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Quantum Tunneling in Dissipative Systems at Finite Temperatures

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A quantum system which can tunnel out of a metastable state, and which interacts with an environment at temperature T, is considered. It is found that heat enhances the tunneling probability at $T=0$ by a factor $\exp[A(T)M\omega_0 q_0^2/\hbar]$, where M is the mass of the system, ω_0 is the frequency of small oscillations about the metastable state, and q_0 is the tunneling distance. For an undamped system $A(T)$ is exponentially small, $A(T) \propto \exp(-\hbar\omega_0/k_B T)$, whereas for a dissipative system $A(T)$ grows algebraically with temperature.

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There has been recent experimental and theoretical work on the question of whether a macroscopic system can be shown to tunnel out of a metastable state.[1] In macroscopic systems, the tunneling probability is strongly influenced by the interaction with the environment. This coupling is often so strong that the motion in the classically accessible region is heavily damped. Caldeira and Leggett[2] have shown that damping suppresses the tunneling rate at $T=0$. Their results are in qualitative agreement with recent experiments on Josephson systems.[3] A more detailed comparison should have regard to the temperature dependence of the tunneling probability which is investigated theoretically in this Letter. We have found that the thermal enhancement of the tunneling rate at low temperatures sensitively depends on the details of the coupling to the environment. Our predictions should be experimentally testable and render a crucial check of currently discussed theoretical models.

Specifically we consider a particle of mass M moving in a potential $V(q)$ with a metastable minimum; we choose the axes so that this lies at $q=0$, $V=0$. To tunnel out of the metastable state, the particle has to penetrate a potential barrier of width q_0 [that is, $V(q_0)=0$] before reaching the region of lower potential. The system is assumed to be coupled linearly to its environment which at low temperatures can be replaced by a bath of harmonic oscillators.[1] Feynman's method[4] of integrating away the environmental modes leaves a one-dimensional problem, the partition function of which is given in terms of an effective action[1,5]

$$S[q(\tau)] = \int_{-\theta/2}^{\theta/2} d\tau \left[\tfrac{1}{2}M\dot{q}^2 + V(q)\right] + \tfrac{1}{2}\int_{-\theta/2}^{\theta/2} d\tau \int_{-\theta/2}^{\theta/2} d\tau'\, k(\tau-\tau')\, q(\tau)\, q(\tau'), \tag{1}$$

where $q(\tau)$ is a path in "imaginary time" τ with period θ, $q(\tau+\theta)=q(\tau)$, where $\theta=\hbar/k_B T$. The potential $V(q)$ includes the shift due to the coupling. The final term in (1) introduces dissipation. $k(\tau)$ is a θ-periodic kernel given by[1,5]

$$k(\tau) = \theta^{-1} \textstyle\sum_m K(\nu_m) \exp(i\nu_m \tau),$$

where $\nu_m = 2\pi m/\theta$, and

$$K(\nu) = \frac{1}{\pi}\int_0^\infty d\omega \frac{2\nu^2}{\nu^2+\omega^2}\frac{J(\omega)}{\omega}.$$

Here and in the sequel sums over the index m run from $-\infty$ to $+\infty$. The spectral density $J(\omega)$ is proportional to the density of environmental modes at frequency ω and proportional to the square of the strength of their coupling to the tunneling system.[1]

To determine the tunneling probability we employ the "bounce" technique originally used by Langer[6] and popularized by Coleman.[7] The "bounce" trajectory is a saddle point of the action (1) which starts from the metastable region at $\tau = -\theta/2$, traverses the potential barrier (which is a valley in imaginary time), and returns to the metastable region at $\tau = \theta/2$. As long as $k_B T$ is small compared with $\hbar\omega_0$, where ω_0 is the frequency of small oscillations about the metastable equilibrium, the WKB approximation applies, and the tunneling probability may be written

$$\Gamma = N \exp(-S_B/\hbar), \tag{2}$$

where S_B is the action (1) evaluated along the "bounce" trajectory, and N is a prefactor which can be calculated from the small fluctuations about this path. A derivation of the decay rate formula (2) has been given by Coleman[7] for an undamped system at zero temperature and the extension to the dissipative case has been expounded by Caldeira and Leggett.[1] They also have estimated the effect of interbounce interactions and have shown that they may be neglected at low temperatures even for the dissipative case. Furthermore, we have analyzed the decay rate for temperatures near the crossover temperature to thermal hopping and have found that for damping of arbitrary strength the one-bounce contribution to the decay rate always matches smoothly with the Arrhenius factor. It seems therefore natural to conjecture that the formula (2) holds in the whole temperature regime where tunneling prevails.

