Phase transitions in the problem of the decay of a metastable state

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The decay of a metastable state is studied by means of a functional-integral approach. Depending on the shape of the potential barrier, the crossover from thermal activation to thermally assisted quantum tunneling is either a first- or second-order phase transition on temperature. Below the crossover temperature, first-order transitions between different tunneling regimes are possible. The general features of these transitions, and the possibilities to observe them, are discussed.

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Consider a particle of mass M in a metastable state formed by the potential $V(q)$, Fig. 1. The probability of the escape is assumed to be exponentially small, providing that the particle is in a thermodynamic equilibrium with the environment. At high temperature, the decay of the metastable state is determined by processes of thermal activation, which are governed by the Boltzmann factor, $\exp(-E_0/k_BT)$. At $T=0$ the particle can escape from the metastable state due to quantum tunneling, the rate of which goes as $\exp(-B)$, B being the WKB exponent. The crossover from the thermal to the quantum regime has been intensively studied in the last decade. Goldanskii [1] long ago suggested that the crossover occurs at $k_BT_0=\hbar/\tau_0$, where τ_0 is the period of small oscillations near the bottom of the inversed potential, Fig. 1. Based upon the functional-integral approach of Langer [2] and Callan and Coleman [3], Affleck [4] and Larkin and Ovchinnikov [5] demonstrated that a second-order phase transition from the thermal to the quantum regime takes place at $T=T_0$. In terms of the escape rate, $\Gamma(T)$, this means that, in the steepest-descent approximation, $\Gamma(T)$ and its first derivative $\Gamma'(T)$ are continuous, while the second derivative, $\Gamma''(T)$, is discontinuous at $T=T_0$. Quantum fluctuations, of course, smear this transition in a narrow temperature region near T_0. Interaction between the particle and the dissipative environment renormalizes T_0 but does not affect the general features of the transition. A rigorous solution to that problem was given by Grabert and Weiss [6], Larkin and Ovchinnikov [7], Zwerger [8], and Riseborough, Hänggi, and Freidkin [9]. This allowed Clarke *et al.* [10] to perform a detailed comparison between the theory and experiment on macroscopic quantum tunneling [11] in Josephson junctions. Other areas where similar phenomena may occur include tunneling of magnetization in solids, low-temperature diffusion of defects, chemical reactions, and nuclear physics. In this Brief Report, I show that the crossover from the thermal to the quantum regime can quite generally be the first-order transition [12] that takes place at $T_c>T_0$. Moreover, first-order transitions are possible between different thermally assisted tunneling regimes below T_c.

The statistical average of the transition probability over a time $t=t_f-t_i$ is

$$P=\frac{\sum_{i,f}\left|\langle\psi_f|\exp\left[-\frac{i}{\hbar}\int_{t_i}^{t_f}dt\,\hat{\mathcal{H}}\right]|\psi_i\rangle\right|^2\exp(-E_i/k_BT)}{\sum_i\exp(-E_i/k_BT)}\,, \tag{1}$$

where $\mathcal{H}$ is the Hamiltonian of the system, E_i are energy levels of the particle, and ψ_i and ψ_f are the wave functions of the initial and final states. According to Feynman [13], this is equivalent [14] to the computation of the functional integral

$$\int D\{q(\tau)\}\exp\left\{-\frac{1}{\hbar}\oint d\tau\,\mathcal{L}[q(\tau)]\right\}, \tag{2}$$

where $\mathcal{L}[q(\tau)]$ is the imaginary-time ($\tau=it$) classical Lagrangian of the system, the functional integration is performed over $q(\tau)$ trajectories which are periodic in τ with the period $\tau_p=\hbar/k_BT$, the integral in the exponent is taken over the period τ_p.

