Dynamics of a particle in a two-well potential

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The density-matrix method is used to investigate the dynamics of a particle in a symmetric two-well potential. In second order of perturbation theory an expression is obtained for the relaxation rates and renormalization of the frequency of oscillations of the elements of the density matrix. The ground state of the system is investigated in the same approximation. It is shown that the so-called incoherent terms damp exponentially at large times. The simple picture of the renormalizations, leading to localization at $T = 0$ and for a sufficiently strong interaction with the thermostat, is also incorrect.

INTRODUCTION

The dynamics of a quantum particle in a two-well potential in the presence of interaction with a thermostat has recently been under active study. The main results were obtained in Refs. 1–3 and the review Ref. 4. Either the Hamiltonian method for a two-level system is used,[4] or the assumption is made that there is a discontinuous solution in the path-integral method.[5]

However, in the justification of the existence of a discontinuous solution there arise certain difficulties associated with the fact that the amplitude of fluctuations about the extremal path grow as the temperature is lowered. The eigenvalue of the operator $\delta^2 S[q]/\delta q^2$ (S is the effective action and q is the particle coordinate), responsible for the growth of fluctuations in the symmetric two-well potential, tends to zero with decrease of the temperature, exponentially in the absence of viscosity and as a power in the presence of viscosity. Therefore, in the decay problem the method of instantons requires further improvement. To study the rate of relaxation in the approximation of a two-level system it is necessary to perform extremely laborious summations. Here one makes a number of additional assumptions, which, apparently, are incorrect. With decrease of the temperature there is a sharp slowing of the rate of relaxation of a particle in a symmetric two-well potential.[1–4] The assumption that localization appears at $T = 0$ and at a value of the viscosity greater than a certain threshold value seems to us to be incorrect. To verify this assertion we shall investigate the relaxation process at a low temperature and low viscosity. Using perturbation theory we shall find corrections to the oscillation frequency up to terms $\sim \eta^2$ and shall show that the simple picture of the renormalizations in Refs. 1–4, which leads to localization, is incorrect. We note also that even for comparatively small values of the viscosity at low temperatures the ground state changes substantially. The difficulties in the calculation of the dynamics of a particle in a symmetric two-level potential are connected, apparently, with the change of the relaxation regime from a situation with weak damping, when the inverse relaxation time Γ is proportional to Δ—the splitting of the levels in the two-well potential (or to the temperature T, if $T \gg \Delta$), to the situation when coherent processes are unimportant and $\Gamma \sim \Delta^2$.

1. EQUATION FOR THE DENSITY MATRIX OF A PARTICLE INTERACTING WITH A THERMOSTAT

The dynamics of a particle interacting with a thermostat can be described using the density matrix $\hat{\rho}(t, \varphi, \tilde{\varphi})$ which depends on the time and the coordinates φ and $\tilde{\varphi}$. The advantage of this method is that fast processes are taken into account exactly in the zeroth approximation. The value of the density matrix at time t_f is expressed in terms of its value at time t_i by means of the path integral

$$\hat{\rho}(t_f, \varphi, \tilde{\varphi}) = \int D\varphi\, D\tilde{\varphi} \exp\{iA[\varphi, \tilde{\varphi}]\} \hat{\rho}(t_i, \varphi, \tilde{\varphi}). \tag{1}$$

Here the path integral is taken over all values of φ and $\tilde{\varphi}$ at the times from t_i to t_f. The effective action $A[\varphi, \tilde{\varphi}]$ can be represented in the form

$$A[\varphi, \tilde{\varphi}] = A_0[\varphi] - A_0[\tilde{\varphi}] + A_2[\varphi, \tilde{\varphi}], \tag{2}$$

where $A_0[\varphi]$ is the effective action in the absence of interaction with the thermostat:

$$A_0[\varphi] = \int_{t_i}^{t_f} \left[\frac{m}{2} \left(\frac{\partial \varphi}{\partial t} \right)^2 - V(\varphi) \right] dt. \tag{3}$$

The functional $A_2[\varphi, \tilde{\varphi}]$ is determined by the interaction of the quantum particle with the thermostat. For a tunnel junction, shunted by a normal resistance R_N, the functional $A_2[\varphi, \tilde{\varphi}]$ is equal to[6]

$$\begin{aligned} iA_2[\varphi, \tilde{\varphi}] = &-\frac{2\pi}{R_N e^2} \int_{t_i}^{t_f} dt \int_{t_i}^{t} dt_1 \Big\{ g^{>}(t, t_1)\, g^{<}(t_1, t) \\ &\times \sin^2 \left[\frac{\varphi(t) - \varphi(t_1)}{2} \right] \\ &+ g^{<}(t, t_1)\, g^{>}(t_1, t) \sin^2 \left[\frac{\tilde{\varphi}(t) - \tilde{\varphi}(t_1)}{2} \right] \Big\} \\ &+ \frac{2\pi}{R_N e^2} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} dt_1\, g^{<}(t, t_1)\, g^{>}(t_1, t) \sin^2 \left[\frac{\varphi(t) - \tilde{\varphi}(t_1)}{2} \right]. \end{aligned} \tag{4}$$

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The functions $g^{>(<)}(t,t_1)$ depend only on the difference of the times, and their Fourier components are equal to

$$g^{>}(\varepsilon)=1+\operatorname{th}(\varepsilon/2T),\quad g^{<}(\varepsilon)=-1+\operatorname{th}(\varepsilon/2T), \tag{5}$$

where T is the temperature of the thermostat. In the following we shall need only the convolution of these functions:

$$\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}g^{<}(\varepsilon)g^{>}(\varepsilon+\omega)=-\left[1+\operatorname{th}\left(\frac{\omega}{2T}\right)\right]M(\omega), \tag{6}$$

where

$$M(\omega)=\frac{\omega}{\pi}\operatorname{cth}\left(\frac{\omega}{2T}\right). \tag{7}$$