Since the temperature dependence of the prefactor N is negligible, we find from (2) that to a good approximation the tunneling probability $\Gamma(T)$ at low temperatures may be written

$$\Gamma(T) = \Gamma_0 \exp[\Delta S_B(T)/\hbar], \tag{3}$$

where Γ_0 is the tunneling probability at $T=0$ (including the influence of dissipation) and $\Delta S_B(T) = S_B(0) - S_B(T)$.

We have evaluated (3) for various potentials. Our principal findings for the behavior at low temperatures of the thermal enhancement of the tunneling probability are as follows.

(i) The thermal enhancement factor may be written

$$\Gamma(T)/\Gamma_0 = \exp[A(T) M\omega_0 q_0^2/\hbar], \tag{4}$$

where $A(T)$ is a dimensionless quantity characterizing the influence of thermal fluctuations.

(ii) For an undamped system, $A(T)$ is exponentially small, $A(T) = a\exp(-\hbar\omega_0/k_B T)$, where a is a numerical factor which depends on the potential. This is in agreement with results of Affleck[8] and of Weiss and Haeffner[9] which have been obtained on different lines involving a Boltzmann average of energy-dependent rates.

(iii) For a system with linear frequency-independent damping whose classical equation of motion is $M\ddot{q} + \eta\dot{q} + \partial V/\partial q = 0$, the spectral density $J(\omega)$ must have the form $J(\omega) = \eta\omega$.[1] Then $A(T)$ increases quadratically with temperature, $A(T) = a(\alpha)(k_B T/\hbar\omega_0)^2$, where $a(\alpha)$ is a function of the dimensionless damping parameter $\alpha = \eta/2M\omega_0$. This function depends on the form of the potential. The low-temperature power law $A \propto T^2$, however, holds for all metastable potentials and is a distinctive feature of "Ohmic dissipation," that is a dissipative mechanism characterized by a damping coefficient which becomes frequency independent at low frequencies.

(iv) For tunneling centers in solids, the spectral density $J(\omega)$ is typically proportional to ω^3 for small frequencies.[10] Then $A(T)$ grows as the fourth power of temperature.

(v) If the environmental spectrum has a low-frequency cutoff, as in the oxide junction model of Ambegaokar, Eckern, and Schön,[11] the thermal enhancement is exponentially small as in undamped systems.

(vi) The increase of $A(T)$ with temperature is intimately connected with the asymptotic behavior for $\tau \to \infty$ of the "bounce" trajectory $q(\tau)$ at zero temperature. Both of these asymptotic forms can be related to the long-time behavior of the zero-temperature kernel $k(\tau)$.

There is space here only to give the general outline of our calculations. Let us first consider a simple model potential

$$V(q) = \begin{cases} \frac{1}{2}M\omega_0^2 q^2 & \text{for } q < q_0, \\ -\infty & \text{for } q > q_0, \end{cases} \tag{5}$$

which is the limit for $n \to \infty$ of the smooth potential

$$V(q) = \tfrac{1}{2}M\omega_0^2 q_0^2 [(q/q_0)^2 - (q/q_0)^n].$$

The motion in "imaginary time" in the potential $V(q)$ corresponds to a motion in real time in the inverted potential $-V(q)$.[7] The saddle-point trajectory reaches q_0 at $\tau = 0$ and bounces off the infinitely high barrier of the inverted potential. Hence, the "bounce" trajectory has a cusp at $\tau = 0$ with $\dot{q}(0^-) = -\dot{q}(0^+) = v$. Taking this discontinuity of the velocity into account, and expanding the saddle-point trajectory into a Fourier series

$$q(\tau)=(2\pi/\theta)\sum_m Q_m \exp(i\nu_m\tau), \qquad (6)$$

we obtain from the equation of motion

$$(\nu_m^2+\omega_0^2+\zeta_m)Q_m=v/\pi,$$

where $\zeta_m=K(\nu_m)/M$, and where v is determined by the requirement $q(0)=(2\pi/\theta)\sum Q_m=q_0$. Thus, our results for the "bounce" trajectory $q(\tau)$ and for the action $S_B(T)$ of this path are

$$q(\tau)=q_0\Omega(T)\theta^{-1}\times\sum_m \exp(i\nu_m\tau)(\nu_m^2+\omega_0^2+\zeta_m)^{-1}, \qquad (7)$$

$$S_B(T)=\tfrac{1}{2}M\Omega(T)q_0^2=\tfrac{1}{2}\hbar q_0^2/\langle q^2\rangle_h, \qquad (8)$$

where $\langle q^2\rangle_h=\hbar/M\Omega(T)$ is the dispersion of a harmonic oscillator with frequency ω_0 which is damped by the same dissipative mechanism as the tunneling system, and where

$$\Omega(T)^{-1}=\theta^{-1}\sum_m(\nu_m^2+\omega_0^2+\zeta_m)^{-1}. \qquad (9)$$