Consider the imaginary-time action

$$S(T)=\oint d\tau\,\mathcal{L}=\oint d\tau[\tfrac{1}{2}M\dot{q}^2+V(q)] \tag{3}$$

with $V(q)$ of the shape shown in Fig. 1, and $\dot{q}\equiv dq/d\tau$. According to (2), the decay rate in a semiclassical limit ($S\gg\hbar$), with an exponential accuracy, is

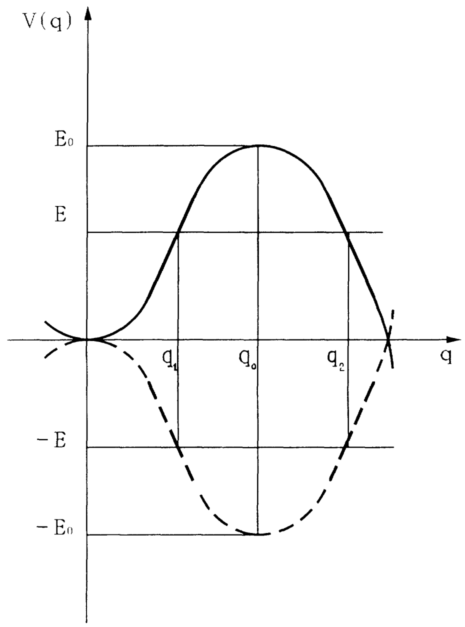

FIG. 1. The shape of the potential $V(q)$ (solid line) and the shape of the inverted potential $-V(q)$ (dashed line).

$$\Gamma \propto \exp(-S_{\min}/\hbar) , \tag{4}$$

where $S_{\min}(T)$ is evaluated along the $q(\tau)$ trajectory with $\tau_p = \hbar/k_B T$ that minimizes Eq. (3) [15]. Such trajectories satisfy

$$M\ddot{q} = \frac{dV}{dq} . \tag{5}$$

Periodic, with $\tau_p = \hbar/k_B T$, solutions of this equation belong to two classes: a constant, $q = q_0$, and $q(\tau)$ satisfying

$$\tfrac{1}{2}M\dot{q}^2 = V(q) - E(\tau_p) . \tag{6}$$

The first solution, $q = q_0$, corresponds to the particle in rest at the bottom of the inversed potential (Fig. 1). The second solution, $q(\tau)$ given by Eq. (6), corresponds to the periodic motion of the particle in the inversed potential between $q_1(E)$ and $q_2(E)$ (Fig. 1), with E determined by the condition that the period of the motion equals $\hbar/k_B T$. I will call this trajectory the "thermon." At $T = 0$, that is, $\tau_p = \infty$, $E = 0$, the thermon becomes a regular instanton of Eq. (6) which determines the WKB exponent of quantum tunneling at zero temperature.

For $q = q_0$ one obtains from Eq. (3)

$$S_{\min} = S_0 = V(q_0)\tau_p = \hbar E_0/k_B T \tag{7}$$

and the escape rate

$$\Gamma_0 \propto \exp(-S_0/\hbar) = \exp(-E_0/k_B T) , \tag{8}$$

that is, the Boltzmann formula representing a pure thermal activation. The thermodynamic action S_0 should be compared with the thermon action, S_T. Since both S_0 and S_T are assumed to be large compared to $\hbar$, the smallest of the two determines the actual escape rate of Eq. (4).

With the help of Eq. (6), S_T can be written as

$$S_T = 2(2M)^{1/2} \int_{q_1(E)}^{q_2(E)} dq[V(q) - E]^{1/2} + E\tau_p(E) , \tag{9}$$

where

$$\tau_p(E) = (2M)^{1/2} \int_{q_1(E)}^{q_2(E)} dq[V(q) - E]^{-1/2} . \tag{10}$$

From Eqs. (7), (9), and (10) one obtains

$$\frac{dS_0}{d\tau_p} = E_0, \quad \frac{dS_T}{d\tau_p} = E > 0 . \tag{11}$$

This allows one to analyze the temperature dependence of $S_{\min}$ based upon the dependence of the thermon period $\tau_p = \hbar/k_B T$ on energy E. Note that dE/dT (which is proportional to the second derivative of the action) can be interpreted as the specific heat of the system. I will study here nonexotic potentials having a regular parabolic shape near the top ($q = q_0$) and the bottom ($q = 0$). Even in this case, τ_p may have a nontrivial dependence on E.