For a linear interaction of the quantum particle with a set of oscillators[4,5] the functional $A_2[\varphi,\tilde{\varphi}]$ has the same form (4) with the replacement

$$\sin^2\left[\frac{\varphi(t)-\varphi(t_1)}{2}\right]\to-\frac{\varphi(t)\varphi(t_1)}{2}. \tag{8}$$

Below we shall assume that the interaction with the thermostat is effectively cut off at frequencies $\omega_c\sim\Omega_p$, where Ω_p is the frequency of small oscillations about the minimum of the potential $V(\varphi)$:

$$m\Omega_p^2=\partial^2V/\partial\varphi^2. \tag{9}$$

We shall assume also that the potential $V(\varphi)$ is an even function of φ, having two minima lying at the points $\pm\varphi_0$. In this case, in the absence of interaction with the thermostat, the splitting of the levels is determined by the transparency of the barrier,[7] and for the particular case of a potential formed from two parabolas,

$$V(\varphi)=\frac{m\Omega_p^2}{2}\begin{cases}(\varphi+\varphi_0)^2, & \varphi<0\\ (\varphi-\varphi_0)^2, & \varphi>0\end{cases} \tag{10}$$

the magnitude δE_N of the splitting of the Nth level is equal to

$$\delta E_N=\frac{2\Omega_p}{(2\pi)^{1/2}}\frac{[\varphi_0(2m\Omega_p)^{1/2}]^{2N+1}}{\Gamma(N+1)}\exp(-m\Omega_p\varphi_0^2), \tag{11}$$

where $\Gamma(N)$ is the Euler gamma-function.

The interaction with the thermostat leads to a rearrangement of the ground state, to a change in the magnitude of the splitting, and to relaxation to the ground state. At low temperatures ($T\ll\Omega_p$) we can neglect the presence of the upper excited states and take only the transitions between the two lowest levels into account. Henceforth we shall denote these lowest levels by the numbers 1 and 2.

We represent the density matrix $\hat{\rho}$ in the form

$$\hat{\rho}(t,\varphi,\tilde{\varphi})=\sum_{m,n}\rho_n^m(t)\psi_m(\varphi)\psi_n^*(\tilde{\varphi})\exp[-i(E_m-E_n)t], \tag{12}$$

where $\psi_m(\varphi)$ are the eigenfunctions of the zeroth Hamiltonian with potential $V(\varphi)$. The density-matrix elements ρ_n^m satisfy the condition

$$\rho_n^m(t)=\rho_m^n(t)^*. \tag{13}$$

Since we neglect the occupation of the upper levels, we have

$$\rho_1^1(t)+\rho_2^2(t)=1. \tag{14}$$

The probability $W(1)$ of finding the particle in the left well and the probability $W(2)$ of finding it in the right well are expressed in terms of the density-matrix elements, with allowance for the formula (14), as follows:

$$\begin{aligned}W(1)&={}^1/_2[1+\rho_2^1(t)\exp(i\Delta t)+\rho_1^2(t)\exp(-i\Delta t)],\\ W(2)&={}^1/_2[1-\rho_2^1(t)\exp(i\Delta t)-\rho_1^2(t)\exp(-i\Delta t)],\end{aligned} \tag{15}$$

where the quantity Δ is the spacing between the levels 2 and 1:

$$\Delta=E_2-E_1 \tag{16}$$

in the absence of interaction with the thermostat.

To understand the relaxation process it is useful to consider not only the situation in which, at the initial time, the particle was in one of the wells (in this case, $\rho_2^1(0)=\rho_1^2(0)=1/2$), but also the situation when, at $t=0$, there exists a nonzero flux from one well to the other.

As follows from formula (15), the probability of finding the particle in one of the wells is determined entirely by the nondiagonal elements ρ_2^1 and ρ_1^2 and does not depend on the magnitude of the diagonal element ρ_1^1. However, the character of the rearrangement of the ground state is determined by the element ρ_1^1, and for this reason we shall also find this density-matrix element below.

Substituting the expression (12) for the density matrix into formula (1), we obtain

$$\rho_f^j(t_f)=\int d\varphi_1\int d\varphi_2\,\psi_j^*(\varphi_1)\psi_f(\varphi_2)\int D\varphi\,D\tilde{\varphi}\exp\{iA[\varphi,\tilde{\varphi}]\}$$
$$\times\hat{\rho}(t_i,\varphi_1,\varphi_2)\exp[i(E_j-E_f)t_f]. \tag{17}$$

We shall seek an expression for the elements $\rho_f^j(t_f)$ of the density matrix using perturbation theory in the coupling constant of the quantum particle with the thermostat.

2. PERTURBATION THEORY IN THE COUPLING CONSTANT

In the formula (17) we shall substitute the expression (2) for the quantity $A[\varphi,\tilde{\varphi}]$ and expand the exponential in powers of $A_2[\varphi,\tilde{\varphi}]$. As a result we obtain for the density-matrix elements $\rho_f^j(t_f)$ a perturbation-theory series in the interaction of the quantum particle with the thermostat. In the perturbation-theory calculations it is necessary to bear in mind that with the time varying in the interval t_2, t_1 ($t_2>t_1$) we have the equality

$$\int D\varphi\exp[iA_0[\varphi]]\psi_j(\varphi)=\exp[-iE_j(t_2-t_1)]\psi_j(\varphi), \tag{18}$$

where ψ_j is an eigenfunction of the zeroth Hamiltonian and E_j is the corresponding eigenvalue.