To proceed further we need to particularize the coupling to the environmental modes. Let us first consider an undamped, or free, system where $J(\omega)=0$. We then have $\langle q^2\rangle_h=(\hbar/2M\omega_0)\coth(\theta\omega_0/2)$ which by virtue of (8) leads to a thermal enhancement factor of the form (4), where

$$A(T)=2\exp(-\hbar\omega_0/k_BT)$$

at low temperatures. From (7) we obtain for the saddle-point trajectory at zero temperature $q(\tau)=q_0\exp(-\omega_0|\tau|)$ which for large τ shows the same asymptotic behavior as $A(T)$ for large $\theta=\hbar/k_BT$.

Next we consider the case of a system with linear Ohmic dissipation where $J(\omega)=\eta\omega$.[1] Then $\zeta_m=\eta|\nu_m|/M$, and one has

$$\Omega(T)^{-1}=M\langle q^2\rangle_h/\hbar = (\theta\omega_0^2)^{-1}+[\pi(\lambda_1-\lambda_2)]^{-1}\times[\psi(1+\theta\lambda_1/2\pi)-\psi(1+\theta\lambda_2/2\pi)].$$

The psi function, $\psi(z)$, is the logarithmic derivative of the gamma function,[12] and $\lambda_{1,2}=\omega_0[\alpha\pm(\alpha^2-1)^{1/2}]$, where $\alpha=\eta/2M\omega_0$. Using the asymptotic expansion of $\psi(z)$ for large $|z|$,[12] we find

$$S_B(T)=\tfrac{1}{2}M\Omega_0q_0^2[1-\tfrac{2}{15}\pi^3(\eta\Omega_0/M\omega_D^2)\times(k_BT/\hbar\omega_0)^4]$$

where terms of order $(k_BT/\hbar\omega_0)^4$ have been disregarded, and where $\Omega_0=\Omega(0)$. This shows that

$$A(T)=\tfrac{1}{3}\pi_\alpha(\Omega_0/\omega_0)^2(k_BT/\hbar\omega_0)^2$$

increases proportional to T^2 at low temperatures. At $T=0$, the asymptotic behavior of the "bounce" trajectory for $\tau\rightarrow\infty$ reads $q(\tau)=(2/\pi)\alpha(\Omega_0/\omega_0)q_0(\omega_0\tau)^{-2}$. This algebraic decay obeys the same power law as the decrease of $A(T)$ as a function of θ for $\theta\rightarrow\infty$.

The coupling of tunneling centers in solids to the phonon mode[10] can frequently be described by a spectral density of the form[13] $J(\omega)=\eta\omega^3/(\omega^2+\omega_D^2)$. We now have $\zeta_m=\eta\nu_m^2/M(\omega_D+|\nu_m|)$, and one finds after some algebra

$$S_B(T)=\tfrac{1}{2}M\Omega_0q_0^2[1-\tfrac{2}{15}\pi^3(\eta\Omega_0/M\omega_D^2)\times(k_BT/\hbar\omega_0)^4]$$

where terms of order $(k_BT/\hbar\omega_0)^6$ have been disregarded, and where $\Omega_0=\Omega(0)$, which depends on η, ω_0, and ω_D. The quantity $A(T)$ defined in (4) now increases proportional to T^4 at low temperatures.

As a last example, we consider a case where the environmental spectrum has a low-frequency cutoff ω_c: $J(\omega)=0$ for $\omega<\omega_c$, $J(\omega)=\eta\omega$ for $\omega>\omega_c$. In this case, one has $K(\nu)=(2\eta\nu/\pi)\arctan(\nu/\omega_c)$. Since $K(\nu)$ has no cusp at $\nu=0$, one finds that the zero-temperature kernel $k(\tau)$ decays exponentially for large τ. This leads to an increase of $A(T)$ with temperature which is exponentially small as in a free system.

