Quantum tunneling with dissipation

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Dissipative processes reduce the probability for quantum tunneling. The temperature dependence of the probability for the decay of a metastable state is analyzed.

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As a classical particle moves through a dissipative medium, a friction force proportional to the velocity of the particle arises. We are interested in how this force affects the probability for the particle to tunnel through a semiclassical barrier. This problem has been solved previously[1] for the case of a zero temperature; in the present letter we generalize to arbitrary temperatures. At sufficiently high temperatures the quantum tunneling is inconsequential, and the barrier is overcome in a classical fashion, involving an activation energy. The transmission probability W is described by an Arrhenius equation with an activation energy which is generally a smooth function of the temperature. At low temperatures, tunneling through the barrier is more probable. The transition from one regime to the other may be either a first-order or second-order transition. The general form of the temperature dependence of the lifetime of the system in the metastable state is found for a temperature near the critical temperature. An analytic solution is derived for arbitrary temperatures for the case in which viscous forces are much stronger than inertial forces, and the potential barrier is a cubic parabola.

We assume that it is possible to single out in the dissipative system a single semiclassical coordinate q, which interacts with a large number of quantum coordinates Q. The Hamiltonian of such a system can be written

$$\hat{H} = p^2/2m + V(q, Q); \qquad V(q, Q) = V(q) + qQ + H(Q). \tag{1}$$

It may be that there is neither a starting potential energy $V(q)$ nor a starting kinetic energy, and these energies arise only as a result of the interaction. For definiteness, we describe the Hamiltonian of the temperature reservoir, $H(Q)$, as a set of a large number of simple harmonic oscillators. Many of the results are independent of this assumption.

We assume that the tunneling probability is quite low, so that the system manages to reach thermal equilibrium while the coordinate q is in the classically allowed region on one side of the barrier. The average transition probability over a time t in this case is

$$W = Z^{-1} \sum_{i,f} |\langle \psi^f | \exp\left(-i \int_{t_i}^{t_f} dt\, \hat{H}\right) | \psi^i \rangle|^2 \exp(-E_i/T); \; Z = \sum_i \exp(-E_i/T). \tag{2}$$

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Here ψ^f, ψ^i, and E_i are the wave functions and energies of the final (f) and initial (i) states. These wave functions and energies should be found in the zeroth approximation in the barrier transmission. Expression (2) can be written as a path integral over the variable q:

$$W = \int Dq(t) Sp_Q \exp\left\{ i \int_C \left[\frac{m}{2}\dot{q}^2 - V(q,Q)\right] dt \right\}. \qquad (3)$$

Here the contour $\widetilde{C}$ is a broken line connecting the points $(t_i + i/2T, t_i, t_f, t_i, t_i - i/2T)$.

In this letter we will be content with calculating the transition probability with an exponential accuracy. For this purpose we need to find the extreme path along which we see the system go from one metastable state to another.

There are no such paths if there is motion only in real time. We displace the vertical part of the contour to the imaginary axis, so that the final points $t = \pm i/2T$ correspond to a state of the system in the semiclassical region on one side of the barrier, while the point $t = 0$ corresponds to the other side of the barrier. We put the origin of the time scale between t_i and t_f. On the extreme path the coordinate q satisfies the condition

$$q(t + i\tau) = q(t - i\tau). \qquad (4)$$

In the calculation of Sp_Q, Green's phonon functions arise on a Keldysh contour.[2] Diagrams in which at least one end of a Green's phonon function lies on a part of the contour running parallel to the real axis cancel out. This cancellation results from the symmetry property (4) for the coordinate q and from the different signs of the increments in time on the parts of the contour running parallel to the real axis. These parts of the contour contribute to W only if q deviates from its extreme value. As a result, the coefficient of the exponential function is proportional to $t_f - t_i$. After the substitution $t = -i\tau$ we find, with exponential accuracy.

$$W = \exp(-A); \quad A = \ln \mathrm{Sp}_Q \exp\left\{ \int_{-1/2T}^{1/2T} d\tau \left[\frac{m}{2}\left(\frac{\partial q}{\partial \tau}\right)^2 + V(q,Q)\right]\right\}. \qquad (5)$$

The function $q(\tau)$ in (5) is determined from the condition for an extremum of the functional A, and it satisfies the boundary condition $q(1/2T) = q(-1/2T)$. At sufficiently high temperatures, the functional A reaches its extreme value for the function $q(\tau) = q_0 = \mathrm{const}$:

$$A_0 = F(q_0)/T, \qquad (6)$$

where $F(q_0)$ is the extreme value of the free energy as a function of the parameter q. In quantum-mechanical tunneling we would have

$$q(\tau) = q_0 + \sum_{n=0}^{\infty} a_n \cos(2\pi T n \tau). \qquad (7)$$

If the transition from the classical case to the quantum-mechanical tunneling is a second-order transition, the coefficients a_n are small near the transition temperature

T_0, and the action A can be written

$$A = A_0 + \alpha a_1^2 + B a_1^4 . \tag{8}$$

The transition point T_0 is determined from the condition $\alpha(T_0) = 0$. We have assumed that as the temperature is lowered the coefficient of a_1^2 is the first to vanish. In this case, we have $|a_{n\neq 1}| \ll |a_1|$ near T_0.

