [5].

Caldeira and Leggett [3] have investigated the decay rate of a metastable state at $T=0$, in the two extreme limits of weak damping and infinitely large damping. The generalization of these results to finite temperatures has lead to many different and contradicting results, some of these results even do not reduce to those in Ref. 3 in the limit of zero temperature.

We shall in this article, study the low damping limit in order to shed some light onto many of the results in the existing literature. We find results that do agree with the exact analytical results of Affleck [6], at finite temperatures and zero damping. The results for the zero temperature, small damping are in agreement with the results in Ref. 3, while for finite low temperatures and finite damping the leading temperature dependence of the decay rate is in perfect agreement with the general results obtained by Grabert, Weiss and Hänggi [7].

This is in direct contrast to several other articles on the subject [10].

In Sect. II, we shall very briefly outline the general formalism of the approach. The decay rate is calculated to be of the form

$$\Gamma = A \exp[-B]. \tag{1.1}$$

The exponential term will be calculated in Sect. III, and the prefactor A is calculated in Sect. IV. We discuss our results in Sect. V.

II. General Formulation

We consider a system which consists of a particle of mass M, which is described by a coordinate q and moves in a potential field $V(q)$. The particle is coupled to the normal modes of a thermal reservoir.

The Lagrangian of the system is described by

$$\mathscr{L}=\frac{M}{2}\left(\frac{\partial q}{\partial t}\right)^2-V(q)+\sum_{n=1}^{N}\left\{\frac{m_n}{2}\left(\frac{\partial \varphi_n}{\partial t}\right)^2-\frac{m_n\omega_n^2}{2}\varphi_n^2\right\}-\sum_{n=1}^{N}\lambda_n\varphi_n q-\sum_{n=1}^{N}\frac{\lambda_n^2}{2m_n\omega_n^2}q^2 \tag{2.1}$$

where the first two terms represent the Lagrangian of the particle moving in the effective potential $V(q)$. The second two terms represent the Lagrangian of the normal modes of the thermal reservoir. The last two terms represent the coupling between the particle and the thermal reservoir. The last term is included to ensure that the potential $V(q)$ will coincide with the effective potential. This type of Lagrangian was first considered by Ullersma [8].

The variables of the thermal reservoir can be eliminated by standard methods. The motion of the particle coupled to the heat bath can then be described by an effective action $S_{\text{eff}}[q(t)]$

$$S_{\text{eff}}[q(t)]=\int_{-\frac{T}{2}}^{\frac{T}{2}}\mathrm{d}t\left[\frac{M}{2}\left(\frac{\partial q}{\partial t}\right)^2-V(q)\right]+\frac{1}{2}\int_{-\frac{T}{2}}^{\frac{T}{2}}\mathrm{d}t\int_{-\frac{T}{2}}^{\frac{T}{2}}\mathrm{d}t'\,K(t-t')[q(t)-q(t')]^2. \tag{2.2}$$

The first term represents the motion of the particle in an effective potential. The second term represents the dynamical aspects of coupling to the environment. The function $K(t)$ is given by

$$K(t)=\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}J(\omega)\{[1+N(\omega)]\,\mathrm{e}^{\mathrm{i}\omega t}+N(\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}\}$$

where $N(\omega)$ is the Bose-Einstein distribution function.

The properties of the particle-thermal reservoir coupling are contained entirely in the function

$$J(\omega)=\frac{\pi}{2}\sum_{n=1}^{N}\frac{\lambda_n^2}{m_n\omega_n}\delta(\omega-\omega_n)$$

the spectral density.

As Sethna [9] pointed out, considerable advantage may be gained by analytically continuing from real times to imaginary times $t\to i\tau$, since this eliminates troublesome oscillating behavior in $K(t)$. After analytic continuation to imaginary times, one finds

$$-iS_{\text{eff}}[q(\tau)]=\int_{-\frac{\theta}{2}}^{\frac{\theta}{2}}\mathrm{d}\tau\left[\frac{M}{2}\left(\frac{\partial q}{\partial \tau}\right)^2+V(q)\right]+\frac{1}{2}\int_{-\frac{\theta}{2}}^{\frac{\theta}{2}}\mathrm{d}\tau\int_{-\infty}^{\infty}\mathrm{d}\tau'\,k(\tau-\tau')[q(\tau)-q(\tau')]^2 \tag{2.3}$$

where

$$k(\tau)=\int_0^{\infty}\frac{\mathrm{d}\omega}{2\pi}J(\omega)\,\mathrm{e}^{-\omega|\tau|}$$

and θ is related to the inverse temperature of the heat bath through

$$\theta=\frac{\hbar}{K_B T}.$$

The paths $q(\tau)$ have been periodically continued outside the region $-\frac{\theta}{2}<\tau<\frac{\theta}{2}$. Therefore, in the expression for the effective action, only periodic paths

$$q(\tau+\theta)=q(\tau)$$

are to be considered.

The decay rate is given in terms of the space diagonal, imaginary time Greens function. The Greens function is calculated using Feynman's functional integral formulation of quantum mechanics. The functional integrals are calculated by a generalization of the method of steepest descents, as applied by Langer [4] and Coleman [5].

We shall specialize our considerations to the case considered by Caldeira and Leggett [3], that of a cubic potential (see Fig. 1)

$$V(q)=M\left\{\frac{\omega_0^2 q^2}{2}-\frac{u q^3}{3}\right\}$$

and ohmic dissipation

$$J(\omega)=M\eta\omega.$$

In the next section we shall examine the trajectories which extremize the action $S[q(\tau)]$ and evaluate the exponential term in the decay rate. The discussion of the prefactor is delayed until Sect. IV.