After simple calculations, for the first-order terms in the right-hand side of formula (17) we obtain

$$\left(\frac{\pi}{R_Ne^2}\right)\rho_n^m(t_i)$$
$$\times\left\{i\langle m|\varphi|k\rangle\langle k|\varphi|j\rangle\delta_{nf}\int\frac{d\varepsilon}{2\pi}\frac{[1+\operatorname{th}(\varepsilon/2T)]M(\varepsilon)}{E_k-E_m+\varepsilon-i\nu}\right.$$
$$\times\left[\int_{t_i}^{t_f}dt\exp[i(E_j-E_m)t]\right.$$
$$+i\frac{\exp[it_f(E_j-E_k-\varepsilon)]-\exp[it_i(E_j-E_k-\varepsilon)]}{E_j-E_k-\varepsilon}$$

$$\times \exp(it_i(E_k-E_m+\varepsilon))\Big]-i\langle n|\varphi|k\rangle\langle k|\varphi|f\rangle\cdot$$

$$\times\delta_{mj}\int\frac{d\varepsilon}{2\pi}\frac{[1+\mathrm{th}(\varepsilon/2T)]M(\varepsilon)}{E_k-E_n+\varepsilon+i\nu}\Big[\int_{t_i}^{t_f}dt\exp[i(E_n-E_f)t]$$

$$+i\frac{\exp[it_f(E_k-E_f+\varepsilon)]-\exp[it_i(E_k-E_f+\varepsilon)]}{E_k-E_f+\varepsilon}$$

$$\times\exp[it_i(E_n-E_k-\varepsilon)]\Big]+\langle n|\varphi|f\rangle\langle m|\varphi|j\rangle$$

$$\times\Big[\Big(1+\mathrm{th}\Big(\frac{E_n-E_f}{2T}\Big)\Big)M(E_n-E_f)$$

$$\times\int_{t_i}^{t_f}dt\exp[i(E_j-E_f+E_n-E_m)t]$$

$$-\int\frac{d\varepsilon}{2\pi}\Big(1+\mathrm{th}\Big(\frac{\varepsilon}{2T}\Big)\Big)$$

$$\times M(\varepsilon)\frac{\exp[it_f(E_j-E_m+\varepsilon)]-\exp[it_i(E_j-E_m+\varepsilon)]}{E_j-E_m+\varepsilon}$$

$$\times\Big(\frac{\exp[it_i(E_n-E_f-\varepsilon)]}{E_f-E_n+\varepsilon+i\nu}-\frac{\exp[it_f(E_n-E_f-\varepsilon)]}{E_f-E_n+\varepsilon-i\nu}\Big)\Big]\Big\}.\qquad(19)$$

Setting $t_f-t_i\gg\Delta$ (Δ is the spacing between levels 1 and 2) and retaining only terms proportional to t_f-t_i in formula (19), we obtain the well-known equation for the density matrix[4,8]

$$\frac{\partial\rho_1^{\,1}}{\partial t}=\frac{\alpha\pi^2}{2}\Big[-2M(\Delta)\rho_1^{\,1}+\Big(1+\mathrm{th}\Big(\frac{\Delta}{2T}\Big)\Big)M(\Delta)\Big]$$

$$\times\frac{\partial\rho_2^{\,1}}{\partial t}=-\frac{\alpha\pi^2}{2}\rho_2^{\,1}[M(\Delta)+2i\Delta I],\qquad(20)$$

where

$$\alpha=\frac{2}{\pi R_N e^2}\langle 1|\varphi|2\rangle^2\qquad(21)$$

is the effective coupling constant of the quantum particle with the thermostat, and

$$I=\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\frac{M(\varepsilon)}{\varepsilon^2-\Delta^2}.\qquad(22)$$

From formula (21) we find the renormalization of the oscillation frequency and the magnitudes of the inverse relaxation times $\gamma_{1,2}$ of the density-matrix elements in first order in α:

$$\tilde{\Delta}=\Delta(1-\alpha\pi^2 I),\qquad(23)$$

$$\gamma_1=\alpha\pi^2M(\Delta),\qquad\gamma_2=\alpha\pi^2M(\Delta)/2$$

(γ_1 is the inverse relaxation time of the diagonal element of the density matrix, and γ_2 is that for the nondiagonal element).

It follows from formula (19) that, apart from the terms proportional to t_f-t_i, there appear terms that do not depend on t_f-t_i and terms that damp as $(t_f-t_i)^{-2}$ at $T=0$. The latter have been named incoherent terms.[4] The time-independent terms are important for the determination of the frequency correction of second order in α and of the damping correction of first order in α. Rather cumbersome calculations of the second-order terms lead to a qualitatively new phenomenon—the appearance of damping in the incoherent terms, and the appearance of incoherent terms of a new type. For the density-matrix element $\rho_2^1(t_f)$ we find

$$\rho_2^{\,1}(t_f)=\rho_2^{\,1}(t_i)(B_1+B_2)\exp[(t_f-t_i)(-\gamma_2+i(\tilde{\Delta}-\Delta))]$$

$$+\frac{\alpha^2\pi^4}{4}\rho_2^{\,1}(t_i)(C_1+C_2)\exp[(t_f-t_i)(-\gamma_2-i(\Delta+\tilde{\Delta}))]$$

