

Destruction of coherence in quantum systems with dissipation

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The dynamics of a quantum particle in the presence of dissipation is investigated. The cases of symmetric double-well and periodic potentials are considered. The quantum coherence is destroyed in the region $0 < \alpha < \frac{1}{2}$ (α is the parameter characterizing the dissipation). In the region $\frac{1}{2} < \alpha < 1$ incoherent relaxation occurs, which, in the case of the double-well potential, proceeds according to an exponential law at sufficiently large t . The probability of finding the particle in the i th minimum of the periodic potential is $W_i \propto t^{\alpha-1}$; coherent oscillations of $W_i(t)$ also occur in the region of moderate t in the case when $\alpha \ll 1$. In the case of the periodic potential the quantity $\langle q^2(t) \rangle$ varies in time according to the power law $\langle q^2 \rangle \propto t^{2(1-\alpha)}$ for all $\alpha < 1$, which corresponds to a transition of the system into a localized state for $\alpha > 1$.

1. INTRODUCTION

At present the investigation of the effect of dissipation on the phenomenon of quantum coherence is attracting much attention. There is now the possibility in principle of experimentally observing such a phenomenon in macroscopic systems (Josephson junctions, SQUIDS), and this is arousing further interest in this investigation.

It is well known that the process of tunneling of a quantum particle through a potential barrier between two degenerate (or near-degenerate) minima is a coherent process. In a symmetric potential this leads to the lifting of the degeneracy of the energy levels and to an oscillating time dependence of the correlator $\langle q(0)q(t) \rangle$ (where q is the particle coordinate). The coherence of the wave function is destroyed when interaction with a medium takes place. As shown in Refs. 1 and 2, even a fairly weak dissipation leads to a significant change in the behavior of the system. Thus, the particle can be localized in one of the potential minima at $T \rightarrow 0$. The case of a periodic potential is considered in Refs. 3–5. In such a system there occurs at $T \rightarrow 0$ and a certain value of the effective viscosity η a sharp change in the mobility of the particle, i.e., there occurs a transition between two phases, one of which corresponds to diffusion and the other, to localization of the particle.³ A more accurate phase diagram of a dissipative quantum system is obtained in Refs. 4 and 5.

In the present paper we propose a procedure for investigating the temporal evolution of the density matrix of a dissipative quantum system located in a potential with several minima. The method is then used to describe the dynamics of such a system for the cases of two, and an infinite number of, minima. These two cases are of the greatest physical interest in connection with the study of the macroscopic quantum phenomena that occur in superconducting weak links and SQUIDS. Furthermore, the partition function of a system with two energetically close potential minima is, in the low-temperature limit, equivalent to that of a two-level system, which is extensively used as a model in the description various physical phenomena. The case of the periodic potential

may also be of interest in connection with the investigation of the problem of the diffusion of heavy particles in a solid and some other problems. It should be noted that the study of the dynamics of a dissipative two-level system described by the so-called spin-boson Hamiltonian was initiated in Ref. 6 (see also Ref. 7). In that paper the dissipative contribution to the tunneling amplitude is computed by separating out the trajectories corresponding to successive instantaneous flippings of the spin. Although such an approach is a physically natural one within the framework of the phenomenological spin-boson Hamiltonian, from our viewpoint it needs to be justified through a direct computation of the density matrix of the original dissipative system, since the identity (at low temperatures) of the equilibrium properties of such a system and those of a system described by the model two-level Hamiltonian does not, generally speaking, yet imply that their nonequilibrium properties are equivalent. Furthermore, the trajectories used in Ref. 6, i.e., those describing the spin flipping in real time, are not extremal trajectories for the action of a quantum particle in a double-well potential, and, consequently, do not make the decisive contribution to the functional integral for the density matrix. Nevertheless, as will be shown, the description obtained in Ref. 6 of the process of coherence destruction in the region $\alpha < \frac{1}{2}$ (see below) coincides in the $T \rightarrow 0$ limit of interest to us here with the result that is furnished by the direct computation of the density matrix of the original system.

2. DYNAMICS OF A QUANTUM SYSTEM IN THE PRESENCE OF TUNNELING

The dynamics of a quantum system can be studied with the aid of the obvious relations

$$\rho(q_+, q_-) = \int dq_+^i dq_-^i J(q_+^i, q_-^i, q_+^i, q_-^i) \rho(q_+^i, q_-^i),$$
$$J = \int \mathcal{D}q \exp\{iS_c\}, \quad (1)$$

where ρ is the density matrix. The effective action functional S_c on a Keldysh contour C (Ref. 8) for a particle interacting with a heat bath has the form

$$iS_C = iS_+ - iS_- + \ln F, \quad S_{\pm} = \int_{t_i}^{t_f} dt_{\pm} \left[\frac{m}{2} \left(\frac{\partial q}{\partial t_{\pm}} \right)^2 - V(q(t_{\pm})) \right], \quad (2)$$

$$\ln F = \int_{t_i}^{t_f} \int_{t_i}^{t_f} dt dt' [q_+(t) - q_-(t)] [f(t, t') q_+(t') - f^*(t, t') q_-(t')],$$

where m is the particle mass, $V(q)$ is the potential, and F is the influence functional.^{9,10} The expression for the quantity $f(t, t')$ is easily found under the assumption that the heat bath consists of a large number of harmonic oscillators. We have¹¹

$$f(t, t') = \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon(t-t')} \eta \varepsilon \left(1 + \text{cth} \frac{\varepsilon}{2T} \right). \quad (3)$$

The expressions (2) and (3) for S_C also follow in a number of limiting cases from the microscopic expression for the effective action of superconducting junctions with tunneling¹² and direct¹³ conductivity.

In Ref. 14 the present authors propose a method of describing the quantum decay of a metastable state in real time. Here we shall use this method to study the dynamics of a quantum system in a potential with several degenerate minima. The state of a particle in such a potential at low temperatures can be described by a matrix ρ_{ij} in which the number of different values of i and j is equal to the number of minima. The diagonal element ρ_{ii} of this matrix determines the probability of finding the particle in the vicinity of the i th minimum.