III. The Extremal Trajectories

The action $S[q(\tau)]$ is a functional of the trajectories $q(\tau)$. The trajectories for which the action is extremal, i.e. $\delta S[q(\tau)]=0$, is determined by the Euler-Lagrange equation

$$-M\ddot{q}(\tau)+\frac{\partial V}{\partial q}+\frac{\eta M}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\tau'\frac{\partial q(\tau')}{\partial \tau'}\cdot\left\{\frac{1}{\tau-\tau'+i\delta}+\frac{1}{\tau-\tau'-i\delta}\right\}=0. \tag{3.1}$$

This equation has two trivial solutions. Only the solution $q(\tau)=0$, with the corresponding action $S(0)=0$, enters into the discussion of the low temperature decay rate. The other solution $q(\tau)=\frac{\omega_0^2}{u}$ which corresponds to the top of the potential barrier has an action $S\left(\frac{\omega_0^2}{u}\right)=V_{\max}\theta$ which is intimately connected to the high temperature Arrhenius decay rate [7].

The non-trivial solution of the Euler-Lagrange Eq. (3.1) is well known for $\eta=0$. This simplifies at $T=0$, to yield

$$q_B^{(0)}(\tau)=\frac{3}{2}\frac{\omega_0^2}{u}\operatorname{sech}^2\frac{\omega_0\tau}{2}$$

and the corresponding action is

$$S_B=\frac{6}{5}M\omega_0\left(\frac{\omega_0^2}{u}\right)^2.$$

We shall calculate the corrections to these results to first order in the dissipation η.

We shall decompose $q_B(\tau)$ into terms representing the higher order corrections

$$q_B(\tau)=\sum_{n=0}^{\infty}q_B^{(n)}(\tau).$$

The linear term in η is found from the equation

$$-\ddot{q}_B^{(1)}(\tau)+\omega_0^2 q_B^{(1)}(\tau)-2u\,q_B^{(0)}(\tau)\,q_B^{(1)}(\tau)+\frac{\eta}{2\pi}\int_{-\infty}^{\infty}d\tau'\frac{\partial q_B^{(0)}(\tau')}{\partial\tau'}\left\{\frac{1}{\tau-\tau'+i\delta}+\frac{1}{\tau-\tau'-i\delta}\right\}=0. \quad (3.2)$$

The inhomogeneous term can be represented as

$$f(\tau)=3\omega_0^2\left(\frac{\omega_0^2}{u}\right)\left(\frac{\eta}{2\omega_0}\right)\cdot\int_0^{\infty}\frac{dk}{\pi}\cos\frac{k\omega_0\tau}{2}\,k\left\{\frac{\frac{\pi k}{2}}{\sinh\frac{\pi k}{2}}\right\}. \quad (3.3a)$$

The solution of the linear inhomogeneous equation can be found by standard methods since all the solutions of the homogeneous eigenvalue equation are known (cf. Appendix 1). In particular, one finds a solution of the homogeneous form of Eq. (3.2) is given by

$$\varphi_C(\tau)=\operatorname{sech}^2\frac{\omega_0\tau}{2}\tanh\frac{\omega_0\tau}{2}. \quad (3.3b)$$

A second solution of the homogeneous version of Eq. (3.2) can be found by integration as

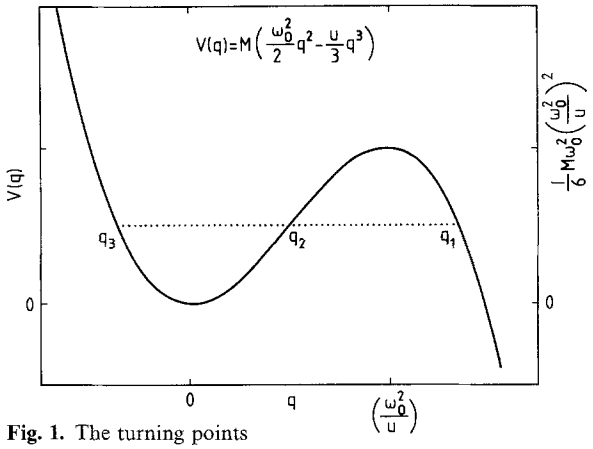

Fig. 1. The turning points

$$\varphi_D(\tau)=\frac{1}{8}\left\{2\cosh^2\frac{\omega_0\tau}{2}+5+15\operatorname{sech}^2\frac{\omega_0\tau}{2}\left(\frac{\omega_0\tau}{2}\tanh\frac{\omega_0\tau}{2}-1\right)\right\}. \quad (3.3c)$$

The Wronskian of these solutions is $\frac{\omega_0}{2}$. Hence the general solution of Eq. (3.2) is

$$q_B^{(1)}(\tau)=\frac{2}{\omega_0}\left[\varphi_D(\tau)\int_0^{\tau}d\tau'\,\varphi_C(\tau')\,f(\tau')-\varphi_C(\tau)\int_0^{\tau}d\tau'\,\varphi_D(\tau')\,f(\tau')\right]+C\varphi_C(\tau)+D\varphi_D(\tau)$$

where C and D are arbitrary constants. We fix C and D by the requirement that the bounce trajectory be an even function of τ, and that it vanishes as $\tau\to\infty$. Thus

$$q_B^{(1)}(\tau)=\frac{2}{\omega_0}\left[\varphi_D(\tau)\int_{-\infty}^{\tau}\varphi_C(\tau')\,f(\tau')\,d\tau'-\varphi_C(\tau)\int_0^{\tau}\varphi_D(\tau')\,f(\tau')\,d\tau'\right]. \quad (3.3d)$$

We shall now argue that this contribution $q_0^{(1)}(\tau)$ does not contribute to the action S_B in first order in the damping. Nevertheless, we shall require $q_B^{(1)}(\tau)$ in Sect. IV when we evaluate the prefactor.

The action S_B for this trajectory, when evaluated to first order in η, is given only by the dissipative part of the action. Since the undamped bounce trajectory extremizes the undamped action, the undamped action will remain unaltered, to first order in η, if the damped bounce trajectory is substituted into the expression. Therefore, the first order corrections to the action are contained entirely within the dissipative part of the action, and since this explicitly contains a factor of η it must be calculated using the undamped bounce.