$$+\frac{\alpha\pi^2}{2}\rho_2^{\,1}(t_i)C_3\exp[-(t_f-t_i)(\gamma_1+i\Delta)]$$

$$+\frac{\alpha\pi^2}{2}\rho_1^{\,2}(t_i)\{(F+F_1)\exp(-2i\Delta t_f)$$

$$\times\exp[-(t_f-t_i)(\gamma_2+i(\tilde{\Delta}-\Delta))]$$

$$+(F^*+F_1^*)\exp(-2i\Delta t_i)\exp[-(t_f-t_i)(\gamma_2-i(\tilde{\Delta}-\Delta))]$$
$$-D\exp[-i\Delta(t_f+t_i)]\exp[-\gamma_1(t_f-t_i)]\},\qquad(24)$$

where the coefficients $B_{1,2}$, $C_{1,2,3}$, F, F_1, and D are equal to

$$B_1=1-\frac{\alpha\pi^2}{2}\Big[-\!\!\!\!\!\!\int\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta)^2}-iM'(\Delta)\Big]$$

$$+\frac{\alpha^2\pi^4}{4}\Big\{I\int\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta+i\nu)^2}$$

$$\times\Big(\frac{4\Delta}{\varepsilon-\Delta+i\nu}-1\Big)+\int\frac{d\varepsilon}{\pi}M(\varepsilon)\int\frac{d\varepsilon_1}{2\pi}M(\varepsilon_1)\Big[\frac{1}{(\varepsilon+\varepsilon_1+i\nu)^2}$$

$$\times\Big(\frac{2}{(\varepsilon+\Delta+i\nu)(\varepsilon-\Delta+i\nu)}+\frac{1}{(\varepsilon_1+\Delta+i\nu)(\varepsilon-\Delta+i\nu)}$$

$$-\frac{1}{(\varepsilon+\Delta+i\nu)^2}\Big)$$

$$-\frac{1}{(\varepsilon+\varepsilon_1+i\nu)(\varepsilon_1-\Delta+i\nu)^2(\varepsilon-\Delta+i\nu)}$$

$$+\frac{1}{(\varepsilon_1-\varepsilon-2\Delta+i\nu)(\varepsilon+\Delta-i\nu)(\varepsilon_1-\Delta+i\nu)^2}$$

$$+\frac{1}{(\varepsilon+\Delta-i\nu)^2}\Big(\frac{2}{(\varepsilon_1-\Delta+i\nu)^2}+\frac{1}{(\varepsilon_1+\Delta+i\nu)^2}\Big)\Big]$$

$$+\frac{M^2(\Delta)}{4\Delta^2}\Big[1-\mathrm{th}^2\Big(\frac{\Delta}{2T}\Big)\Big]$$

$$+i\int\frac{d\varepsilon}{2\pi}\frac{M^2(\varepsilon)[1-\mathrm{th}^2(\varepsilon/2T)]}{(\varepsilon-\Delta+i\nu)^2}\Big(\frac{1}{\varepsilon-\Delta+i\nu}$$

$$-\frac{1}{\varepsilon+\Delta+i\nu}\Big)-iM(\Delta)\int\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)}{(\varepsilon+\Delta-i\nu)^3}-\frac{iM(\Delta)}{2\Delta}\int\frac{d\varepsilon}{2\pi}M(\varepsilon)$$

$$\times\Big[1+\mathrm{th}\Big(\frac{\varepsilon}{2T}\Big)\Big]\Big(\frac{1+\mathrm{th}(\Delta/2T)}{(\varepsilon+\Delta-i\nu)^2}+\frac{1-\mathrm{th}(\Delta/2T)}{(\varepsilon-\Delta+i\nu)^2}\Big)\Big\},$$

$$B_2=\frac{\alpha^2\pi^4}{4}\Big\{\int\frac{d\varepsilon}{\pi}\int\frac{d\varepsilon_1}{\pi}M(\varepsilon)M(\varepsilon_1)\frac{\exp[i(t_f-t_i)(\varepsilon+\varepsilon_1)]}{(\varepsilon+\varepsilon_1+i\nu)^2}$$

$$\times\Big(\frac{1}{(\varepsilon_1+\Delta+i\nu)^2}+\frac{1}{(\varepsilon_1+\Delta+i\nu)(\varepsilon+\Delta+i\nu)}\Big)-i\int\frac{d\varepsilon}{2\pi}\int\frac{d\varepsilon_1}{2\pi}$$

$$\times\int_0^{t_f-t_i}dt\frac{M(\varepsilon)M(\varepsilon_1)}{(\varepsilon+\Delta-i\nu)(\varepsilon_1-\Delta+i\nu)}\exp[i\varepsilon_1 t-i\varepsilon(t_f-t_i-t)]$$

$$\times\left(\frac{1}{\varepsilon-\Delta-i\nu}-\frac{1}{\varepsilon+\Delta-i\nu}\right)\Bigg\},$$

$$C_1=\left[I+\frac{iM(\Delta)}{2\Delta}\right]^2,$$

$$C_2=\left[\int\frac{d\varepsilon}{2\pi}\frac{M(\varepsilon)\exp[i\varepsilon(t_f-t_i)]}{(\varepsilon-\Delta+i\nu)^2}\right]^2$$