Further, we shall everywhere consider the $T \rightarrow 0$ limit, which is the most interesting one. At values of the parameter $\alpha \equiv \eta q_0^2 / 2\pi > 1$ (q_0 is the distance between the nearest minima) the particle is localized in one of the minima of the potential¹⁻⁵ $V(q)$. Clearly, the description of the dynamics of the system has meaning in the region of delocalization, i.e., in the region $0 < \alpha < 1$. Taken together with the condition $V_0 \gg \omega_0$ (where V_0 is the potential barrier between neighboring minima and ω_0 is the frequency of small oscillations of the particle in the vicinity of the minimum), this means that the dissipation weakly affects the particle motion in the classically accessible regions, $\eta \ll m\omega_0$. Let us show that in this case the quantity $\rho_{ii}(t)$ can be represented in the form of a series in even powers of the amplitude $\Delta/2$ of the tunneling between neighboring minima, where¹⁾

$$\Delta \sim \omega_0 A^{1/2} e^{-A}, \quad A \sim V/\omega_0 \gg 1, \quad \text{i.e. } \Delta \ll \omega_0.$$

For definiteness, we shall assume that, at zero time, the particle is localized in the vicinity of the i th minimum. In order to evaluate the functional integral (1), (2), we must determine the contribution of the trajectories describing all possible transitions between the states ρ_{ij} . At sufficiently small times $t \equiv t_f - t_i$ (but $t \gg \tau_0 \equiv \omega_0^{-1}$) we can, in determining the $\rho_{ij}(t)$, limit ourselves to considering the contributions of the transitions of the type $\rho_{ii} \rightarrow \rho_{i+1i} \rightarrow \rho_{ii}$ to the functional integral

$$N^{-1} \int \mathcal{D}q \exp\{iS_C\},$$

where N is the normalization constant. Following Ref. 14, we introduce the parametrization $\tau_{\pm}(t_{\pm})$, which is such that $d\tau_{\pm}/dt_{\pm} = \pm i$. This parametrization is convenient,

since it allows us to easily separate out the expression for A , an expression which goes over in the limit as $\eta \rightarrow 0$ into the WKB result. The quantity A is given by the value of the action functional on the trajectory $\tilde{q}(\tau_{\pm}(t_{\pm}))$ describing the tunneling between neighboring minima, and satisfying the condition $\delta S/\delta \tilde{q}(\tau) = 0$. We use $\tau_+(t_+ - t_1)$ to describe the transition $\rho_{ii} \rightarrow \rho_{i+1i}$ and $\tau_+(t_+ - t_2)$ ($0 < t_1 < t_2 < t$) to describe the inverse transition $\rho_{i+1i} \rightarrow \rho_{ii}$. The integration over the deviations $\delta q(t) = q(t) - \tilde{q}(\tau_+(t_+ - t_{1,2}))$ reduces, as usual, to integration over the coefficients of the expansion of δq in terms of the eigenfunctions of the operator $\delta^2 S/\delta q(\tau)\delta q(\tau')$. The separation of the zero eigenvalue is carried out in much the same way as was done in Ref. 14; the integration over the remaining eigenvalues yields a preexponential factor in the expression for Δ . As a result, for the contribution to the functional integral (1)–(3) of the trajectories describing the transitions $\rho_{ii} \rightarrow \rho_{i+1i} \rightarrow \rho_{ii}$ we obtain

$$-\left(\frac{\Delta}{2}\right)^2 \int_0^t dt_2 \int_0^{t_2-\tau_0} dt_1 \exp\left(-2\alpha \ln \frac{t_2-t_1}{\tau_0}\right) e^{i\pi\alpha}. \quad (4)$$

The contribution of the transitions $\rho_{ii} \rightarrow \rho_{ii+1} \rightarrow \rho_{ii}$ differs from (4) only by the sign of the imaginary unit, and is obtained from it by making the substitution $i\pi\alpha \rightarrow -i\pi\alpha$. It is the sum of the contributions of the trajectories describing these two sets of transitions that governs the evolution of the quantity ρ_{ii} in the region of small t . The notation of the upper limit in the t_1 integral has, to some extent, a symbolic form, and indicates that the instanton trajectories $\tilde{q}[\tau(t - t_{1,2})]$ have meaning only when $t_2 - t_1 \gg \tau_0$. We shall see below that the behavior of the system will not be sensitive to the choice of a specific method of truncation.

For not too small t , it is no longer sufficient to consider just the contribution of the simplest instanton configurations of the type (4). Allowance for more complicated configurations leads to the appearance of terms of higher order in Δ . As a result, the quantity $\rho_{ii}(t) \equiv W_i(t)$ can be represented in the form of a series in even powers of Δ . Here we shall consider two important particular cases: the cases of double-well and periodic potentials.

3. THE SYMMETRIC DOUBLE-WELL POTENTIAL $V(q) = V(-q)$

We shall assume in the case of a potential with two minima $i(j) = 1, 2$ that at the initial time $t = 0$ the particle is localized in the first well. We have

$$W_1(t) = 1 - W_2(t) = [1 + P(t)]/2.$$

We should, in deriving the expression for $P(t)$, take account of the pair-wise interaction between the instantons located both on the same, and on different, contours τ_+ and τ_- .