The first order corrections to the action originate entirely from the dissipative term. The most convenient way of evaluating this is found by expressing the bounce trajectory in terms of its Fourier components. The dissipative part of the action is evaluated in the form

$$\pi\eta \sum_{n=-\infty}^{\infty} |n|\, q_B^{(0)}(n)\, q_B^{(0)}(-n). \tag{3.4}$$

This need only be calculated with the Fourier components of the undamped bounce, since it is already of order η. These are found to be given by

$$q_B^{(0)}(n) = 3\frac{\omega_0^2}{u}\left(\frac{2\pi}{\omega_0\theta}\right)\left\{\frac{\left(\frac{2\pi n}{\omega_0\theta}\right)}{\sinh\left(\pi\left(\frac{2\pi n}{\omega_0\theta}\right)\right)}\right\}$$

(cf. Appendix 2). (3.5)

The summation over n can be performed using the Euler-McLaurin summation formulae.

We find that the total action can be written as

$$S_B(\theta) = \frac{36}{5}\frac{V_{\max}}{\omega_0}\left[1+\left(\frac{\eta}{2\omega_0}\right)\right.$$
$$\left.\cdot\left\{\frac{45\xi(3)}{\pi^3} - \frac{5}{2\pi}\left(\frac{2\pi}{\omega_0\theta}\right)^2 - \frac{\pi}{12}\left(\frac{2\pi}{\omega_0\theta}\right)^4 + \ldots\right\} + \ldots\right]. \tag{3.6}$$

The zero temperature limit yields the action calculated by Caldeira and Leggett [3]. This is in disagreement with the zero temperature limit calculated by Zwerger [10].

The effect of temperature is to decrease the action. The temperature dependence is intimately connected with the damping. In the absence of the damping, the action only depends on the temperature exponentially. As seen in the work of Affleck [6], this is due mainly to thermal activation between the virtually bound levels of the metastable potential minima. The presence of the damping procedures a closely packed continuum of levels which can be thermally activated, and therefore results in power laws. We see that the first temperature dependence is of the form T^2. This and the numerical value of the coefficient is in agreement with the general calculation of Grabert, Weiss and Hänggi [7]. By contrast Zwerger [10] has performed quasi-phenomenological calculations with the same model and found only a T^4 dependence.

The exponential term of the decay rate is given by the formula

$$B = [S_B - S_0]/\hbar$$

where S_B is the extremal action evaluated with the bounce trajectory and S_0 is the action evaluated with the trivial trajectory $q(\tau)=0$. The prefactor A is given by the ratio of the eigenvalues of the second variation of the action evaluated about these same trajectories. In the next section we shall evaluate the prefactor.

IV. Fluctuations about the Extrema

An arbitrary path, quite close to an extremal path $\tilde{q}(\tau)$, can be represented in terms of a complete, orthogonal set of functions $\varphi_n(\tau)$ through an expansion

$$q(\tau) = \tilde{q}(\tau) + \sum_{n=1}^{N} C_n \varphi_n(\tau). \tag{4.1}$$

The set of functions $\varphi_n(\tau)$ will be chosen, such that the action is diagonalized up to the terms quadratic in C_n.

$$S[q(\tau)] = S[\tilde{q}(\tau)] + \sum_{n=1}^{N} \frac{\Lambda_n C_n^2}{2} + \ldots. \tag{4.2}$$

The small fluctuations which diagonalize the action, as well as the eigenvalues Λ_n are given by the solutions of the equation

$$-\frac{\partial^2\varphi_n}{\partial\tau^2} + \omega_0^2\varphi_n - 2u\tilde{q}(\tau)\varphi_n + \frac{\eta}{2\pi}\int_{-\infty}^{\infty} d\tau' \frac{\partial\varphi_n(\tau')}{\partial\tau'}$$
$$\cdot\left\{\frac{1}{\tau-\tau'+i\delta} + \frac{1}{\tau-\tau'-i\delta}\right\} = \frac{\Lambda_n}{M}\varphi_n \tag{4.3}$$

with periodic boundary conditions.

The solution of Eq. (4.3) with $\eta=0$, is given in Appendix 1.

The path integral can be approximated in terms of an integral around the extremal paths and the Gaussian fluctuations about those paths. The path integral in the neighborhood of an extremal trajectory $\tilde{q}(\tau)$ can be written as

$$\exp\left[-\frac{S[\tilde{q}(\tau)]}{\hbar}\right]\prod_{n=1}^{N}\int_{-\infty}^{\infty}\frac{dC_n}{(2\pi\hbar)^{\frac{1}{2}}}\exp\left[-\frac{\Lambda_n C_n^2}{2\hbar}\right]. \tag{4.4}$$

Thus the Gaussian fluctuations can be related to the product of eigenvalues.

$$\left\{\prod_{n=1}^{N}\Lambda_n\right\}^{-\frac{1}{2}}. \tag{4.5}$$

The prefactor of the decay rate is related to the ratio of the eigenvalues for the two extremal trajectories

$$\tilde{q}(\tau) = 0$$

and

$$\tilde{q}(\tau)=q_B(\tau).$$

The product over the eigenvalues, which we need to calculate can be written as

$$\prod_{n=1}^{N}\left\{\left(\frac{\Lambda_n^0}{\Lambda_n^B}\right)^{\frac{1}{2}}\right\}.$$

This is rewritten in terms of a product over the bound state eigenvalues (b.s.) times a product over the continuum eigenvalues.

$$=\prod_{\substack{n=1\\ \{\text{b.s.}\}}}^{3}\left\{\left(\frac{M\omega_0^2}{\Lambda_n^B}\right)^{\frac{1}{2}}\right\}\exp\left[-\frac{1}{2}\sum_{n=4}^{\infty}\log_e\frac{\Lambda_n^B}{M\omega_0^2}\right.$$
$$\left.+\frac{1}{2}\sum_{n=1}^{\infty}\log_e\frac{\Lambda_n^0}{M\omega_0^2}\right]$$

where the continuum eigenvalue spectrum starts at $M\omega_0^2$. This can be rewritten in terms of the Green's function as

$$=\prod_{\substack{n=1\\ \{\text{b.s.}\}}}^{3}\left\{\left(\frac{M\omega_0^2}{\Lambda_n^B}\right)^{\frac{1}{2}}\right\}$$
$$\cdot\exp\left[-\frac{\mathrm{Im}}{2\pi}\int_{M\omega_0^2}^{\infty}\mathrm{d}\Lambda\{G^B(\Lambda)-G^0(\Lambda)\}\log_e\frac{\Lambda}{M\omega_0^2}\right]$$