$$+\int\frac{d\varepsilon}{\pi}\int\frac{d\varepsilon_1}{2\pi}\frac{M(\varepsilon)M(\varepsilon_1)\exp[i(\varepsilon+\varepsilon_1)(t_f-t_i)]}{(\varepsilon-\Delta+i\nu)(\varepsilon_1-\Delta+i\nu)^2(\varepsilon+\varepsilon_1-2\Delta+i\nu)} \tag{25}$$

$$C_3=\int\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)\exp[i\varepsilon(t_f-t_i)]}{(\varepsilon-\Delta+i\nu)^2}-\frac{\alpha\pi^2}{2}\Bigg\{\int\frac{d\varepsilon}{\pi}$$

$$\times\frac{M(\varepsilon)\exp[i\varepsilon(t_f-t_i)]}{(\varepsilon-\Delta+i\nu)}\Bigg(\frac{4\Delta I}{(\varepsilon-\Delta+i\nu)^2}$$

$$-\frac{2\Delta I}{(\varepsilon-\Delta+i\nu)(\varepsilon+\Delta+i\nu)}$$

$$+\frac{2\Delta I-iM(\Delta)\operatorname{th}(\Delta/2T)}{4\Delta(\varepsilon+\Delta+i\nu)}-\frac{I}{\varepsilon-\Delta+i\nu}$$

$$-i\frac{[1+\operatorname{th}(\Delta/2T)]M'(\Delta)}{(\varepsilon-\Delta+i\nu)}$$

$$-i\frac{M(\Delta)}{(\varepsilon-\Delta+i\nu)2T\operatorname{ch}^2(\Delta/2T)}+i\frac{M(\varepsilon)+2M(\Delta)}{2(\varepsilon-\Delta+i\nu)}$$

$$\times\left(\frac{1}{\varepsilon-\Delta+i\nu}-\frac{1}{\varepsilon+\Delta+i\nu}\right)\Bigg)+\int\frac{d\varepsilon}{\pi}\int\frac{d\varepsilon_1}{\pi}M(\varepsilon)M(\varepsilon_1)$$

$$\times\exp[i\varepsilon(t_f-t_i)]$$

$$\times\Bigg[\frac{1}{(\varepsilon-\Delta+i\nu)^2}\left(\frac{5}{4(\varepsilon_1+\Delta+i\nu)^2}+\frac{1}{(\varepsilon_1+\Delta-i\nu)^2}\right)$$

$$+\frac{1}{2(\varepsilon+\varepsilon_1+i\nu)(\varepsilon-\Delta+i\nu)(\varepsilon_1+\Delta+i\nu)}$$

$$\times\left(\frac{1}{\varepsilon+\Delta+i\nu}-\frac{1}{\varepsilon-\Delta+i\nu}\right)\Bigg]\Bigg\},$$

$$F=I+\frac{iM(\Delta)}{2\Delta}-\frac{\alpha\pi^2}{2}$$

$$\times\int\frac{d\varepsilon}{\pi}\int\frac{d\varepsilon_1}{\pi}\frac{M(\varepsilon)M(\varepsilon_1)}{(\varepsilon-\Delta-i\nu)^2(\varepsilon_1-\Delta-i\nu)(\varepsilon+\varepsilon_1-i\nu)},$$

$$F_1=-\frac{\alpha\pi^2}{2}\int\frac{d\varepsilon}{\pi}\int\frac{d\varepsilon_1}{\pi}\frac{M(\varepsilon)M(\varepsilon_1)\exp[i(\varepsilon+\varepsilon_1)(t_f-t_i)]}{(\varepsilon_1-\Delta+i\nu)^2(\varepsilon-\Delta+i\nu)(\varepsilon+\varepsilon_1+i\nu)},$$

$$D=\int\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)\exp[i\varepsilon(t_f-t_i)]}{(\varepsilon+\Delta+i\nu)(\varepsilon-\Delta+i\nu)}$$

$$-\alpha\pi^2\int\frac{d\varepsilon}{\pi}M(\varepsilon)\exp[i\varepsilon(t_f-t_i)]$$

$$\times\Bigg(\frac{4\Delta^2I}{(\varepsilon+\Delta+i\nu)^2(\varepsilon-\Delta+i\nu)^2}+\frac{1}{(\varepsilon+\Delta+i\nu)(\varepsilon-\Delta+i\nu)}$$

$$\times\fint\frac{d\varepsilon_1}{\pi}\frac{M(\varepsilon_1)}{(\varepsilon_1-\Delta)^2}\Bigg)$$

The quantities $\hat{\Delta}$ and γ_2, to within terms of second order in α, are equal to

$$\tilde{\Delta}=\Delta\Bigg\{1-\alpha\pi^2I-\frac{\alpha^2\pi^4}{4}\Bigg[2I^2-2I\fint\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta)^2}$$

$$+\frac{M^2(\Delta)}{4\Delta^2}\left(3-5\operatorname{th}^2\left(\frac{\Delta}{2T}\right)\right)+\frac{M(\Delta)M'(\Delta)}{\Delta}\left(2\operatorname{th}^2\left(\frac{\Delta}{2T}\right)-1\right)$$

$$+\frac{M^2(\Delta)\operatorname{th}(\Delta/2T)}{\Delta T\operatorname{ch}^2(\Delta/2T)}\Bigg]\Bigg\}, \tag{26}$$

$$\gamma_2=\frac{\alpha\pi^2}{2}M(\Delta)-\frac{\alpha^2\pi^4}{4}\Bigg[2\Delta IM'(\Delta)+M(\Delta)$$

$$\times\left(\fint\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta)^2}-2I\right)$$

$$+\fint\frac{d\varepsilon}{\pi}M^2(\varepsilon)\left(1-\operatorname{th}^2\left(\frac{\varepsilon}{2T}\right)\right)\left(\frac{1}{\varepsilon^2-\Delta^2}-\frac{1}{(\varepsilon-\Delta)^2}\right)\Bigg]$$