The coefficient a_1 is found from the condition for a minimum of expression (7). Above the transition point we have $A = A_0$, while below it we have

$$A - A_0 = -\alpha^2/4B = -(\alpha')^2 (T - T_0)^2/4B . \tag{9}$$

For the model described by Hamiltonian (1), we have

$$A[q(\tau)] = \int_{-1/2T}^{1/2T} d\tau \left[\frac{m}{2}\left(\frac{\partial q}{\partial \tau}\right)^2 + V(q) + \frac{1}{2}\int_{-1/2T}^{1/2T} d\tau_1\, q(\tau) q(\tau_1) D(\tau - \tau_1) \right], \tag{10}$$

where $D(\tau)$ is the Matsubara Green's function,

$$D(\tau) = T \sum_{\omega_n} D(\omega_n) \exp(-i\omega_n \tau); \quad D(\omega_n) = -\sum_k \frac{C_k^2}{\omega_k^2 + \omega_n^2}; \quad \omega_n = 2\pi T n . \tag{11}$$

Substituting expression (7) for the function $q(\tau)$ into (10), and expanding it in powers of a_n, we find

$$\alpha = \pi^2 T m + V''/4T + (D_1 - D_0)/4T,$$

$$B = \frac{1}{64T}\frac{\partial^4 V}{\partial q^4} - \frac{(\partial^3 V/\partial^3 q)^2}{32 T V''}\left(1 + \frac{V''}{2(16\pi^2 T^2 m + V'' + D_2 - D_0)}\right). \tag{12}$$

The derivatives are evaluated at the point q_0. If the coefficient B is greater than zero, the transition at $T = T_0$ is a second-order transition. It follows from (12) that the cubic term in the expansion of the potential in powers of $q - q_0$ corresponds to the onset of the second-order transition. The oscillators with frequencies ω_k greater than the reciprocal tunneling time cause a renormalization of the mass m and of the potential $V(q)$. The interaction with low-frequency phonons gives rise to the viscosity. It follows from the derivation of the Langevin equation in the classically allowed region[3] that the viscosity coefficient η is related to the Green's function D at low frequencies by

$$D(\omega_n) = D_0 + \eta |\omega_n| . \tag{13}$$

Renormalizing the mass and the potential in (10), using (13), we find

$$A[q(\tau)] = \int_{-1/2T}^{1/2T} d\tau \left\{ \frac{m^*}{2}\left(\frac{\partial q}{\partial \tau}\right)^2 + V^*(q) + \frac{\eta}{4\pi}\int_{-\infty}^{\infty} d\tau_1 \frac{(q(\tau) - q(\tau_1))^2}{(\tau_1 - \tau)^2} \right\}. \tag{14}$$

The function $q(\tau)$ in (14) is continued periodically: $q(\tau + 4/T) = q(\tau)$. At $T = 0$, expression (14) becomes the same as that derived in Ref. 1.

Let us examine the interesting case in which $V^*(q)$ is a cubic parabola:

$$V(q) = 3 V_0 (q/q_0)^2 \left(1 - \frac{2}{3}\frac{q}{q_0}\right). \tag{15}$$

We further assume that the viscosity η is large, $(\eta q_0)^2 \gg 6m^* V_0$, so that we may ignore the first term in (14). In this limiting case $q(\tau)$ satisfies the equation

$$-\frac{6V_0 q}{q_0^2}(1-q/q_0)+\frac{\eta}{\pi}\fint_{-\infty}^{\infty} d\tau_1 \frac{\partial q(\tau_1)}{\partial \tau_1}\frac{1}{\tau_1-\tau}=0 . \qquad (16)$$

The solution of Eq. (16) is of the form in (7), with

$$a_0=-q_0\,(1-T/T^*), \qquad a_n = 2q_0\, T/T^* \exp(-bn),$$
$$T^* = 3V_0/\pi\eta q_0^2 , \qquad \operatorname{cth} b = T^*/T . \qquad (17)$$

Substituting this value of $q(\tau)$ into (14), we find

$$A=\frac{V_0}{T_0}\left[\frac{3}{2}-\frac{1}{2}(T/T_0)^2\right], \qquad T_0=T^*\,(1-6m^* V_0/\eta^2 q_0^2). \qquad (18)$$

In (18) we have retained terms of first order in m^*. At $T=0$, this expression agrees with the result of Refs. 4 and 5.

These results apply to the case in which the system is nearly at thermal equilibrium before the tunneling occurs. The method used here can also be applied to tunneling in nonequilibrium systems.

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