We first consider the $\alpha < 1/2$ case. As in (4), we shall assume that the cutoff parameter for the interaction between the instantons at small distances is equal to τ_0 . Below we shall investigate the question of the magnitude of this parameter in greater detail. For $\alpha < 1/2$ this question is not important, since the quantity $P(t)$ for such α values is determined by the region of large t (i.e., the dominant contribution to $P(t)$ is

made by the configurations in which the instantons are located far from each other). Finally, we have ($\alpha \leq \frac{1}{2}$)

$$P(t) = \sum_{n=0}^{\infty} (-2)^{-n} \Delta^{2n} \int_0^t dt_{2n} \int_0^{t_{2n}-\tau_0} dt_{2n-1} \dots \int_0^{t_2-\tau_0} dt_1 \times \text{Sp}_{s_{2r}} \exp \left\{ 2\alpha \sum_{k>l}^{2n} s_k s_l \ln \frac{t_k - t_l}{\tau_0} \right\} (\cos \pi \alpha)^n, \quad (5)$$

where $s_{2r} = \pm 1$ is the "spin" variable; $s_{2r-1} = -s_{2r}$, $r = 1, 2, \dots, n$. This expression actually coincides with the result obtained by Chakravarty and Leggett⁶ with the aid of a two-level spin-boson Hamiltonian.

Let us compute the quantity $P(t)$ in the approximation in which only the interaction between the nearest instanton pairs (the instanton-antiinstanton interaction) is taken into account, i.e., let us retain in the sums over k and l in (5) only those terms for which $k = l + 1 = 2r$. In this approximation the series (5) is easy to sum (see Ref. 6):

$$P(t) = E_{2(1-\alpha)}[-(\Delta_r t)^{2(1-\alpha)}] = \frac{1}{1-\alpha} \cos \left[\Delta_r t \cos \left(\frac{\pi \alpha}{2(1-\alpha)} \right) \right] \times \exp \left[-\Delta_r t \sin \left(\frac{\pi \alpha}{2(1-\alpha)} \right) \right] + P_1(t), \quad (6)$$

$$\Delta_r(\alpha) = \Delta (\Delta/\omega_0)^{\alpha/(1-\alpha)} [\Gamma(1-2\alpha)]^{1/2(1-\alpha)}, \quad (7)$$

where $E_\nu(x)$ is the Mittag-Leffler function¹⁶ and the function $P_1(t)$ is negative and, for $\Delta_r t \gg 1$, equal to

$$P_1(t) \approx (\Delta_r t)^{-2(1-\alpha)} / \Gamma(2\alpha - 1). \quad (8)$$

As shown in Appendix 1, the approximation we used in the $A \gg 1$ case works well, at least at times

$$\Delta_r t \ll \max\{\alpha^{-1}, A\}. \quad (9)$$

At very small values of $\alpha < A^{-1}$ the difference between the expression for $P(t)$ in the region (9) and $\cos \Delta t$ is negligible, i.e., the dissipation is insignificant under such conditions. For $A^{-1} \ll \alpha \ll 1$ the formulas (6) and (8) describe both the coherent $P(t)$ oscillations, which occur at times $t \leq (\Delta_r \alpha)^{-1}$, and the incoherent relaxation of $P(t)$ to zero, a relaxation which, as follows from (6) to (8), is governed by the power law $t^{-2(1-\alpha)}$. Practically no coherent oscillations occur for $t \gtrsim 1/3$, and the function $P(t)$ coincides with $P_1(t)$, (8), in a broad time interval. Thus, the simple approximation used in the evaluation of the series (5) for $P(t)$ is quite a fruitful approximation for the description of the evolution of the density matrix of the system in question. The formulas (6) and (8) may not be correct when the condition (9) is violated. The description of the region $\Delta_r t \gtrsim \max\{\alpha^{-1}, A\}$ apparently requires additional investigation. In this connection the fact that the problem of the computation of $P(t)$, (5), can, as shown in Appendix 1, be precisely reduced to an effective-field-theory analysis may turn out to be useful.

In the $\alpha \rightarrow \frac{1}{2}$ limit $P(t)$ is not described by the formulas (6) and (8), since for such α both large and small interinstanton separations are important.

Let us again consider the transitions $\rho_{11} \rightarrow \rho_{21} \rightarrow \rho_{11}$. The separation of the zero mode t_2 yields, in complete agreement with Ref. 14, the expression

$$i \int_0^t dt_2 K(\tau(t_2)), \quad K(\tau) = \left(\frac{\Delta}{2} \right)^2 \int_0^{\tau(t_2)} d\tau' \left(\frac{\tau'}{\tau_0} \right)^{-2\alpha} \quad (10)$$

The formal parameter τ' plays the role of interinstanton "separation," and is the second "quasizero" mode (it is a zero mode only in the $\alpha \rightarrow 0$ limit). Integrating over τ' , and then going over to the variable t_2 , we obtain in the case when $\alpha < \frac{1}{2}$ a result that coincides with (4). At $\alpha = \frac{1}{2}$ (and in fact for $|\frac{1}{2} - \alpha| \lesssim 1/4A$ in the broad time interval in which the principal changes in $P(t)$ occur) $K(\tau) = \ln(\tau(t_2)/\tau_0)$. Going over to t_2 , and integrating, we obtain from (10) the expression

$$-t \frac{\pi}{8} + i \int_0^t dt_2 \frac{\Delta^2}{4\omega_0} \ln \frac{t_2}{\tau_0}. \quad (11)$$

The direct summation of the contributions of the transitions between the ρ_{ij} states in all orders in Δ^2 for $\alpha = \frac{1}{2}$ yields²⁾

$$P(t) = \exp(-\Delta_r t), \quad \Delta_r = \frac{\pi}{2} \frac{\Delta^2}{\omega_0}. \quad (12)$$

Clearly, the expression (12) for Δ_r coincides with (7) in the $\alpha \rightarrow \frac{1}{2}$ limit. Nevertheless, as has already been noted, the relation (5) does not describe $P(t)$ in this limit, so that, strictly speaking, the formulas (12) cannot be obtained from (5) through passage to the $\alpha \rightarrow \frac{1}{2}$ limit. Note also that the result (12) is exact in the region $t \gg \tau_0$.

