Crossover from Thermal Hopping to Quantum Tunneling

Hermann Grabert and Ulrich Weiss
Institut für Theoretische Physik, Universität Stuttgart, D-7000 Stuttgart 80, Germany
(Received 5 June 1984)

Consider a macroscopic system rendered unstable by both thermal fluctuation and quantum tunneling. Kramers's classical theory of the rate of decay by thermal activation is extended to lower temperatures where quantum tunneling prevails. By means of a functional-integral approach, a general formula for the decay rate is derived which describes the transition between the high- and low-temperature regimes. The influence of dissipation on the decay rate is emphasized.

PACS numbers: 05.30.−d, 05.40.+j

The decay of metastable states in macroscopic systems plays a central role in many areas of physical sciences including low-temperature physics, nuclear physics, and chemical kinetics. Since Kramers,[1] a popular model of such systems has been a Brownian particle of mass M moving in a metastable potential $V(q)$ while coupled to an environment at temperature T. At sufficiently high temperatures the potential barrier separating the metastable minimum from the region of lower potential is surmounted in a classical fashion by thermal activation, and the decay rate is given by the familiar Arrhenius law.[1] On the other hand, at low temperatures tunneling through the barrier becomes more probable, and the decay rate is given by the tunneling rate. Recently, Caldeira and Leggett[2] have shown that this quantum decay rate is strongly affected by the frictional influence of the environment. In this Letter we turn our attention to the transition from one region to the other.

We employ a functional-integral approach which is convenient because it allows the inclusion of dissipation as a nonlocal term in the effective action.[2] In the transition region the functional integral cannot be done by steepest descents but requires a more careful treatment which will be presented here.

The partition function of a Brownian particle may be written as a functional integral[3] over periodic paths where the path probability is weighted according to the Euclidean action[2,4]

$$S[q]=\int_0^{\hbar\beta} d\tau[\tfrac{1}{2}M\dot{q}^2+V(q)]+\tfrac{1}{2}\int_0^{\hbar\beta} d\tau\int_0^{\hbar\beta} d\tau' k(\tau-\tau')q(\tau)q(\tau'), \quad (1)$$

where $\beta=1/k_BT$. The first term in (1) describes the reversible motion while the second term describes the frictional influence of the environment. The damping kernel $k(\tau)$ may be expressed as a Fourier series[4]

$$k(\tau)=(M/\hbar\beta)\sum_{n=-\infty}^{+\infty}\zeta_n\exp(i\nu_n\tau),$$

where $\nu_n=\nu n$, $\nu=(2\pi/\hbar\beta)$, and where $\zeta_n=\gamma\times(i|\nu_n|)|\nu_n|$ is related to the frequency-dependent damping coefficient $\gamma(\omega)$. In the important case of Ohmic dissipation we simply have $\zeta_n=\gamma|\nu_n|$.

Consider now a potential $V(q)$ which has a metastable minimum at $q=0$, $V=0$, and a barrier of height $V_b=V(q_b)$ (Fig. 1). For a particle in the metastable well, the partition function must be defined by an analytical continuation from a stable to the unstable situation.[5] This leads to an (exponentially small) imaginary part of the free energy F which is proportional to the decay rate.[5,6] We expect this connection to remain unchanged in the dissipative case for reasons given below.

At high temperatures the imaginary part of F comes from the contribution of the "saddle point" $q(\tau)=q_b$. Continuing the integral over the unstable mode into the complex plane, one finds

$$\mathrm{Im}F=(1/2\beta)[D_0/|D_b|]^{1/2}\exp(-\beta V_b), \quad (2)$$

where D_0 and D_b are determinants of second-order variation operators given by

$$D_0=\prod_{n=-\infty}^{+\infty}\nu_n^2+\omega_0^2+\zeta_n;\quad D_b=\prod_{n=-\infty}^{+\infty}\lambda_n$$

in which $\lambda_n=\nu_n^2-\omega_b^2+\zeta_n$. The frequencies ω_0 and ω_b are given by $\omega_0^2=V''(0)/M$ and $\omega_b^2=-V''(q_b)/M$.