where G^0 is the unperturbed Green's function evaluated with $\tilde{q}(\tau)=0$. Finally, after expressing the G^B in terms of the T matrix, we obtain the form

$$=\prod_{\substack{n=1\\ \{\text{b.s.}\}}}^{3}\left\{\left(\frac{M\omega_0^2}{\Lambda_n^B}\right)^{\frac{1}{2}}\right\}$$
$$\cdot\exp\left[-\int_{M\omega_0^2}^{\infty}\frac{\mathrm{d}\Lambda}{2\pi}\frac{\partial}{\partial\Lambda}\{\delta(\Lambda)\}\log_e\frac{\Lambda}{M\omega_0^2}\right] \tag{4.6}$$

where $\frac{1}{\pi}\frac{\partial}{\partial\Lambda}\{\delta(\Lambda)\}$ is just the change in the continuum density of states expressed in terms of the phase shift $\delta(\Lambda)$.

The bound states produce problems, since one eigenvalue is negative while another is zero. The integration over the coefficient corresponding to the negative eigenvalue eigenfunction is analytically continued to produce a factor of

$$\frac{i}{2}\left(\frac{M\omega_0^2}{|\Lambda_1^B|}\right)^{\frac{1}{2}}. \tag{4.7}$$

The zero eigenvalue eigenfunction represents a Goldstone like mode. It is related to the arbitrariness of the bounce. The zero eigenvalue is replaced by a factor of

$$\frac{\theta}{(2\pi\hbar)^{\frac{1}{2}}}\left\{\int_{-\frac{\theta}{2}}^{\frac{\theta}{2}}\mathrm{d}\tau\left(\frac{\partial q_B}{\partial\tau}\right)^2\right\}^{\frac{1}{2}}(M\omega_0^2)^{\frac{1}{2}} \tag{4.8}$$

by a standard method [4]. This corresponds to an integration over the initial phase of the bounce.

In zeroth order in the dissipation strength ($\eta=0$), one can evaluate the prefactor analytically. This was first done by Affleck [6], using a different method, and later reported by Caldeira and Leggett [3]. We shall reproduce the results here, since it provides the basis for further calculations with non-zero dissipation.

The zeroth order expressions for the phase shift can be obtained by using the solutions φ_n given in Appendix 1. The lowest order phase shift is given by

$$\delta^{(0)}(\Lambda)=2\left\{\tan^{-1}\frac{1}{k}+\tan^{-1}\frac{2}{k}+\tan^{-1}\frac{3}{k}\right\}$$

where

$$\Lambda=M\omega_0^2\left(1+\frac{k^2}{4}\right).$$

This phase shift satisfies Levinson's theorem since there are only three bound states and

$$\frac{1}{\pi}\{\delta^{(0)}(M\omega_0^2)-\delta^{(0)}(\infty)\}=3.$$

On evaluating the continuum contribution to the product in (4.6) we arrive at a factor of 15/2.

$$\exp\left[-\frac{1}{2\pi}\int_{M\omega_0^2}^{\infty}\mathrm{d}\Lambda\frac{\partial}{\partial\Lambda}\{\delta^{(0)}(\Lambda)\}\log_e\frac{\Lambda}{M\omega_0^2}\right]=\frac{15}{2}. \tag{4.9}$$

The two non-zero bound state eigenvalues contribute a factor of

$$\frac{i}{2}\left(\frac{16}{15}\right)^{\frac{1}{2}}. \tag{4.10}$$

While the Goldstone-like mode contributes the factor (4.8), which is evaluated as

$$\frac{\theta}{(2\pi)^{\frac{1}{2}}}\omega_0\left\{\frac{6}{5}\frac{M\omega_0^2}{\hbar\omega_0}\left(\frac{\omega_0^2}{u}\right)^2\right\}^{\frac{1}{2}}. \tag{4.11}$$

This results in the same $T=0$, undamped prefactor found in the work of Affleck [6] and reported by Caldeira and Leggett [3]. Our main task in this section is to calculate the leading corrections to the prefactor, in powers of damping and temperature.

The lowest order corrections to the undamped eigenvalues and eigenfunctions can be determined

from Eq. (4.3) together with the substitution

$$\tilde{q}(\tau)=q_B^{(0)}(\tau)+q_B^{(1)}(\tau)$$

where $q_B^{(1)}(\tau)$ is linearly proportional to η. The first order corrections $\Delta\Lambda_n^{(1)}$ to the undamped bound state eigenvalues are given by standard perturbation theory as

$$\frac{\Delta\Lambda_n^{(1)}}{M}=\frac{\eta}{2\pi}\int_{-\infty}^{\infty}d\tau\int_{-\infty}^{\infty}d\tau'\varphi_n^{(0)}(\tau)^*\frac{\partial}{\partial\tau'}\varphi_n^{(0)}(\tau')\cdot\left\{\frac{1}{\tau-\tau'+i\delta}+\frac{1}{\tau-\tau'-i\delta}\right\}-2u\int_{-\infty}^{\infty}d\tau\,\varphi_n^{(0)}(\tau)^*q_B^{(1)}(\tau)\varphi_n^{(0)}(\tau). \tag{4.12}$$

The first term of Eq. (4.12) can be evaluated analytically, by expressing the bound state wavefunctions in terms of their Fourier transforms. The integral over the linear correction to the bounce trajectory may be approximated, since we note that the bound states are localized and have a strong exponential fall off. We note that only the behavior of $q_B^{(1)}(\tau)$ near $\tau=0$ is important, thus τ can be set to zero in intermediate integrals. The final results are

$$\Lambda_1=-M\omega_0^2\left[\frac{5}{4}+1.16\left(\frac{\eta}{2\omega_0}\right)\right],$$

$$\Lambda_3=M\omega_0^2\left[\frac{3}{4}-4.07\left(\frac{\eta}{2\omega_0}\right)\right]. \tag{4.13}$$

The zero-mode normalization is calculated with the same approximation yielding a linear η correction to (4.11). The factor (4.11) becomes

$$\frac{\theta}{(2\pi)^{\frac{1}{2}}}\omega_0\left\{\frac{36}{5}\frac{V_{\max}}{\hbar\omega_0}\right\}^{\frac{1}{2}}\left\{1+1.60\left(\frac{\eta}{2\omega_0}\right)\right\} \tag{4.14}$$

where $V_{\max}$ is the maximum height of the potential barrier.