At $T=0$ the expression (26) for γ_2 coincides with the result of Ref. 4, but that for $\tilde{\Delta}$ does not agree with Ref. 4.
For the density-matrix element ρ_1^1 in the same approximation we obtain

$$\rho_1^1(t_f)=\rho_1^1(eq)[1-\exp(-\gamma_1(t_f-t_i))]$$

$$+\Bigg[\rho_1^1(t_i)\left(1-\alpha\pi^2\fint\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta)^2}\right)$$

$$+\frac{\alpha\pi^2}{2}\int\frac{d\varepsilon}{\pi}\frac{M(\varepsilon)(1+\operatorname{th}(\varepsilon/2T))}{(\varepsilon-\Delta)^2}\Bigg]$$

$$\times\exp[-\gamma_1(t_f-t_i)]+\frac{\alpha\pi^2}{2}\rho_1^1(t_i)\exp[-\gamma_2(t_f-t_i)]$$

$$\times\int\frac{d\varepsilon}{\pi}M(\varepsilon)\left[\frac{\exp(i(\varepsilon-\tilde{\Delta})(t_f-t_i))}{(\varepsilon-\Delta+i\nu)^2}+\frac{\exp(-i(\varepsilon-\tilde{\Delta})(t_f-t_i)}{(\varepsilon-\Delta-i\nu)^2}\right]$$

$$-\frac{\alpha\pi^2}{4}\int\frac{d\varepsilon}{\pi}\left[1+\operatorname{th}\left(\frac{\varepsilon}{2T}\right)\right]M(\varepsilon)$$

$$\times\left[\frac{\exp(i(\varepsilon-\tilde{\Delta})(t_f-t_i))}{(\varepsilon-\Delta+i\nu)^2}+\frac{\exp(-i(\varepsilon-\tilde{\Delta})(t_f-t_i))}{(\varepsilon-\Delta-i\nu)^2}\right]$$

$$\times\exp[-\gamma_2(t_f-t_i)]. \tag{27}$$

The equilibrium value $\rho_1^1(eq)$ of the element ρ_1^1 is equal to

$$\rho_1^1(eq)=\frac{1}{2}\Bigg\{1+\operatorname{th}\left(\frac{\Delta}{2T}\right)-\alpha\pi^2\Bigg[\left(1+\operatorname{th}\left(\frac{\Delta}{2T}\right)\right)$$

$$\times\left(\fint\frac{ds}{\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta)^2}-I\right)$$

$$+\frac{\Delta I}{M(\Delta)}\left(\left(1+\operatorname{th}\left(\frac{\Delta}{2T}\right)\right)M'(\Delta)+\frac{M(\Delta)}{2T\operatorname{ch}^2(\Delta/2T)}\right)\Bigg]$$

$$+\alpha\pi^2\fint\frac{d\varepsilon}{2\pi}\frac{[1+\operatorname{th}(\varepsilon/2T)]M(\varepsilon)}{(\varepsilon-\Delta)^2}\Bigg\}. \tag{28}$$

To terms of order α^2 the coefficient γ_1 is equal to

$$\gamma_1=\alpha\pi^2M(\Delta)-\alpha^2\pi^4\Bigg[\Delta IM'(\Delta)-M(\Delta)I+M(\Delta) \tag{29}$$

$$\times\fint\frac{d\varepsilon}{2\pi}\frac{M(\varepsilon)}{(\varepsilon-\Delta)^2}\Bigg].$$

In the leading logarithmic approximation the functions B_1, F, $\hat{\Delta}$, γ_1, γ_2, and $\rho_1^1(eq)$ are equal to

$$\tilde{\Delta}=\Delta\left\{1-\alpha\pi^2 I+\frac{\alpha^2\pi^4 I^2}{2}-\dots\right\},$$

$$\begin{aligned}\gamma_1&=\alpha\pi^2[M(\Delta)-\alpha\pi^2\Delta M'(\Delta)I+\dots],\\ \gamma_2&=\frac{\alpha\pi^2}{2}[M(\Delta)-\alpha\pi^2\Delta M'(\Delta)I+\dots],\end{aligned}\qquad(30)$$

$$\rho_1{}^1(eq)=\frac{1}{2}\left\{1+\text{th}\left(\frac{\Delta}{2T}\right)-\alpha\pi^2 I\left[\text{th}\left(\frac{\Delta}{2T}\right)\right.\right.$$
$$\left.\left.+\frac{\Delta M'(\Delta)}{M(\Delta)}\left(1+\text{th}\left(\frac{\Delta}{2T}\right)\right)+\frac{\Delta}{2T\,\text{ch}^2\,(\Delta/2T)}\right]\right\},$$
$$B_1=1-\alpha\pi^2 I+3\alpha^2\pi^4 I^2/4,\quad F=I(1-\alpha\pi^2 I).$$

It follows from these formulas that even at zero temperature the dependence on the coupling constant in the leading logarithmic approximation is different for the different quantities. Physically, it is rather obvious that the function $\rho_1^1(eq)$ should remain greater than 0.5 with increase of the parameter α. In this way, in the leading logarithmic approximation, substantially different series arise. Evidently, localization should imply that at $T=0$, at a certain value $\alpha=\alpha_{cr}$, the quantity $\rho_1^1(eq)$ becomes equal to 1/2 and does not change with further increase of α. Such behavior contradicts the analyticity of $\rho_1^1(eq)$ as a function of α.