Let us now consider the $\alpha > \frac{1}{2}$ case. This region of values of the parameter α is actually not considered in Ref. 6. The simplest way to compute the quantity $P(t)$ is, as in the $\alpha < \frac{1}{2}$ case, to consider only the pairwise interaction between the $2n$ and $2n - 1$ instantons. In this case each power-series term, which is proportional to Δ^{2n} , contains n zero and n "quasizero" modes. The integration over the n quasizero modes can be carried out in much the same way as was done in (10). As a result, as in the $\alpha < \frac{1}{2}$ case, this approximation yields (Δ_r is defined in (7))

$$P(t) = E_{2(1-\alpha)}(-(\Delta_r t)^{2(1-\alpha)}). \quad (13)$$

This function is a monotonically decreasing function when $\alpha \gtrsim \frac{1}{2}$ (for greater details, see Ref. 16), and coincides with the function $P(t) \propto t^{2(1-\alpha)}$, (8), when $(\Delta_r t)^{2(1-\alpha)} \gg 1$. We now go beyond the simple approximation that leads to (13). Let the characteristic time scale of the variation of $P(t)$ be denoted by τ_c , and show that those transitions between the ρ_{ij} states which have frequencies $\gtrsim \tau_c^{-1}$ lead to the renormalization of the bare parameters Δ and α . This circumstance, as we shall see, should be taken into account in the determination of the form of $P(t)$ at times $t \gtrsim \tau_c$. Group all the possible instanton configurations in the manner shown in Fig. 1, i.e., divide all the trajectories into two classes, one of which describes the "fast" and the other the "slow" transitions. Sum over all the trajectories differing only in the numbers of "fast" instantons. At $t \gg \tau_c$ we can neglect the interaction between such instantons located on different contours τ_+ and τ_- . This enables us to sum the contributions of the indicated trajectories on the two contours separately. A similar sum is evaluated in Ref. 17 by the renormalization-group method in connection with the Kondo

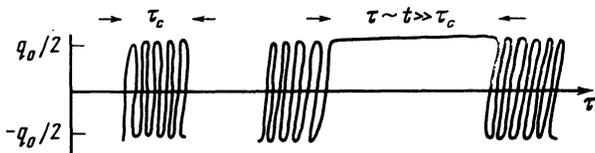


FIG. 1.

problem. According to the renormalization-group equations,¹⁷ the quantity α decreases in the course of the renormalization (as τ is increased), and attains the value $\tilde{\alpha} = \frac{1}{2}$ at $\tau = \tilde{\tau} = 0.783\tilde{\Delta}^{-1}$ ($\tilde{\alpha}$ and $\tilde{\Delta}$ are the renormalized values of α and Δ). Renormalizing to this value $\tau = \tilde{\tau}$, and then using for the sum of the contributions with larger τ the exact result (12) for $\alpha = \tilde{\alpha} = \frac{1}{2}$, we find

$$P(t) = \exp\left(-\frac{\pi}{2}\tilde{\Delta}^2\tilde{\tau}t\right). \quad (14)$$

As follows from (14), the characteristic time scale of the $P(t)$ variation is the quantity $\tau_c \approx \tilde{\tau} \sim \Delta(\Delta/\omega_0)^{\alpha/(1-\alpha)}$. Thus, for sufficiently large values of $t \gtrsim \Delta_r^{-1}$ and $\alpha > \frac{1}{2}$ the approximation based on considering only the interaction between the nearest instanton pairs, and leading to (13), does not allow us to obtain the correct result for $P(t)$. This approximation furnishes at $\alpha > \frac{1}{2}$ a good description only for the region of t smaller than, or of the order of, Δ_r^{-1} . Notice, however, that, as α tends to unity, Δ_r decreases, i.e., the expression (13) remains valid at larger and larger t .

The relation (7) gives the dependence $\Delta_r(\alpha)$ in the region $\Delta^2\tau_0^2 \ll 1 - \alpha \ll 1$. For $1 - \alpha \lesssim \Delta^2\tau_0^2$ the nonlinear terms in the renormalization-group equations are important for the determination of the $\Delta_r(\alpha)$ function.¹⁴ It should be noted in this connection that, strictly speaking, the transition into the localized state occurs not at the point $\alpha = 1$, but at the point $\alpha = 1 + \delta$, where $\delta \sim \Delta\tau_0$ (see, for example, Ref. 18). But the study of the dynamics of the system for such a narrow region of α values around unit is apparently not of great interest.

As has already been noted, the dynamics of a dissipative two-level system has been studied by Chakravarty and Leggett⁶ (at $T = 0$ in the region of values of $\alpha \leq \frac{1}{2}$). These authors describe the transitions between the various ρ_{ij} states with the aid of trajectories that have the form of θ functions of real time. (Such trajectories are not extremal trajectories, and (in the absence of dissipation) do not give the correct expression for Δ .) They introduce the quantity Δ phenomenologically, which permits the reproduction of the correct result at $\alpha < \frac{1}{2}$. As to the extremal trajectories for the action, they are close to the θ functions in the Euclidean space with parameter³⁾ τ . Let us also note that for $\alpha > \frac{1}{2}$ the study of the dynamics within the framework of the approach employed in Ref. 6 meets with considerable difficulties, and in fact the dynamics was not investigated for $T \rightarrow 0$ in that paper.

4. THE PERIODIC POTENTIAL $V(q) = V(q + q_0)$

As has already been pointed out, another physically important case is the case of the periodic potential. Here $i(j) = 0, \pm 1, \pm 2, \dots$. At the initial time $t = 0$ let the parti-

cle be localized in the vicinity of the $i = 0$ minimum. We shall be interested in the temporal evolution of the diagonal elements $W_i(t)$ of the density matrix. To determine them, we should, as before, consider all the possible transitions between the various ρ_{ij} states. As a result, for $\alpha \leq \frac{1}{2}$ we shall have

$$W_i(t) = \sum_{n=|i|}^{\infty} (-1)^{n+i} \left(\frac{\Delta}{2}\right)^{2n} \sum_{m=1}^M \int_0^t dt_{2n} \int_0^{t_{2n-1}} dt_{2n-1} \dots \times \int_0^{t_{2n-1}} dt_1 \exp\left\{2\alpha \sum_{k>l} f_m^i(k, l) \ln \frac{t_k - t_l}{\tau_0} + ip_m^i \pi \alpha\right\}. \quad (15)$$