When the temperature is lowered one of the eigenvalues λ_n goes through 0 at a certain temperature. For all models of the dissipative mechanism of interest, λ_1 is the first eigenvalue changing sign. The relation $\lambda_1(T_c)=0$ defines a crossover temperature T_c which, e.g., for Ohmic dissipation is given by

$$T_c=(\hbar/2\pi k_B)[(\omega_b^2+\gamma^2/4)^{1/2}-\gamma/2].$$

Note that dissipation lowers T_c so that quantum

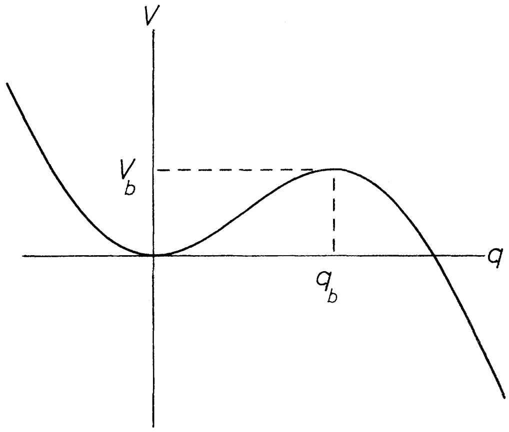

FIG. 1. Form of the metastable potential.

tunneling effects are diminished by the damping. The high-temperature formula (2) holds above T_c, and in this region the decay rate Γ is related to ImF by[6] $\Gamma = (2/\hbar)(\beta/\beta_c)\mathrm{Im}F$ which gives

$$\Gamma = \frac{\nu_c \omega_0}{2\pi\omega_b} \prod_{n=1}^{\infty} \frac{\nu_n^2 + \omega_0^2 + \zeta_n}{\nu_n^2 - \omega_b^2 + \zeta_n} \exp(-\beta V_b), \quad (3)$$

where $\nu_c = 2\pi/\hbar\beta_c = 2\pi k_B T_c/\hbar$. The result (3) has been obtained by Wolynes[7] following a different line of reasoning.

In the classical limit ($T >> T_c$) one finds $\Gamma = (\nu_c \omega_0/2\pi\omega_b)\exp(-\beta V_b)$ which for Ohmic dissipation gives the familiar result found by Kramers.[1] On the other hand, putting $\lambda_1 = a(\nu - \nu_c)/\nu_c$ where $a = \nu_c(\nu + \nu_c + \gamma)$ for Ohmic dissipation, we find

$$\Gamma = (\nu_c/2\pi) A T_c (T - T_c)^{-1} \exp(-\beta V_b), \quad (4)$$

where we have introduced the dimensionless quantity

$$A = \frac{\omega_0}{\omega_b} \frac{\nu^2 + \omega_0^2 + \zeta_1}{a} \prod_{n=2}^{\infty} \frac{\nu_n^2 + \omega_0^2 + \zeta_n}{\nu_n^2 - \omega_b^2 + \zeta_n}. \quad (5)$$

Thus, as noted by Wolynes,[7] the result (3) diverges at $T = T_c$. This divergence will be removed by the more detailed analysis presented below.

At temperatures below T_c the partition-function integral has another saddle point, the so-called bounce trajectory[8] $q_B(\tau) = q_b + x(\tau)$. The fluctuation modes about this trajectory include a zero mode, $\dot{x}(\tau)$, and an unstable mode. Deforming the integration contour with respect to the negative mode, one finds[2,4]

$$\mathrm{Im}F = \frac{\hbar}{2}\left(\frac{S_0}{2\pi\hbar}\right)^{1/2}\left(\frac{D_0}{|D_B'|}\right)^{1/2}\exp\left(\frac{-S_B}{\hbar}\right)$$

where D_B' is the product of eigenvalues of bounce-fluctuation modes with the zero eigenvalue omitted. S_0 is a zero-mode normalization factor

$$S_0 = M\int_0^{\hbar\beta} d\tau \dot{x}^2, \quad (6)$$

and S_B is the action (1) evaluated along the bounce trajectory.