We note also that at $T=0$, even in the logarithmic approximation, in the functions C_3 and D the second-order corrections do not reduce to a renormalization of the quantity Δ. It follows from the formulas (30) that the coefficients in the expansion of the functions $\gamma_{1,2}$ determining the rate of relaxation to equilibrium, and the coefficients in the expansion of the function $\rho_1^1(eq)$, depend in an essential way on the temperature, while for the functions $\hat{\Delta}$, B_1, and F in the leading logarithmic approximation, only the factor under the logarithm depends on the temperature.

For sufficiently large values of the coupling constant α, when the coherent processes become unimportant, the relaxation rate γ can be found from the imaginary part of the partition function Z (Refs. 9, 10). For a potential of the form (10) with $V(\varphi)=0$ for $\varphi>\varphi_0$, after straightforward calculations we find

$$\gamma=B\exp(-A).\qquad(31)$$

The exponent A and the pre-exponential factor B are determined by the formulas

$$A=\frac{2m\Omega_p{}^2\varphi_0{}^2}{\pi^2}T\sum_{N=2k+1}S_N\left(4\pi^2+\frac{2\pi\eta}{m|N|T}\right),\qquad(32)$$

$$B=4\varphi_0\Omega_p{}^2\left(\frac{m}{2\pi}\right)^{1/2}\left(T\sum_{N=2k+1}S_N\right)\left(T\sum_{N=2k}S_N-T\sum_{N=2k+1}S_N\right)^{-1/2},\qquad(33)$$

where

$$S_N=[(2\pi TN)^2+\Omega_p{}^2+2\pi T|N|\eta/m]^{-1},\quad k=0,\pm1\dots,\qquad(34)$$

in which $\eta=1/R_N e^2$ is the viscosity coefficient, connected with the coefficient α by the relation

$$\alpha=\frac{2\eta}{\pi}\varphi_0{}^2.\qquad(35)$$

As was noted above, one (negative) eigenvalue of the operator $\delta^2 S[\varphi]/\delta^2\varphi$ tends to zero as $T\to0$. This eigenvalue Λ_- satisfies the equation

$$T\sum_{N=2k+1}S_N=T\sum_{N=2k}\{S_N{}^{-1}-\Lambda_-/m\}^{-1}\qquad(36)$$

and, at low temperatures ($T\ll\Omega_p$) and low viscosities $\eta\ll\eta_2$ ($\eta_2=m\Omega_p$), is equal to

$$-\frac{\Lambda_-}{m}=2\Omega_p{}^2\left[4\exp\left(-\frac{\Omega_p}{2T}\right)+\frac{\eta}{\pi m\Omega_p}\left(\frac{2\pi T}{\Omega_p}\right)^2\right].\qquad(37)$$

The decrease of the negative eigenvalue with lowering of the temperature leads to growth of the fluctuations about the extremal path and to inapplicability of the method of instantons in its simplest form at low temperatures.

At low temperatures ($T\ll\Omega_p$) and low viscosities ($\eta\ll\eta_2$), from the formulas (32) and (33) we find

$$\begin{aligned}A&=2m\Omega_p\varphi_0{}^2\,\text{th}\left(\frac{\Omega_p}{4T}\right)+\frac{4\varphi_0{}^2\eta}{\pi}\left[C-\frac{1}{2}+\ln\left(\frac{\Omega_p}{\pi T}\right)\right],\\ B&=\varphi_0\Omega_p\left(\frac{m}{2\pi}\right)^{1/2}\left[\frac{1}{\Omega_p}\exp\left(-\frac{\Omega_p}{2T}\right)+\frac{\eta\pi T^2}{m\Omega_p{}^4}\right]^{-1/2},\end{aligned}\qquad(38)$$

where $C=0.577$ is the Euler constant.

The splitting Δ of the ground-state level in the potential (10) is equal to

$$\Delta=2\Omega_p(m\varphi_0{}^2\Omega_p/\pi)^{1/2}\exp(-m\Omega_p\varphi_0{}^2).\qquad(39)$$

From the formulas (31), (38), and (39) for $T\ll\Omega_p$, we find

$$\gamma=\frac{\Delta^2}{4T(\pi\alpha)^{1/2}}\exp\left\{-2\alpha\left[C-\frac{1}{2}+\ln\left(\frac{\Omega_p}{\pi T}\right)\right]\right\}.\qquad(40)$$

The formula (40) coincides with the result of Ref. 2 with the special choice of cutoff frequency ω_c.

We shall compare the expression for the quantity γ (formula (40)), which is valid for sufficiently large values of the parameter α and not too low temperatures, with the quantity γ_1 for small values of the parameter α.

From the formulas (7) and (26) we find

$$\gamma_1=\alpha\pi^2 M(\Delta)-\alpha^2\pi^4\left\{\Delta IM'(\Delta)+\frac{ia}{2\pi^2}M(\Delta)\right.$$
$$\left.\times[\psi'(-ia)-\psi'(ia)]\right\},\qquad(41)$$

where a $=\Delta/2\pi T$ and $\psi(x)$ is the logarithmic derivative of the Γ-function. In the limiting cases of high ($T\gg\Delta$) and low ($T\ll\Delta$) temperatures, from formula (41) we find

$$\gamma_1=2\alpha\pi T+\frac{\alpha\pi\Delta^2}{6T}\left\{1-2\alpha\pi^2\left[I-\frac{3\zeta(3)}{\pi^4}\right]\right\},\quad T\gg\Delta,\qquad(42)$$

$$\gamma_1=\alpha\pi\Delta\left\{1-\alpha\pi^2\left[I-\frac{1}{\pi^2}+\frac{2T^2}{3\Delta^2}\right]\right\},\quad T\ll\Delta.\qquad(43)$$

Comparing the formulas (40) and (42), we see that summation over the powers of α in formula (42) should reduce to zero the terms that do not depend on Δ, and should reduce to the appearance of an exponential dependence on α in the term proportional to Δ^2.