Here $M = M(i, n)$ is the number of all the possible realizations of the transition from the zeroth into the i th minimum for a given n , the p_m^i are whole numbers, and $f_m^i(k, l)$ is a function determining the sign of the interaction between each pair of instantons for a given realization. Clearly, $W_i = W_{-i}$, so that below we shall assume that $i \geq 0$. Simple combinatorial calculations of the quantity $M(i, n)$ yield

$$M(i, n) = (2n!) / (n!)^2 (n+i)! (n-i)! \quad (16)$$

For the purpose of illustrating the approximation that will be used in evaluating the series (15) for $\alpha < \frac{1}{2}$, consider the simplest types of configurations, which occur in fourth order in Δ (see Fig. 2). In the configurations of the type $+ - + -$ and $+ - - +$, we shall, as in the case of the double-well potential, consider the interaction between the charge pairs 1-2 and 3-4, and in the configurations of the type $+ + - -$ we shall consider the interaction between the pairs 1-4 and 2-3. Proceeding in similar fashion in the computation of the terms of higher order in Δ , we obtain

$$W_i(t) = \sum_{n=i}^{\infty} \frac{(-1)^{n+i} (\Delta_r t)^{2n(1-\alpha)} M(i, n)}{4^n \Gamma[2n(1-\alpha) + 1]}. \quad (17)$$

As before, the approximation used in the $\alpha < \frac{1}{2}$ case will be valid at least up to times of the order of $\Delta_r t \sim \max\{\alpha^{-1}, A^{1/(1-\alpha)}\}$. But in the case of a periodic potential this restriction is not important. The behavior of $W_i(t)$ at large t is also described well by the expression (17). Below we shall discuss this question in greater detail.

First let $\alpha = 0$. In this case the expression (17) coincides exactly with (15), and can easily be evaluated. We have

$$W_i(t) = J_i^2(\Delta t), \quad (18)$$

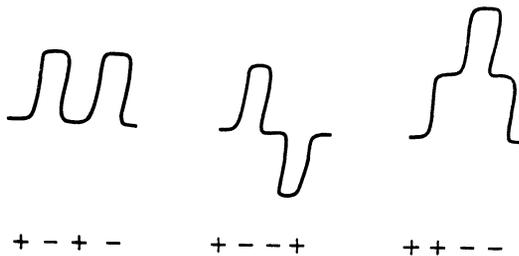


FIG. 2.

where the $J_i(x)$ are Bessel functions.¹⁵ For $\Delta t \gg i$ we obtain $W_i \approx (2/\pi\Delta t) \cos^2(\Delta t - \pi/2 - \pi/4)$. The series (17) for $\alpha < \frac{1}{2}$ is evaluated in Appendix 2. For $(\Delta_r t)^{1-\alpha} \gg i$ (Δ_r is defined in (7)) the calculation yields

$$W_i(t) = \frac{(\Delta_r t)^{\alpha-1}}{\pi\Gamma(\alpha)} \left\{ (1-\alpha) [\ln(\Delta_r t) - \psi(\alpha)] + \psi(1) + \ln 2 - \psi\left(i + \frac{1}{2}\right) \right\} + \frac{2(-1)^i(1-\alpha)}{\pi\Delta_r t} \cos[\Delta_r t \sin \beta - \beta] \exp[-\Delta_r t \sin(\alpha\beta)],$$

$$\Delta_r = \Delta_r \cdot 2^{1/(1-\alpha)}, \quad \beta = \pi/2^{(1-\alpha)}. \quad (19)$$

Here $\psi(x)$ is the psi-function.¹⁵ For $i \gg (\Delta_r t)^{1-\alpha}$ the quantities $W_i(t)$ are exponentially small, i.e., the wave-packet front propagates in the case when $\alpha < \frac{1}{2}$ according to the law $q(t) \sim (\Delta_r t)^{1-\alpha}$. For $\alpha \rightarrow \frac{1}{2}$ the approximation (17) ceases to hold, but, as in the case of the double-well potential, the expression (15) for $W_i(t)$ can be evaluated exactly at the point $\alpha = \frac{1}{2}$ (and in fact for $|\alpha - \frac{1}{2}| \lesssim 1/4A$ provided $A \gg 1$):

$$W_i(t) = \frac{4(\Delta_r t)^i}{\pi} \frac{\Gamma^2(i+1/2)}{\Gamma(2i+1)\Gamma(i+1)} {}_2F_2\left(i + \frac{1}{2}, i + \frac{1}{2}, 2i+1, i+1, -4\Delta_r t\right), \quad (20)$$

where ${}_2F_2(a, b, c, d, x)$ is the generalized hypergeometric series.¹⁵ In the limit $(\Delta_r t)^{1-\alpha} \gg i$ we have from (20) the estimate

$$W_i(t) \approx \frac{1}{2\pi(\pi\Delta_r t)^{1/2}} [\ln(\Delta_r t) - C + 4 \ln 2 - 2\psi(i+1/2)], \quad (21)$$

where $C \approx 0.577$ is the Euler constant.¹⁵

The approximation used by us in the determination of $W_i(t)$ in the region $\alpha < \frac{1}{2}$ works well in the region $\alpha > \frac{1}{2}$ as well. In order to verify this, let us first determine the characteristic time over which a substantial change occurs in the quantities $W_i(t)$. The direct application of the above-indicated approximation leads, as before, to the relation (17), from which we immediately obtain in the case when $\frac{1}{2} < \alpha < 1$ and $(\Delta_r t)^{\alpha-1} \gg i$ the expression

$$W_i(t) = \frac{(\Delta_r t)^{\alpha-1}}{\pi\Gamma(\alpha)} [\dots], \quad (22)$$