The continuum of eigenvalues is treated with the aid of the observation that the phase shift $\delta(k)$ for potential scattering is unchanged with respect to the k dependence, to leading order in the dissipation. However the eigenvalue is changed to

$$\Lambda=M\omega_0^2\left\{1+\frac{k^2}{4}+\left(\frac{\eta}{2\omega_0}\right)\frac{|k|}{2}\right\}.$$

To prove this, we consider the eigenvalue equation

$$(\hat{H}_0+\hat{H}_1)\psi=\frac{\Lambda}{M}\psi \tag{4.15}$$

in which $\hat{H}_0$ represents the scattering from a potential $-2u\tilde{q}(\tau)$, in the absence of dissipation. The operator $\hat{H}_0$ is the form of the left hand side of the Eq. (4.3) with $\eta=0$. The term $\hat{H}_1$ represents the nonlocal dissipation term in (4.3) which is proportional to η.

The solutions of the undamped eigenvalue equation are given by

$$\hat{H}_0\varphi_k=\frac{\tilde{\Lambda}_k}{M}\varphi_k. \tag{4.16}$$

The forward travelling components of the solutions of (4.16) have the asymptotic form

$$\operatorname*{Limit}_{\tau\to-\infty}\varphi_k(\tau)=e^{ik\frac{\omega_0\tau}{2}},$$

$$\operatorname*{Limit}_{\tau\to\infty}\varphi_k(\tau)=e^{ik\frac{\omega_0\tau}{2}+i\delta(k)}$$

where

$$\tilde{\Lambda}_k=M\omega_0^2\left(1+\frac{k^2}{4}\right). \tag{4.17}$$

We shall look for solutions of the damped eigenvalue Eq. (4.15) that are expressed in terms of the undamped solutions (4.17) in the form

$$\psi(\tau)=\exp[iV(\tau)]\,\varphi_k(\tau)$$

where V is the linear or higher order in η.

On substituting this form of the eigenvalue equation, and noting the large $|\tau|$ asymptotic behavior of $\varphi_k(\tau)$ we find that

$$\hat{H}_1\varphi_k(\tau)=\omega_0^2\left(\frac{\eta}{2\omega_0}\right)\frac{|k|}{2}\varphi_k(\tau).$$

To linear order in η, the solution $V(\tau)=$const. satisfies the equation

$$\frac{\Lambda}{M}\psi=\exp[iV(\tau)]\cdot\left\{\omega_0^2\left(1+\frac{k^2}{4}+\left(\frac{\eta}{2\omega_0}\right)\frac{|k|}{2}\right)\varphi_k(\tau)-2i\varphi_k'(\tau)V'(\tau)-i\varphi_k(\tau)V''(\tau)+\varphi_k(\tau)V'(\tau)^2\right\}$$

if

$$\frac{\Lambda}{M}=\omega_0^2\left(1+\frac{k^2}{4}+\left(\frac{\eta}{2\omega_0}\right)\frac{|k|}{2}\right)$$

which proves our assertion, since $V=$const. does not yield a phase shift.

The remaining problem is therefore to determine the phase shift $\delta(k)$ for fluctuations about the total bounce trajectory. Since we can expand $q_B(\tau)$ in powers of η, as done in Eq. (3.2), the task can be

simplified to that of finding the extra phase shift introduced by the potential

$$-2u\,q_B^{(1)}(\tau)$$

since the phase shift due to $q_B^0(\tau)$ has already been determined. We again express the solution in the form

$$\varphi_k(\tau)=\varphi_k^{(0)}(\tau)\,e^{i\tilde{V}(\tau)}$$

where $\varphi_k^{(0)}(\tau)$ are given in Appendix A. We find that $\tilde{V}(\tau)$ must satisfy the equation

$$2i\,\tilde{V}'(\tau)\frac{\varphi_k'^{(0)}(\tau)}{\varphi_k^{(0)}(\tau)}+i\,\tilde{V}''(\tau)-\tilde{V}'^2(\tau)=-2u\,q_B^{(1)}(\tau). \quad (4.18)$$

Since $\tilde{V}'(\tau)^2$ is at least of order η^2 we may neglect it. We shall also assume that $\tilde{V}(\tau)$ is a slowly varying function of τ, and therefore we shall also neglect the term $\tilde{V}''(\tau)$, in analogy with the W.K.B. approximation. Thus we obtain,

$$\tilde{V}'(\tau)=\frac{i\,u\,q_B^{(1)}(\tau)\,\varphi_k^{(0)}(\tau)}{\varphi_k'^{(0)}(\tau)}. \quad (4.19)$$

This introduces an extra contribution to the phase shift of

$$\delta^{(1)}(k)=\tilde{V}(\infty)-\tilde{V}(-\infty). \quad (4.20)$$

We note that since the dissipation does not introduce any extra bound states then $\delta^{(1)}(k)$ vanishes as $k\to 0$, in accordance with Levinson's theorem.