For temperatures near T_c the bounce trajectory can be determined perturbatively. Expanding the potential $V(q)$ about the barrier top

$$V(q) = V_b - \tfrac{1}{2}M\omega_b^2 x^2 + \sum_{j=3}^{\infty} (Mc_j/j)x^j,$$

where $x = q - q_b$, we can determine the coefficients $X_n = X_{-n}$ of the Fourier representation of the bounce trajectory

$$q_B(\tau) = q_b + \sum_{n=-\infty}^{+\infty} X_n \exp(i\nu_n\tau). \quad (7)$$

For small $(\beta - \beta_c)/\beta_c$ we then find for the bounce action

$$S_B = \hbar\beta V_b - \tfrac{1}{2}\hbar M a^2(\beta - \beta_c)^2/\beta_c B \quad (8)$$

and for the zero-mode factor (6)

$$S_0 = 8\pi^2 M a(\beta - \beta_c)/\hbar\beta_c^2 B,$$

where we have assumed that the coefficient

$$B = 4c_3^2/\omega_b^2 - 2c_3^2/\lambda_2 + 3c_4$$

is positive which is the case for most metastable potentials of interest. The result (8) has also been obtained by Larkin and Ovchinnikov.[9] To study the fluctuation modes, we put $q(\tau) = q_B(\tau) + y(\tau)$ and expand $y(\tau)$ in a Fourier series:

$$y(\tau) = \sum_{n=-\infty}^{+\infty} Y_n \exp(i\nu_n\tau).$$

The fluctuation $y(\tau)$ leads to a change ΔS of the action (1). Near T_c we may diagonalize the second-order variation operator which gives

$$\Delta S = \tfrac{1}{2}M\hbar\beta[-\omega_b^2\hat{Y}_0^2 + \sum_{n=2}^{\infty} 2\lambda_n \hat{Y}_n \hat{Y}_{-n} + a\beta_c^{-1}(\beta - \beta_c)(Y_1 + Y_{-1})^2], \quad (9)$$

where $\hat{Y}_0 = Y_0 - 2c_3\omega_b^{-2}X_1(Y_1 + Y_{-1})$, $\hat{Y}_{\pm 2} = Y_{\pm 2} + 2c_3\lambda_2^{-1}X_1 Y_{\pm 1}$, while the remaining Fourier coefficients remain unchanged. This yields

$$D_B' = -2a\omega_b^2\beta_c^{-1}(\beta-\beta_c)\prod_{n=2}^{\infty}\lambda_n^2.$$

Now, below T_c the decay rate Γ is related to the imaginary part of the free energy by[6] $\Gamma=(2/\hbar)\mathrm{Im}F$. Collecting the results we find

$$\Gamma = A\,(2\pi S_B''/\hbar)^{1/2}\exp[-\beta V_b + \tfrac{1}{2}\hbar S_B''(\beta-\beta_c)^2], \tag{10}$$

where

$$S_B'' = -\left.\frac{\partial^2 S_B}{\partial(\hbar\beta)^2}\right|_{\beta=\beta_c} = \frac{1}{2\pi}\frac{M\nu_c a^2}{B}.$$

Since the bounce has been determined perturbatively, the result (10) holds only near T_c, more precisely, for $|T-T_c| << T_c\omega_b^2/a$ where ω_b^2/a is a factor of order 1. However, very close to T_c, for[10] $|T-T_c| \lesssim T_c(\nu_c/2\pi)(\hbar/S_B'')^{1/2}$, the fluctuation $\frac{1}{2}(Y_1+Y_{-1})$ of the bounce amplitude is of the same order of magnitude as the amplitude X_1, and the functional integral cannot be done by steepest descents. This crossover region will be studied in the following.

For $T \lesssim T_c$ the fluctuation modes about the bounce trajectory include two dangerous modes whose contribution to the partition function cannot be calculated by the method of steepest descent: the zero mode, $\dot{x}(\tau)$, which describes phase fluctuations of the bounce, and a quasi zero mode describing amplitude fluctuations. The eigenvalue of this latter mode vanishes at T_c. To proceed we must determine the increase of action ΔS caused by a fluctuation $y(\tau)$ more accurately as in (9) by taking into account terms of the third and fourth order in the amplitudes of the dangerous modes, i.e., in Y_1 and Y_{-1}. These higher-order terms include nonlinear couplings between the dangerous modes and the other modes. Having performed this expansion, we integrate out the stable modes $[Y_{\pm n}, n\geqslant 2]$ by steepest descents and integrate over the unstable mode along a contour deformed in the usual way.[5] We then are left with an effective action of the dangerous fluctuations which is given by

$$\Delta S_1 = \tfrac{1}{2}MB\hbar\beta[X_1^2(Y_1+Y_{-1})^2 + 2X_1(Y_1+Y_{-1})Y_1Y_{-1} + (Y_1Y_{-1})^2].$$