where the expression in the square brackets exactly coincides with the expression in the first square brackets in the formula (19). As follows from (22), in the case when $\alpha > \frac{1}{2}$ the wave-packet front also propagates according to the law $(\Delta_r t)^{1-\alpha}$. Thus, the characteristic time scale of the $W_i(t)$ variation in this case also coincides in order of magnitude with Δ_r^{-1} . Now, just as we did earlier in the study of the dynamics of a particle in a double-well potential, we go beyond the simple approximation (17), and sum the contributions of all the "fast" ($\tau < \tilde{\tau} \sim \Delta_r^{-1}$) trajectories, using for this purpose the renormalization-group equations obtained in Ref. 4. Renormalizing to $\tau = \tilde{\tau}$ in the case when $1 - \alpha \lesssim \Delta^2 \tau_0^2$, we obtain $\tilde{\Delta} \sim \Delta_r \sim \tau$. Now to verify at large $t \gg \Delta_r^{-1}$ the approximation (17), we must make the substitutions $\Delta \rightarrow \tilde{\Delta}$ and $\omega_0 \rightarrow \tilde{\tau}^{-1}$ in the formula (22). It is easy to

verify that both the time scale and the law of variation $W_i(t) \propto (\Delta_r t)^{\alpha-1}$ are left unchanged by these substitutions, and, consequently, the simple approximation (17) works well right up to $1 - \alpha \sim \Delta^2 \tau_0^2$, while the formula (22) determines, at least to within a number of order unity, the dynamics of $W_i(t)$ not only in the region $\Delta_r t \ll A^{1/(1-\alpha)}$, but also at larger t .

Let us recall that, in the case of the double-well potential, allowance for the renormalization of the bare parameters of the system by the "fast" heat-bath oscillators (i.e., those with frequencies $\omega \gtrsim \Delta_r$) for $\alpha > \frac{1}{2}$ substantially changed the form of the function $P(t)$ in the region $t \gg \Delta_r^{-1}$, causing it to decrease according to an exponential, instead of a power, law (cf. (13) and (14)), even though it did not lead to a change in the time scale. In the case of the periodic potential, we verified that this change does not occur. Such a difference is due to the fact that the "fast" fluctuations in a double-well potential renormalize not only the bare tunneling amplitude Δ , but also the strength α of the effective interaction with the heat bath, whereas in the case of the periodic potential allowing for the analogous fluctuation-induced transitions among all the minima (and not just between two nearest ones) does not lead to the renormalization of α (Ref. 4). This circumstance does not, in particular, allow us to use the "double-well" approximation in the construction of the phase diagram of a dissipative quantum system (cf. the results obtained in Refs. 3 and 4). Furthermore, as our results show, the fact that the probability relaxes incoherently at sufficiently large t according to the exponential law (14) is by itself not, generally speaking, enough for the study of the dynamics of a quantum particle in a periodic potential with the aid of simple balance equations for the probability that take account of only the tunneling between nearest minima⁴⁾ (see Ref. 19).

In the narrow region $1 - \alpha \lesssim \Delta^2 \tau_0^2$ the expression (7) for Δ_r is not valid. In this region

$$W_i(t) = \delta_{i0}, \quad t \lesssim \omega_0^{-1} \exp(e^{2A}), \quad A \gg 1. \quad (23)$$

Finally, using (17), we can easily determine the quantity

$$\langle q^2(t) \rangle = q_0^2 \sum_{i=-\infty}^{\infty} i^2 W_i(t). \quad (24)$$

Substituting (17) into (24), we obtain²⁰ ($1 - \alpha \gtrsim \Delta^2 \tau_0^2$)

$$\langle q^2(t) \rangle = q_0^2 (\Delta_r t)^{2(1-\alpha)} / \Gamma(3-2\alpha). \quad (25)$$

The dependence $\langle q^2(t) \rangle \propto t^{2(1-\alpha)}$ is obtained also in Ref. 21, but by a different method. Thus, the quantum diffusion of a wave packet in a periodic potential in which there is friction occurs only at $\alpha = \frac{1}{2}$, and the formula (25) describes the transition from the free motion of the wave-packet front, $q = vt$ ($v \sim q_0 \Delta$), to the localized state for $\alpha > 1$.

5. DISCUSSION OF THE RESULTS

In the present paper we have proposed a method of investigating the dynamics of a dissipative quantum system located in a potential with several degenerate minima. Initially the system is in an essentially nonequilibrium state: the particle is located in one of the minima of the potential. Generally speaking, this circumstance makes it impossible to use

the well-known method of investigating weakly nonequilibrium states, which is based on the analytic continuation to the real time axis of the linear response computed with the imaginary-time technique. The method developed here is used to describe the evolution of the density matrix of a quantum particle in the presence of friction in two cases: the cases of double-well and periodic potentials. In the first case such a system is equivalent in the low-temperature limit to a dissipative two-level system. In such a system the coherent oscillations of the mean value $\langle q(t) \rangle$ of the coordinate occur only at small values of the dimensionless parameter α characterizing the dissipation, and occur right up to times t of the order of $(\Delta_r \alpha)^{-1}$, $\Delta_r \sim \Delta(\Delta/\omega_0)^{\alpha(1-\alpha)}$. At large t the system relaxes incoherently to the equilibrium state according to the law $\langle q(t) \rangle \propto (\Delta_r t)^{-2(1-\alpha)}$, where $\alpha < \frac{1}{2}$. At $t \gtrsim A\Delta_r^{-1}$, where $A \sim \ln(\omega_0/\Delta) \gg 1$, the question of the time dependence of $\langle q(t) \rangle$ requires further investigation, which, by the way, is of interest largely in the region of very small values of $\alpha \lesssim A^{-1}$. Coherent oscillations do not occur at all for $\alpha \gtrsim \frac{1}{2}$, and in this region of α

$$\langle q(t) \rangle \propto \exp(-\Gamma t), \quad \Gamma(\alpha) \sim \Delta_r(\alpha),$$