The continuum contribution to the prefactor, from the terms linear in order η, thus stems from the change in the eigenvalues Λ_k evaluated with $\delta^{(0)}(k)$ and a term from $\delta^{(1)}(k)$ given by Eq. (4.20). The phase shifts are substituted into Eq. (4.6) and integrated over k. The term proportional to $\delta^{(0)}(k)$ is

$$-\frac{1}{\pi}\left(\frac{\eta}{2\omega_0}\right)\int\frac{\frac{\partial}{\partial k}\delta^{(0)}(k)}{4+k^2}k\,dk=0.922\left(\frac{\eta}{2\omega_0}\right).$$

The term proportional to $\delta^{(1)}(k)$ yields a contribution of

$$0.700\left(\frac{\eta}{2\omega_0}\right).$$

Thus, the final result for the continuum contribution to the prefactor results in the factor

$$\frac{15}{2}+1.62\left(\frac{\eta}{2\omega_0}\right). \quad (4.21)$$

On combining the various contributions (4.13), (4.14) and (4.21) we obtain A, the prefactor of the decay rate, as

$$A=12\omega_0\left\{\frac{3}{2\pi}\frac{V_{\max}}{\hbar\omega_0}\right\}^{\frac{1}{2}}\left\{1+5.47\left(\frac{\eta}{2\omega_0}\right)\right\}. \quad (4.22)$$

This result has not been previously derived.

The temperature dependence of the prefactor can be evaluated by using techniques similar to those employed by Grabert and Weiss [11] in their calculation of the exponent. These authors show how the finite temperature bounce trajectory can be expressed in terms of the zero temperature bounce trajectory using an asymptotic low temperature expansion. Using this method, we find that the lowest order change in the bounce trajectory due to finite temperature is

$$-\frac{4}{2\pi}\left(\frac{\eta}{2\omega_0}\right)\left(\frac{2\pi}{\theta\omega_0}\right)^2\left\{q_B(\tau)+\frac{\tau}{2}\frac{\partial q_B(\tau)}{\partial\tau}+\ldots\right\}.$$

This is proportional to both η and T^2. The change in the boundary conditions only give rise to exponentially small temperature corrections which are neglected. We find that the finite temperature, linear η corrections to the prefactor by essentially the same method as was for the $T=0$ case. We shall merely present the results.

The discrete eigenvalues contribute

$$\Lambda_1(T)=\Lambda_1(0)-\frac{3M\omega_0^2}{2\pi}\left(\frac{\eta}{2\omega_0}\right)\left(\frac{2\pi}{\theta\omega_0}\right)^2,$$

$$\Lambda_3(T)=\Lambda_3(0)+\frac{89\,M\omega_0^2}{12\pi}\left(\frac{\eta}{2\omega_0}\right)\left(\frac{2\pi}{\theta\omega_0}\right)^2$$

while the zero-mode normalization becomes

$$\mathcal{N}(T)=\mathcal{N}(0)\left\{1-\frac{5}{2\pi}\left(\frac{\eta}{2\omega_0}\right)\left(\frac{2\pi}{\theta\omega_0}\right)^2\right\}.$$

Finally, the change in the continuous spectrum of eigenvalues results in the factor of

$$\exp\left[-\frac{0.413}{2\pi}\left(\frac{\eta}{2\omega_0}\right)\left(\frac{2\pi}{\theta\omega_0}\right)^2\right].$$

On combining all these results, the full expression for the prefactor can be written as

$$A(T,\eta)=12\omega_0\left\{\frac{3}{2\pi}\frac{V_{\max}}{\hbar\omega_0}\right\}^{\frac{1}{2}}\left[1+\left(\frac{\eta}{2\omega_0}\right)\cdot\left\{5.47-2.49\left(\frac{2\pi}{\theta\omega_0}\right)^2+\ldots\right\}+\ldots\right]. \quad (4.23)$$

This is the main result of this section.

V. Discussion

We have evaluated the lowest order corrections to the quantum decay rate, in powers of the dissipation strength. The decay rate is partitioned into an exponential part and a perfactor.

The exponent agrees precisely with that previously obtained by Caldeira and Leggett [3], at $T=0$. The finite temperature corrections are in complete agreement with the general calculations performed by Grabert, Weiss and Hänggi [7]. The extent to which these calculations are reasonable can be checked by comparison with numerical calculations. Chang and Chakravarty [12] have performed numerical calculations of the rate at $T=0$, and Grabert, Olschowski and Weiss [13] have extended these to finite temperatures. In Table 1, we present a comparison between the analytical expressions with the numerical work for various dissipation strengths $\alpha=\frac{\eta}{2\omega_0}$ and various temperatures $\left(\frac{2\pi}{\theta\omega_0}\right)$. We see that the results for the exponent are in excellent agreement with the numerical values for T close to zero, and for values of α between zero and 0.1. The temperature dependence of the exponent is also quite good for T up to 0.6 of the cross over temperature $\frac{\hbar\omega_0}{2\pi k_B}$. For temperatures above this the non power law dependence on temperature may no longer be ignored.

The prefactor can only be compared directly with the results of numerical calculations. The agreement is not as good as that obtained with the exponent. The results are compared with the zero temperature values of Chang and Chakrararty [12] as well as the finite temperature values of Grabert, Olschowski and Weiss [13] in Table 2.

The results of these calculations can also be directly compared with recent experiments. Devoret, Martinis and Clarke [14] have performed experiments on r.f. SQUIDS. Since the value of the dimensionless damping constant appropriate for these experiments is quite small, good agreement was found with the undamped tunneling rate, reported by Caldeira and Leggett [3]. This same result was previously found by Affleck [6], by a different method. Since Affleck's [6] treatment of the tunneling rate clearly employs the usual transition state assumption, namely that the system maintains thermal equilibrium, and yet neglects the coupling to the thermal reservoir, it is not obvious how this result is relevant to the experiments. As we shall argue, the quantal transition state theory should be reasonable even for extremely small values of the damping strengths. The argument is based on the expectation that, the transition state assumption is appropriate whenever the rate at which the particles redistributes themselves, within the quasi-quantum levels of the metastable well, is much larger than the rate at which the particles decay out from the metastable well. When this condition is satisfied, it seems reasonable to expect that thermal equilibrium will al-

Table 1. The exponent, in units of $\frac{V_{\max}}{\hbar\omega_0}$, for various damping strengths $\alpha=\frac{\eta}{2\omega_0}$ and temperatures $\left(\frac{2\pi}{\omega_0\theta}\right)$. We compare our results with those of the numerical calculations of Grabert, Olschowski and Weiss [13]