As noted above, as the temperature is lowered the negative eigenvalue Λ_- tends to zero, fluctuations about the extremal path grow, and the method of instantaneous becomes inapplicable. We shall find the value of Λ_- at which the fluctuations cease to be small. For this we compare the value obtained for the decay probability γ_{ins} from formulas (32) and (33) for $\alpha=0$:

$$\gamma_{ins}=\varphi_0\Omega_p\left(\frac{m\Omega_p}{\pi}\right)^{1/2}\operatorname{th}\left(\frac{\Omega_p}{4T}\right)\left[\operatorname{sh}\left(\frac{\Omega_p}{2T}\right)\right]^{1/2}$$

$$\times\exp\left[-2m\Omega_p\varphi_0^2\operatorname{th}\left(\frac{\Omega_p}{4T}\right)\right] \tag{44}$$

with its exact quantum-mechanical value

$$\gamma=\Omega_p\left(1-\exp\left(-\frac{\Omega_p}{T}\right)\right)\sum_{n=0}^{\infty}\tilde{\gamma}(n)\exp\left(-\frac{n\Omega_p}{T}\right), \tag{45}$$

where $\Omega_p\tilde{\gamma}_n/2$ is the imaginary part of the energy of the nth level, equal to

$$\tilde{\gamma}_{2k}=2x^{2+8k}\exp(-x^2)\frac{\Gamma(k+1)}{\Gamma^2(2k+1)\Gamma(k+{}^1/_2)(4k+1)^{1/2}},$$

$$\tilde{\gamma}_{2k+1}=x^{6+8k}\exp(-x^2)\frac{\Gamma(k+1)(4k+3)^{1/2}}{2\Gamma^2(2k+2)\Gamma(k+{}^3/_2)},\quad x=\varphi_0(2m\Omega_p)^{1/2}. \tag{46}$$

It follows from the formulas (44), (45), and (46) that there exists a critical temperature T_{cr}, determined from the condition

$$|\Lambda_-|=4\Omega_p/\varphi_0^2, \tag{47}$$

such that for $T<T_{cr}$ the fluctuations about the extremal path become large and the method of instantons it its simplest form becomes inapplicable. Equation (47) for the determination of the critical temperature remains valid even in the presence of a small viscosity $\eta\ll m\Omega_p$. Using for Λ_- the expression (37), we find that formula (40) for the relaxation rate γ is valid only in the temperature range

$$T>\Omega_p/\pi\alpha^{1/2}. \tag{48}$$

At lower temperatures in the region $\alpha\gg 1$ the relaxation rate γ evidently ceases to depend on the temperature.

CONCLUSION

In the problem of the dynamics of a quantum particle in a two-well potential there are several unsolved questions. First of all, the ground state at $T=0$ for an arbitrary value of the coupling constant with the thermostat is not known. The density-matrix element ρ_1^1 characterizing the ground state has been found by us only in first order in the coupling constant α. The transition from small values of α, when the relaxation rate $\gamma\sim\alpha M(\Delta)$, to large values of α has not been investigated. In the region of values of the parameters α and T in which interference effects are unimportant, the relaxation rate γ is determined by the imaginary part of the partition function. We note also that the cutoff frequency ω_c that needs to be introduced in a two-level model turns out to be related in a simple manner to the plasma-oscillation frequency Ω_p (formula (40)): $\ln(\Omega_c/\Omega_p)=C-1/2=0.077$. This question was considered in Ref. 11. It appears to be physically highly plausible that interference effects lead to an increase of the relaxation rate. In any case, this is so for small values of the couplIng constant α. In the absence of interference effects the relaxation rate γ is determined by the formula (40), with emergence to a plateau at a temperature T_{cr} determined by formulas (47) and (48). In view of this, the conclusion that localization arises for $T=0$ and $\alpha=1$ appears to us to be incorrect.

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[1] S. Chakravarty and A. J. Leggett, Phys. Rev. Lett. **52**, 5 (1984).
[2] H. Grabert and U. Weiss, Phys. Rev. Lett. **54**, 1605 (1985).
[3] A. T. Dorsey, M. P. A. Fisher, and M. S. Wartak, Phys. Rev. A **33**, 1117 (1986).
[4] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[5] A. Schmid, Phys. Rev. Lett. **51**, 1506 (1983).
[6] A. I. Larkin and Yu. N. Ovchinnikov, Phys. Rev. B **28**, 6281 (1983).
[7] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, 2nd ed., Pergamon Press, Oxford (1965) [Russ. original, Fizmatgiz, Moscow (1963)].
[8] A. I. Larkin and Yu. N. Ovchinnikov, J. Low Temp. Phys. **63**, 315 (1986).
[9] J. S. Langer, Ann. Phys. (N.Y.) **41**, 108 (1967).
[10] A. I. Larkin and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **86**, 719 (1984) [Sov. Phys. JETP **59**, 420 (1984)].
[11] Yu. Kagan and N. V. Prokof'ev, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 434 (1986) [JETP Lett. **43**, 558 (1986)].

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