i.e., as $\alpha \rightarrow 1$, the quantity $\Gamma(\alpha)$ tends to zero. In the region $\alpha > 1$ (more exactly, for $\alpha > 1 + \delta$, where $\delta \sim \Delta/\omega_0$) the particle is localized in one of the wells, and the mean value of the coordinate is time-independent and equal to $\langle q \rangle = \pm q_0/2 \mp \delta q$, where the quantum correction δq is computed for different values of α in the papers cited in Ref. 22:

$$\delta q = \frac{\lambda \chi(\gamma)}{\pi m \omega_0^2 |\gamma|^{1/2}},$$

$$\chi(\gamma) = \begin{cases} \arctg(\gamma^{1/2}/\eta), & \gamma \geq 0 \\ \frac{1}{2} \ln\{(\eta + (-\gamma)^{1/2})/(\eta - (-\gamma)^{1/2})\}, & \gamma \leq 0 \end{cases},$$

$$\gamma = 4m^2 \omega_0^2 - \eta^2, \quad \lambda = \left| \frac{\partial^3 V(q_0/2)}{\partial (q_0/2)^3} \right|.$$

It should be noted in this connection that such a correction was apparently measured recently by Schwartz *et al.*²³ in macroscopic quantum tunneling experiments, the results obtained in which are in quantitative agreement with the predictions made in Ref. 22.

In the case of a periodic potential with $A \gg 1$ and $T \rightarrow 0$, coherence is also destroyed in the region $0 < \alpha < \frac{1}{2}$. The incoherent relaxation in this region of α values occurs at large $t \gg (\alpha \Delta_r)^{-1}$. In the region $\frac{1}{2} < \alpha < 1$ the incoherent relaxation in a periodic potential, unlike the corresponding process in a double-well potential, occurs according to a power law: $W_i \propto t^{\alpha-1}$. It should be emphasized that this law is not a consequence of the choice of the particular approximation used in the summation of the series (15), and can be obtained with the aid of simple arguments. Indeed, as follows from (15), the probability $W_i(t)$ in the region $\alpha < \frac{1}{2}$ is exponentially small when $i \gg (\Delta_r t)^{1-\alpha}$, and goes through its maximum at $i \sim (\Delta_r t)^{1-\alpha}$. Thus, by the time $t \gg \Delta_r^{-1}$ the particle will be smeared over $2N(t)$ wells, where $N(t) \sim (\Delta_r t)^{1-\alpha}$, from which we immediately obtain

$$W_i(t) \propto (\Delta_r t)^{\alpha-1}, \quad i \ll N(t),$$

as well as the dependence (25) for $\langle q^2(t) \rangle$. The deviation of (17) from the exact expression (15) is small right up to $i \sim A \gg 1$, but even at large t it can only lead to corrections of the order of unity in the numerical coefficients in the corresponding formulas.

The determination of the characteristics of the dynamical behavior of a dissipative quantum system in the region $A \lesssim 1$ requires a separate investigation. Such an investigation in the particular case of a superconducting junction can be complicated by the fact that, generally speaking, the adiabaticity condition, which allows us in a number of cases to reduce the effective action obtained with the aid of the microscopic theory^{12,13} to the simple formulas (2) and (3), is not fulfilled when the junction capacitance is fairly small.

In our paper we have investigated the $T \ll \Delta_r$ case, which is the most interesting case. As has been shown in a number of papers (see, for example, Refs. 2, 6, 7, 18, 19, and 21), for $T \gg \Delta_r$ the system relaxes to the equilibrium state, the relaxation being described by the rate $\Gamma(t) \propto T^{2\alpha-1}$ in a broad range of α values. The transition region $T \sim \Delta_r$ and also the case in which an external force F is present need to be investigated further.

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APPENDIX 1

As follows from the expression (5) for $P(t)$, the interaction between the $2r$ and $2r-1$ ($r = 1, 2, \dots, n$) instantons corresponds to an attraction between them, whereas the sign of the interaction between the remaining pairs of instantons depends on the sign of the "spin" variables s_{2r} . The relation (5) can be written in the following form (cf. Ref. 6):

$$P(t) = \sum_{n=0}^{\infty} (-2)^n \Delta^{2n} \text{Sp}_s \int dt_n \dots \int dt_1$$

$$\times \exp \left[- \sum_{i=1}^n S(t_{2i} - t_{2i-1}) + \frac{1}{2} \sum_{i,j=1}^n \Lambda(t_i, t_j) s_i s_j \right] (\cos \pi \alpha)^n, \quad (\text{A.1})$$

where we have set

$$S(\tau) = 2\alpha \ln(1 + |\tau|/\tau_0), \quad \Lambda(t_i, t_j) = S(t_{2i} - t_{2j-1}) + S(t_{2i-1} - t_{2j})$$

$$- S(t_{2i} - t_{2j}) - S(t_{2i-1} - t_{2j-1}) \quad (\text{A.2})$$

and $t_i = (t_{2i}, t_{2i-1})$, $t_{2i-1} < t_{2i}$. Here we have slightly changed the truncation procedure at short times $\sim \tau_0$. Such a change has no effect whatsoever on the form of the function $P(t)$ at $t \gg \tau_0$. Evidently, the approximation we used in Sec. 3 to compute $P(t)$ consists in making exact allowance for the interaction inside n "molecules" (each of which consists of the $2i$ th and the $(2i-1)$ th instantons) and neglecting the interaction between these "molecules." It is not difficult to estimate the number n_{char} beyond which this approximation fails. To do this, it is sufficient to expand the integrand in (A.1) in a series in powers of α . In first order in α , this expansion will contain only terms describing the interaction inside the "molecules," i.e., at very small values of α the

accuracy of the approximation of noninteracting "molecules" can be terminated only by the region of very long times $t \approx (\Delta\alpha)^{-1}$. At higher values of α we must take account of higher-order terms in the power-series expansion in α . As has already been noted, the dominant contribution in the region $\alpha < \frac{1}{2}$ is made by the configurations in which the instantons are located sufficiently far from each other, i.e., in (2) $|\tau| \gtrsim \Delta_r^{-1}$. For such configurations $\Lambda(t_i, t_j) \sim \alpha$ and $S(t_{2i} - t_{2i-1}) \sim \alpha A$. In the limit $A \gg 1$ the interaction between the "molecules" in the case when the numbers satisfy $n \ll n_{\text{char}} \sim A$ reduces to the renormalization of τ_0 , and can, for such n , be ignored. On the other hand, for a given t only the terms with the numbers $n \lesssim \Delta_r t$ in the formula (A.1) are important, from which it immediately follows that the neglect of the interaction between the "molecules" is legitimate at least for $t \ll \Delta_r^{-1} A$. Naturally, it does not follow from this estimate that the function $P(t)$ for $t \gtrsim \Delta_r^{-1} A$ differs essentially from (8). To investigate this region of times it may be useful to have the exact representation of $P(t)$ in the form of a functional integral. We therefore derive this representation below.