$\left(\frac{2\pi}{\omega_0\theta}\right)$	0.1		0.4		0.6		0.8	
α	Ours	Ref. 13	Ours	Ref. 13	Ours	Ref. 13	Ours	Ref. 13
0.00	7.20	7.20	7.20	7.20	7.20	7.189	7.20	7.036
0.05	7.830	7.830	7.783	7.789	7.722	7.708	–	7.438
0.10	8.458	8.491	8.363	8.390	8.248	8.242	–	7.870

Table 2. The prefactor, in units of $\omega_0\left(\frac{V_{\max}}{\hbar\omega_0}\right)^{\frac{1}{2}}$ for various coupling strengths and temperatures. We compare our results with those of Grabert, Olschowski and Weiss [13]

$\left(\frac{2\pi}{\omega_0\theta}\right)$	0.1		0.4		0.6		0.8	
α	Ours	Ref. 13	Ours	Ref. 13	Ours	Ref. 13	Ours	Ref. 13
0.00	8.292	8.292	8.292	8.292	8.292	8.354	8.292	8.800
0.05	10.56	9.55	10.39	9.45	10.19	9.42	9.90	9.72
0.10	12.83	10.95	12.50	10.78	12.08	10.61	11.50	10.76

ways be maintained by the particles within the metastable well.

A simple fermi golden-rule calculation, for a metastable well containing two quantum levels, indicates that the rate at which thermal eqzilibrium is established is governed by η. The rate for the particle to decay from one quantum level to a lower one, emitting the excess energy into the normal modes of the heat bath is directly proportional to η. Thus, the condition under which quantal transition state theory should be appropriate may be written as

$$\frac{\eta}{\omega_0} \gg \frac{12}{(2\pi)^{\frac{1}{2}}} \left(\frac{3V_{\max}}{\hbar\omega_0}\right)^{\frac{1}{2}} \exp\left[-\frac{36V_{\max}}{5\hbar\omega_0}\right]. \tag{5.1}$$

The assumption of at least two quantum levels are contained within the metastable potential minimum is such that

$$V_{\max} > \tfrac{3}{2}\hbar\omega_0 \tag{5.2}$$

and is consistent with the W.K.B. condition. These conditions are well satisfied in the experiments of Devoret et al. [14]. Due to the largeness of the exponent in the right hand side of Eq. (5.1) we find that even when $V_{\max} = \frac{3}{2}\hbar\omega_0$, quantal transition state theory should be reasonable until

$$\frac{\eta}{\omega_0} \lesssim 2 \cdot 10^{-4}.$$

For smaller values of η/ω_0, one expects deviations from the quantal transition state theory, due to the quantal non-equilibrium effects or preparation of the initial state. In other words, the rate may no longer be well defined.

To summarise, we have found the finite damping and finite temperature corrections for both the exponent and the prefactor of the quantum decay rate. The analytic forms are in reasonable agreement with numerical calculations. The basic assumption of weak damping and thermal equilibrium have been shown to be compatible with recently reported experiments.

This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences through grant no. DE-FG02-84ER 45127 and the U.S. Office of Naval Research, ONR N00014-85-K-0372.

Appendix 1

The Fluctuations about the Bounce

The second variation of the action $\delta^2 S$ with zero dissipation $\eta = 0$, has eigenvalues and eigenfunctions which satisfy the equation

$$-\frac{\partial^2 \psi_k}{\partial \tau^2} + \omega_0^2 \left\{1 - 3\,\mathrm{sech}^2 \frac{\omega_0 \tau}{2}\right\} \psi_k = \frac{\Lambda_k}{M} \psi_k. \tag{A.1}$$

This equation possesses three bound states with discrete eigenvalues, as well as a continuum of scattering states.

The bound state with negative eigenvalue $\Lambda_1 = -\frac{5}{4} M\omega_0^2$ has an eigenfunction

$$\psi_1(\tau) = \frac{\sqrt{30\omega_0}}{8} \mathrm{sech}^3 \frac{\omega_0 \tau}{2}. \tag{A.2}$$

The bound state with zero eigenvalue $\Lambda_2 = 0$ is

$$\psi_2(\tau) = \frac{\sqrt{30\omega_0}}{4} \mathrm{sech}^2 \frac{\omega_0 \tau}{2} \tanh \frac{\omega_0 \tau}{2}. \tag{A.3}$$

The remaining bound state has a positive eigenvalue $\Lambda_3 = \frac{3}{4} M\omega_0^2$ and has the corresponding eigenfunction

$$\psi_3(\tau) = \frac{\sqrt{6\omega_0}}{2} \left\{\mathrm{sech} \frac{\omega_0 \tau}{2} - \frac{5}{4} \mathrm{sech}^3 \frac{\omega_0 \tau}{2}\right\}. \tag{A.4}$$

The continuum of scattering states has eigenvalues

$$\Lambda_k = M\omega_0^2 \left(1 + \frac{k^2}{4}\right)$$

and normalized eigenfunctions

$$\psi_k(\tau) = \mathcal{N}_k \left[ik^3 - 6k^2 \tanh \frac{\omega_0 \tau}{2} - ik\left(11 - 15\,\mathrm{sech}^2 \frac{\omega_0 \tau}{2}\right) + \tanh \frac{\omega_0 \tau}{2} \left(6 - 15\,\mathrm{sech}^2 \frac{\omega_0 \tau}{2}\right)\right],$$

where the normalization $\mathcal{N}_k$ is given by

$$\mathcal{N}_k^2 = \frac{\omega_0}{4\pi} (6^2 + (7k + k^3)^2). \tag{A.5}$$

Appendix 2

The Undamped Bounce Trajectory

The undamped bounce trajectory satisfies the equation

$$-M\ddot{q}(\tau) + M(\omega_0^2 q(\tau) - u q^2(\tau)) = 0 \tag{B.1}$$

with periodic boundary conditions

$$q(\tau + \theta) = q(\tau).$$

The first integral of the motion is

$$-\frac{\dot{q}^2(\tau)}{2} + \left(\frac{\omega_0^2}{2} q^2(\tau) - \frac{u}{3} q^3(\tau)\right) = \frac{E}{M}. \tag{B.2}$$

The turning points of the trajectory are found by solving the equation

$$q^3 - \frac{3}{2}\frac{\omega_0^2}{u} q^2 + \frac{3E}{Mu} = 0$$

for the three roots q_1, q_2 and q_3 (see Fig. 1) where $q_1 > q_2 > q_3$.