Let us start with a class of potentials for which τ_p is monotonically decreasing with E [Fig. 2(a)]. Two most common representatives of this class are potentials $(-q^2 + q^3)$ and $(-q^2 + q^4)$. This case has been studied in great detail [4–9]. In the limit of $E \to E_0$, the thermon reduces to small oscillations near the bottom of the inversed potential (Fig. 1),

$$q(\tau) = q_0 + A(E)\sin(\omega_0 \tau) \tag{12}$$

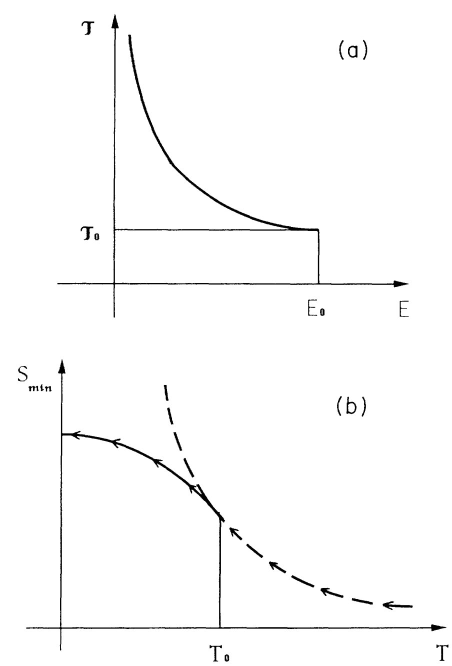

FIG. 2. (a) Monotonic dependence of τ_p on E. (b) Second-order transition from the thermal to the quantum regime. The solid line corresponds to the thermon action, $S_T(T)$. The dashed line corresponds to the thermodynamic action, $S_0(T)$. Arrows show the actual dependence of $S_{\min}(T)$, as temperature is lowered.

with $A(E_0)=0$. This limit corresponds to the approaching crossover temperature,

$$k_B T_0=\hbar/\tau_0=\hbar\omega_0/2\pi \ . \tag{13}$$

Substituting Eq. (12) into Eq. (3) one can easily see that $S_T<S_0$ at $T<T_0$ for $\tau_p(E)$ given by Fig. 2(a). Because $A(E_0)=0$, the thermon action coincides with the thermodynamic action, $S_T(T_0)=S_0$, at $T=T_0$. Equation (11) also gives

$$\left(\frac{dS_T}{dT}\right)_{T=T_0}=\left(\frac{dS_0}{dT}\right)_{T=T_0} . \tag{14}$$

This provides a smooth second-order transition from the thermal regime at $T>T_0$ to thermally assisted tunneling at $T<T_0$, as is shown in Fig. 2(b).

Our next example (Fig. 3) represents a class of potentials which change slowly near the top and the bottom, but are rather steep in the middle. Correspondingly, $\tau_p(E)$ may have a minimum at some $E_1<E_0$, Fig. 3(a). The dependence of $S_T(T)$ for such a potential follows from Eq. (11) and is shown in Fig. 3(b). As one lowers the temperature, the thermon action (solid line) becomes lower than the thermodynamic action (dashed line) at some $T=T_c$ satisfying $T_0<T_c<T_1$, where $k_BT_1=\hbar/\tau_p(E_1)$. The first derivative of $S_{\min}(T)$ is discontinuous at T_c, providing that the crossover from the thermal to the quantum regime is the first-order transition on temperature.

Our final example (Fig. 4) represents potentials for which $\tau_p(E)$ has a form shown in Fig. 4(a). As temperature is lowered, the second-order transition from the thermal to the quantum regime at $T=T_0$ is followed by the first-order transition between different quantum regimes at $T=T_c$.