We now introduce polar coordinates (ρ,ϕ) by $\rho\cos\phi = X_1+\frac{1}{2}(Y_1+Y_{-1})$, $\rho\sin\phi=(1/2i)(Y_1-Y_{-1})$ and find that ΔS_1 is independent of ϕ as it should be. After a corresponding transformation of the integration measure, the ϕ integral is trivial and the ρ integral can be transformed into an error integral. The imaginary part of the free energy then emerges as

$$\mathrm{Im}F = \frac{1}{2\beta}\frac{D_0^{1/2}}{\omega_b\prod_{n=2}^{\infty}\lambda_n}(2\pi M\beta_c/B)^{1/2}\tfrac{1}{2}\mathrm{erfc}[(Ma^2/2B\beta_c)^{1/2}(\beta-\beta_c)]\exp(-S_B/\hbar),$$

where $\mathrm{erfc}(x) = 2\pi^{-1/2}\int_{-\infty}^{x} dt\,\exp(-t^2)$. Now, using $\Gamma=(2/\hbar)\mathrm{Im}F$, we obtain

$$\Gamma = A\,(2\pi S_B''/\hbar)^{1/2}\tfrac{1}{2}\mathrm{erfc}[(\hbar S_B''/2)^{1/2}(\beta-\beta_c)]\exp[-\beta V_b+\tfrac{1}{2}\hbar S_B''(\beta-\beta_c)^2]. \tag{11}$$

Below T_c the function $\frac{1}{2}\mathrm{erfc}[(\hbar S_B''/2)^{1/2}(\beta-\beta_c)]$ approaches 1 very rapidly and we recover our previous result (10). On the other hand, above T_c, we have asymptotically

$$\mathrm{erfc}[(\hbar S_B''/2)^{1/2}(\beta-\beta_c)]\exp[\tfrac{1}{2}\hbar S_B''(\beta-\beta_c)^2] \approx 2(2\pi\hbar S_B'')^{-1/2}(\beta_c-\beta)^{-1}.$$

Hence Γ approaches (4) and matches smoothly onto the high-temperature formula (3). Near T_c the relevant temperature scale is characterized by the dimensionless scaled temperature $\theta=(\pi/\nu_c)(2S_B''/\hbar)^{1/2}(T-T_c)/T_c$, and the rate Γ is conveniently measured in units of the characteristic frequency $\omega_c/2\pi = A_c(\pi S_B''/2\hbar)^{1/2}$ where A_c is the quantity (5) at the crossover temperature. Provided[10] $(\nu_c/2\pi)(\hbar/S_B'')^{1/2} << \omega_b^2/a$, the temperature dependence of the Arrhenius prefactor expressed in these units takes on a universal form which is shown in Fig. 2. There, the classical rate would be represented by a horizontal line with axis intercept $\nu_c\omega_0/\omega_b\omega_c << 1$. As T_c is approached from above, the Arrhenius prefactor grows due to tunneling contributions to the decay rate. Below T_c this growth becomes exponentially fast, and the exponentially growing part of the prefactor is then combined with the Arrhenius exponential factor leading to the "bounce formula" (10) for the decay rate. In the zero-damping limit[11] one has $S_B''=-\partial E/\partial\Theta$ where $\Theta=\hbar\beta$ is the bounce period and $E=\partial S_B/\partial\Theta$ the bounce energy. Then, (11) gives the result found by Affleck[6] by means of a Boltzmann average over energy-dependent decay

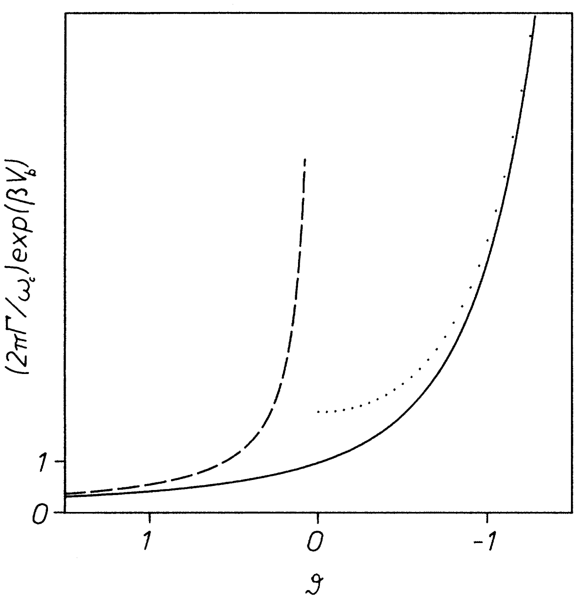

FIG. 2. The Arrhenius prefactor of the decay rate, $\Gamma\exp(\beta V_b)$, in units of $\omega_c/2\pi$ is plotted as a function of the dimensionless temperature $\theta \propto (T-T_c)/T_c$. The high-$T$ formula (3) is shown as a dashed line, and the low-T formula (10) as a dotted line. The solid line shows the formula (11).