The "energy" E is determined by requiring that the motion between the turning points q_1 and q_2 is periodic, with period θ.

Since,

$$\pm\sqrt{\frac{3}{2}\frac{\omega_0^2}{u}}\int^{q(\tau)} \frac{dq}{\sqrt{(q_1-q)(q_2-q)(q_3-q)}} = \omega_0 \int^{\tau} d\tau' \quad \text{(B.4)}$$

we find that the turning points must also satisfy the condition

$$\sqrt{\frac{3\omega_0^2}{2u}}\frac{2}{\sqrt{q_1-q_3}} K\left(\sqrt{\frac{q_1-q_2}{q_1-q_3}}\right) = \frac{\omega_0 \theta}{2}$$

where $K(k)$ is the complete elliptic integral of the first kind [15]. Thus the solution of the bounce trajectory requires finding the value of E such that Eqs. (B.3) and (B.5) are satisfied simultaneously.

The bounce trajectory is found directly from Eq. (B.4) as the solution of

$$\frac{2}{\sqrt{q_1-q_3}}\sqrt{\frac{3\omega_0^2}{2u}} F\left(\varphi; \sqrt{\frac{q_1-q_2}{q_1-q_3}}\right) = \omega_0 \tau$$

where

$$\varphi = \sin^{-1}\sqrt{\frac{q_1-q(\tau)}{q_1-q_2}}$$

and $F(\varphi, k)$ is an elliptic integral of the first kind [15].

This may be formally inverted to yield

$$q(\tau) = q_2 + (q_1-q_2)\ cn^2\left(\frac{\omega_0 \tau}{2}\sqrt{\frac{q_1-q_3}{\left(\frac{3\omega_0^2}{2u}\right)}}\right). \quad \text{(B.7)}$$

Here, $cn(u)$ denotes the Jacobian elliptic function (page 569, 570 in Ref. 15).

This equation was previously derived by Zwerger [10].

The Fourier transform of the bounce trajectory is obtained with the aid of the formula

$$cn^2(u) = \frac{1}{k^2}\left(\frac{\partial}{\partial u}(Zn(u)) + \frac{E(k)}{K(k)}\right) - \frac{1-k^2}{k^2}$$

where $k = \sqrt{\frac{q_1-q_2}{q_1-q_3}}$ and the functions $E(k)$ and $K(k)$ are the complete elliptic integrals. The function $Zn(u)$ is the Jacobi zeta function [16]. The Fourier transform of $Zn(u)$ is obtained from the known expansion as

$$Zn(u) = \frac{\pi}{K(k)}\sum_{n=1}^{\infty} \frac{\sin\left\{\frac{\pi n u}{K(k)}\right\}}{\sinh\left\{\frac{\pi n K'(k)}{K(k)}\right\}}.$$

Hence, we find the result.

$$cn^2(u) = \left(\frac{\pi}{kK(k)}\right)^2 \sum_{n=1}^{\infty} \frac{n\cos\left(\frac{\pi n u}{K(k)}\right)}{\sinh\left(\frac{\pi n K'(k)}{K(k)}\right)} + \frac{1}{k^2}\frac{E(k)}{K(k)} - \frac{(1-k^2)}{k^2}. \quad \text{(B.8)}$$

References

1. a. Kramers, H.A.: Physica (Utrecht) **7**, 284 (1940)
   b. Hänggi, P.: J. Stat. Phys. **42**, 105 (1986)
2. Bailin, D., Love, A.: J. Phys. A**13**, L271 (1980)
3. Caldeira, A.O., Leggett, A.J.: Ann. Phys. (NY) **149**, 374 (1983); **153**, 445, E (1984); Phys. Rev. Lett. **46**, 211 (1981)
4. Langer, J.S.: Ann. Phys. **41**, 108 (1967); Zittartz, J., Langer, J.S.: Phys. Rev. **148**, 741 (1966)
5. Coleman, S.: Phys. Rev. D**15**, 2929 (1977)
   Callan, C.G., Coleman, S.: Phys. Rev. D**16**, 1762 (1977)
6. Affleck, I.K.: Phys. Rev. Lett. **46**, 388 (1981)
7. Grabert, H., Weiss, U., Hänggi, P.: Phys. Rev. Lett. **52**, 2193 (1984)
8. Ullersma, P.: Physica (Utrecht) **32**, 27; 56; 74; 90 (1966)
9. Sethna, J.P.: Phys. Rev. B**25**, 5050 (1982); Phys. Rev. B**24**, 698 (1981)
10. Zwerger, W.: Z. Phys. B - Condensed Matter **51**, 301 (1983)
11. Grabert, H., Weiss, U.: Z. Phys. B - Condensed Matter **56**, 171 (1984)
12. Chang, L.D., Chakravarty, S.: Phys. Rev. B**29**, 130 (1983); **30**, 1566(E) (1984)
13. Grabert, H., Olschowski, P., Weiss, U.: Phys. Rev. B**32**, 3348 (1985)
14. Devoret, M.,Martinis, J., Clarke, J.: Phys. Rev. Lett. **55**, 1543 (1985)
15. Handbook of Mathematical Functions. Abramowitz, M., Stegun, A. (eds.). New York: Dover Publishers 1972
16. Magnus, W., Oberhettinger, F.: Formeln und Sätze für die speziellen Funktionen der mathematischen Physik. In: Grundlagen der Mathematischen Wissenschaften. Bd. 52, p. 150. Berlin, Göttingen, Heidelberg: Springer 1948

E. Freidkin
P.S. Riseborough
Department of Physics
Polytechnic Institute of New York
333 Jay Street
Brooklyn, NY 11201
USA

P. Hänggi
Lehrstuhl für Theoretische Physik
Universität Augsburg
Memmingerstrasse 6
D-8900 Augsburg
Federal Republic of Germany