So far, we have given results for the discontinuous model potential (5) only, which allows for an explicit evaluation of all quantities of interest. However, we have found the same leading dependence of $A(T)$ on temperature for smooth potentials. The reason is as follows. The saddle-point trajectory at low finite temperatures differs from the "bounce" at $T=0$ primarily by the fact that the turning point in the metastable region is reached at a finite "imaginary" time $\tau=\theta/2$ and not only for $\tau\rightarrow\infty$. For large θ, this change in the wings of the trajectory occurs far from the discontinuity of the potential (4). Thus, although the simple model can give poor results for the "bounce" action at $T=0$, it gives correct results for the difference $S_B(T)-S_B(0)$ at low temperatures, apart from a numerical factor which depends on the form of the potential and the strength of the damping but not on temperature.

Let us consider the practically important case of a cubic potential, $V(q)=\tfrac{1}{2}M\omega_0^2q^2-\tfrac{1}{3}Muq^3$, more closely. Inserting the spectral expansion (6) of the saddle-point trajectory into the equation of motion obeyed by the extremal paths of the action (1), one finds

$$(\nu_m^2+\omega_0^2+\zeta_m)Q_m=(2\pi u/\theta)\sum_n Q_{m+n}Q_n. \quad (10)$$

Further, by virtue of (10), the "bounce" action may be written

$$S_B(T)=\tfrac{1}{3}\pi Mu(2\pi/\theta)^2\sum_{m,n}Q_mQ_nQ_{m+n}. \quad (11)$$

At zero temperature, the sums in (10) and (11) are replaced by corresponding integrals. The Euler-Maclaurin expansion[12] of these sums yields the asymptotic expansions of both the form of the saddle-point trajectory and the "bounce" action $S_B(T)$ for large $\theta=\hbar/k_BT$, where the coefficients are given in terms of the Fourier representation

$$Q^0(\nu)=(1/2\pi)\int d\tau\exp(-i\nu\tau)q(\tau)$$

of the "bounce" at $T=0$. This analysis confirms the conclusions drawn from the simple model discussed above.

In the remainder of this Letter, we restrict ourselves to the important case of frequency-independent damping, $J(\omega)=\eta\omega$.[14] To determine the Fourier coefficients Q_m of the saddle-point trajectory at finite T, we compare (10) with its zero-temperature limit using the Euler-Maclaurin formula. The result for Q_m may be inserted into (11) and the sum can be approximated again by means of the Euler-Maclaurin formula. This yields finite-temperature corrections to the bounce action arising both from the discreteness of the sum in (11) and from the corrections to the form of the trajectory. The intermediate result can be simplified by use of the integral equation satisfied by $Q^0(\nu)$. We finally obtain

$$S_B(T)=S_B(0)-\tfrac{2}{3}\pi^3\eta[Q^0(0)k_BT/\hbar]^2, \quad (12)$$

where terms of the fourth order in T have been disregarded.

From (12) we obtain a thermal enhancement factor of the form (4) where

$$A(T)=\tfrac{1}{3}\pi\alpha(k_BT\tau_B/\hbar)^2. \quad (13)$$

Here we have introduced the "bounce length" $\tau_B=q_0^{-1}\int d\tau\, q(\tau)$. The zero-temperature "bounce" trajectory is known explicitly for very weak and for very strong damping.[1] This yields $\tau_B=4/\omega_0$ for $\alpha \ll 1$ and $\tau_B=8\pi\alpha/3\omega_0$ for $\alpha \gg 1$.

At the crossover temperature to thermal hopping $T_0=(\hbar\omega_0/2\pi k_B)[(1+\alpha^2)^{1/2}-\alpha]$ the "bounce" ceases to exist. There $S_B(T)/\hbar$ reaches the value and the slope of the classical Arrhenius factor. In the strong damping limit, where (10) can be solved exactly, the T^2 power law for $A(T)$ holds up to T_0. This overdamped case has also been studied by Larkin and Ovchinnikov.[15,16] In the weak damping limit, the T^2 power law holds only for temperatures below $\hbar\eta/Mk_B$.

These results may be applied to the physically interesting problem of quantum tunneling in SQUID's or current-biased Josephson junctions.[1] An increase of $A(T)$ proportional to T^2 would indicate that these systems are adequately described by the resistively shunted junction model.

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[13] We have chosen a Drude cutoff at large ω but the same low-temperature behavior is found with, e.g., a Debye cutoff.

[14] A more detailed presentation of our method to determine the leading dependence of $S_B(T)$ on temperature in terms of the zero-temperature saddle-point trajectory and a discussion of other potentials and other forms of $J(\omega)$ will be given elsewhere.

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[16] We remark that the discontinuity of the second-order derivative of the exponent of the decay rate is a shortcoming of the WKB approximation and is not associated with a phase transition at $T=T_0$.