rates cut off at $E = V_b$. In a dissipative system, tunneling events are diminished and the transition occurs at lower temperatures where the rate has already reached a much lower value.

So far we have not addressed the important issue of whether the imaginary part of the free energy remains proportional to the decay rate when dissipation is included. We expect the formulas[6] relating Γ to Im F above and below T_c to remain unchanged for the following reasons. The result (3) for Γ based on $\Gamma = (2/\hbar)(\beta/\beta_c)\mathrm{Im}F$ for temperatures above T_c coincides with an earlier result by Wolynes[7] derived by means of a real-time calculation based on a Green-Kubo formula. Further, for temperatures slightly below T_c, the validity of $\Gamma = (2/\hbar)\mathrm{Im}F$ for the dissipative case can be verified by treating the decay in a multidimensional potential which includes the environmental coordinates by conventional methods. Finally, $\Gamma = (2/\hbar)\mathrm{Im}F$ holds for dissipative systems at $T = 0$.[2] These arguments certainly provide strong evidence for the corrections of our approach.

The results derived in this Letter are very general, and they can be applied to analyze experiments on the decay of metastable states in dissipative systems in the temperature range where quantum effects are important. In particular, the problem of macroscopic quantum tunneling in Josephson systems has recently attracted a great deal of experimental and theoretical interest. The crossover from classical to quantal behavior has been observed, e.g., in experiments on the decay of the zero-voltage state in current-driven Josephson junctions.[12] An analysis of our results shows that quantum effects enhance the decay rate by an order of magnitude as compared to the classical rate already at intermediate temperatures $T \approx 3T_c$. This effect is important for the precise determination of the junction parameters, and its consideration leads to an improved agreement between the very low-temperature data and the Caldeira-Leggett theory.[2] We intend to discuss the details of this application elsewhere.

We would like to thank P. Hanggi, A. J. Leggett, and P. Riseborough for interesting discussions.

[1]H. A. Kramers, Physica (Utrecht) **7**, 284 (1940).

[2]A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. **46**, 211 (1981), and Ann. Phys. (N.Y.) **149**, 374 (1983).

[3]R. P. Feynman, *Statistical Mechanics* (Benjamin, New York, 1972).

[4]H. Grabert, U. Weiss, and P. Hanggi, Phys. Rev. Lett. **52**, 2193 (1984); H. Grabert and U. Weiss, Z. Phys. B **56**, 171 (1984).

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

[6]I. Affleck, Phys. Rev. Lett. **46**, 388 (1981).

[7]P. G. Wolynes, Phys. Rev. Lett. **47**, 968 (1981). See also V. I. Mel'nikov and S. V. Meshkov, Pis'ma Zh. Eksp. Teor. Fiz. **38**, 111 (1983) [JETP Lett. **38**, 130 (1983)].

[8]C. Callan and S. Coleman, Phys. Rev. D **16**, 1762 (1977).

[9]A. I. Larkin and Yu. N. Ovchinnikov, Pis'ma Zh. Eksp. Teor. Fiz. **37**, 322 (1983) [JETP Lett. **37**, 382 (1983)].

[10]One can assume $V_b \gg \hbar\omega_0, \hbar\gamma, k_BT$, otherwise, the state $q=0$ would not be metastable. For reasonably smooth potentials one then has $(\nu_c/2\pi)(\hbar/S_B'')^{1/2} \ll \omega_b^2/a$.

[11]This limit must be understood in the same way as the transition-state approximation in the classical case. In the extremely underdamped limit the thermal relaxation time in the metastable well becomes large compared to Γ^{-1} and the quasistationary approximation implicit in our work breaks down.

[12]R. T. Voss and R. A. Webb, Phys. Rev. Lett. **47**, 265 (1981). L. D. Jackel *et al.*, Phys. Rev. Lett. **47** 697 (1981).