The above consideration shows that the "phase diagram" for the decay of a metastable state can be as complex as the behavior of $\tau_p(E)$. The interesting feature is that the transition from the thermal to the quantum regime may quite generally occur as the first-order transition at $T_c>T_0$. The vicinity of the transition point, of course, cannot be investigated by the steepest-descent approximation employed here. It requires a careful analysis of quantum fluctuations in the spirit of Ref. [6]. Another potentially important effect, which has been left out of the picture, is the interaction of the tunneling variable with the dissipative environment. The effects will be studied elsewhere. It seems unlikely, however, that they can change our main conclusion on the possibility of smooth and sharp thermal-to-quantum transitions, depending on the shape of the potential barrier.

To date, the second-order transition from thermal activation to macroscopic quantum tunneling (MQT) has been observed clearly in Josephson junctions [10]. Another area for probing theoretical predictions on

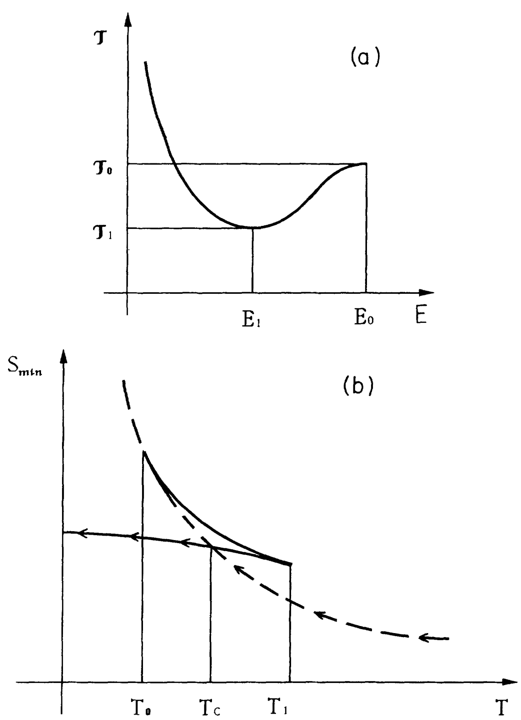

FIG. 3. (a) Nonmonotonic dependence of τ_p on E. (b) First-order transition from the thermal to the quantum regime. The solid line corresponds to the thermon action, $S_T(T)$. The dashed line corresponds to the thermodynamic action, S_0. Arrows show the actual dependence of $S_{\min}(T)$, as temperature is lowered.

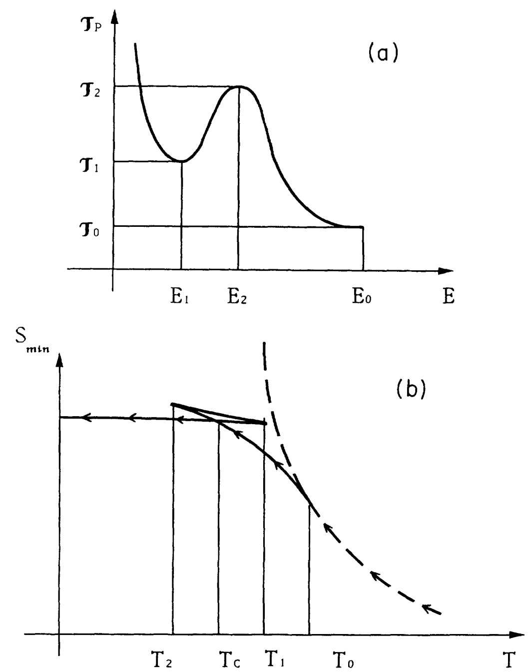

FIG. 4. (a) Another example of nonmonotonic dependence of τ_p on E. (b) As temperature is lowered, the second-order transition from the thermal to the quantum regime at $T=T_0$ is followed by the first-order transition between different quantum regimes at $T=T_c$; $k_BT_n=\hbar/\tau_n$ $(n=0,1,2)$.

MQT, which has recently emerged, is quantum decay of metastable magnetic states in solids [15–19]. Dissipation turns out to be very weak for magnetic tunneling. A large variety and complexity of energy barriers in magnetic systems make them promising candidates for the observation of all kinds of thermal-to-quantum transitions discussed in this Brief Report.

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