Let us define the function $\lambda(t, t')$ by the relation

$$\int dt_i \Lambda(t, t_i) \lambda(t_i, t') = \delta(t - t'). \quad (\text{A.3})$$

Then the function $P(t)$ can be written in the form of a functional integral taken over the field $\varphi(t)$:

$$P(t) = N_0^{-1} \int \mathcal{D}\varphi \exp\{-L_0(\varphi) - L_1(\varphi)\}, \quad (\text{A.4})$$

$$\exp\{-L_1(\varphi)\} = \sum_{n=0}^{\infty} (-1)^n \Delta^{2n} \int dt_n \dots \int dt_1 \exp\left[\sum_{i=1}^n \tilde{S}(t_i)\right] (\cos \pi\alpha)^n,$$

where the normalization factor N_0 is equal to

$$N_0 = \int \mathcal{D}\varphi \exp[-L_0(\varphi)], \quad L_0(\varphi) = \int dt dt' \lambda(t, t') \varphi(t) \varphi(t') \quad (\text{A.5})$$

and we have set

$$\tilde{S}(t_i) = S(t_{2i} - t_{2i-1}) + \ln \text{ch } \varphi(t_i). \quad (\text{A.6})$$

According to (A.4), the interaction of the molecules with each other can be taken into account within the framework of a system of non-interacting molecules by introducing a random interaction \tilde{S} for the instantons forming this molecule. Ignoring the fluctuations in the field $\varphi(t)$, we evaluate the functional integral (A.4) by the method of steepest descent. On a saddle-point trajectory we have $\varphi(t) = 0$, and the results obtained in Sec. 3 can be exactly reproduced in this self-consistent field approximation. By going beyond the self-consistent field approximation in (A.4), we can take account of the interaction of the molecules with each other. To do this, we must take into account the Gaussian fluctuations in the field $\varphi(t)$. Allowing for the contribution of such fluctuations amounts to the multiplication of the expressions (6) and (8) obtained for $P(t)$ in the self-consistent field approximation by the quantity $(\det K)^{-1/2}$, where

$$K(t, t') = \lambda(t, t') + \delta^2 L_1 / \delta\varphi(t) \delta\varphi(t').$$

APPENDIX 2

Using the integral representation¹⁵ for the function $\Gamma^{-1}(y)$, let us write the probability $W_p(t)$, (21) and (20), of finding the particle in the i th well in the form

$$W_p(t) = \frac{i}{2\pi^2} \int_c \frac{dx e^{-x}}{(-x)} (-z)^p \theta_p(z), \quad z = -4 \left(-\frac{\Delta_r t}{x} \right)^{2(1-\alpha)},$$

$$\theta_p(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!} \frac{\Gamma^2(k+p+1/2)}{\Gamma(k+2p+1)}$$

$$= \frac{\Gamma^2(p+1/2)}{\Gamma(2p+1)} F(p+1/2, p+1/2, 2p+1, z). \quad (\text{A.7})$$

The contour C encloses the positive coordinate axis in the plane of the complex variable x (see Ref. 15). The asymptotic ($x \rightarrow \infty$) value of the integral in (A.7) is determined by the singular points, $z = 1$ and $z \rightarrow \infty$, of the function $\theta_p(z)$. Using the asymptotic expression for the hypergeometric function F in (A.7), we extract the character of the singularities of this function:

$$\theta_p(z) = \begin{cases} (-z)^{-p-1/2} [\ln(-z) + 2\psi(1) - 2\psi(p+1/2)], & |z| \rightarrow \infty \\ -\ln(1-z) + 2\psi(1) - 2\psi(p+1/2), & 1-z \ll 1 \end{cases} \quad (\text{A.8})$$

To the singular points of the function $\theta_p(z)$ correspond the values $x_{\pm} = -\Delta_r^* t e^{\pm i\beta}$ and $x \rightarrow \infty$ of the integration variable in (A.7), where Δ_r^* and β are defined in (19). Summing the contributions to the integral in (A.7) from the neighborhoods of the singular points, and using the asymptotic forms (A.8) of the function $\theta_p(z)$, we find the expression (19) for the function $W_p(t)$.

¹ Below we shall also include in the expression for A a term $\sim \eta q_0^2$, which, for $\alpha \lesssim 1$, is of order unity, i.e., is much smaller than A .

² At $\alpha = \frac{1}{2}$ the problem of computing the partition function for the system in question is equivalent to the problem of finding the partition function in the (exactly soluble) "Toulouse limit."¹⁷ The ground-state energy in this limit is equal to $E_g = -\Delta^2 A / 4\omega_0$ at $T \lesssim \Delta_r$. Notice that the second term in (11) for $t \gtrsim \Delta_r^{-1}$ can be represented in the form $i\Delta^2 A t / 4\omega_0 = -iE_g t$.

³ Let us emphasize in this connection that in our paper the integration was performed over trajectories $q(t) \equiv q(\tau(t))$ in real (and not in imaginary) time.

⁴ It can be shown that this approximation is valid for $\alpha > 1$ or at high temperatures and (or) in the presence of a strong external force. It is precisely such a situation that is studied in Ref. 19.

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