On the dynamics of a particle in a two-well potential

B. I. Ivlev

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR, Chernogolovka
(Submitted 10 February 1988)
Zh. Eksp. Teor. Fiz. **94**, 333–343 (July 1988)

The question of the localization of a particle coupled with a thermostat in a two-well potential is investigated. It is shown in a systematic way that the partition function of this system has the same form as for the anisotropic Kondo model, the properties of which are well known. An analysis of these properties points to the localization of the particle in one of the wells at zero temperature if the interaction with the thermostat becomes sufficiently strong.

1. INTRODUCTION

Many papers have been devoted to the quantum dynamics of a particle interacting with a thermostat.[1–12] The interest in this problem is associated primarily with Josephson junctions, the quantum regime of which can be described starting from such ideas.

The behavior of a particle in a symmetric two-well potential arouses particular interest. According to quantum mechanics, in the absence of a thermostat weak splitting of the levels of one well occurs in the quasiclassical approximation. This implies that a particle initially localized in one well will be found after a certain time in the second, and this process will be repeated periodically, with a temporal period inversely proportional to the amount by which the levels move apart.

However, as was first shown in Refs. 4 and 5, as the interaction with the thermostat becomes stronger this picture can change substantially. Namely, if this interaction is sufficiently strong, then at zero temperature a particle localized in one of the wells will not pass over, in time, to the other. Its presence in the neighboring well will involve only a probability that decays exponentially in the coordinate. In this sense we can speak of the localization of the particle in one of the wells. Reference 1 is the most detailed review on this question.

If in the expansion of the exact wavefunction of the "particle plus thermostat" system we confine ourselves to just the two lowest states of the free particle in the two-well potential, this problem reduces to the analysis of a two-level system with a thermostat.[11,13] As shown in Ref. 13, the partition function of such a system has the same form as that for the Kondo model with an anisotropic exchange constant.[14] In the language of this model, the properties of which are well known, the localization corresponds to a phase transition to a state of the ferromagnetic type. The fact of the localization at zero temperature in a two-level system coupled sufficiently strongly with a thermostat is thereby proved.

However, if we reject such a simplifying assumption as the expansion in two states in the initial stage of the solution of the problem, the question of the possibility of localization ceases to be entirely obvious. In fact, for a two-well potential the partition function has been calculated by the instanton method,[4,5] which is approximate. Thus, e.g., in Ref. 12 doubt was cast on the applicability of the method of instantons to the problem of localization. Thus, the question of the localization of a particle in a two-well potential cannot be regarded as fully clarified, and this has served as the starting point for the present paper.

Localization implies degeneracy of levels of different parity (even and odd) with respect to the particle coordinate; this circumstance is reflected in the partition function, and hence it is important to study its properties. In the article we propose a method by which the problem of localization in a two-well potential can be reduced systematically to the analysis of the partition function of the Kondo model. In contrast to Refs. 14, 4, and 5, the result does not require an artificial cutoff of the logarithmic dependence, but takes the restriction on the logarithmic growth into account in a natural manner. As a result, localization occurs also in a real two-well potential, and not only in simplified two-level modeling of it.

The expression for the partition function is found by the method of functional integration in imaginary time $t = -i\tau$. The problem then reduces to the averaging of a certain effective partition function, in which the role of the energies is played by the quasi-energies of the Schrödinger equation with a potential that is periodic in imaginary time. The problem is solved for a two-well potential composed of pieces of parabolas. We demonstrate the applicability of the method to a two-level system, for which it gives the exact expression for its partition function.

2. CHOICE OF MODEL AND BASIC RELATIONS

In the treatment of Josephson junctions the role of the coordinate of the quantum particle is played by the difference in the phases of the order parameter across the junction, and the thermostat is the electron subsystem.[1–3] The detailed properties of the thermostat turn out to be unimportant, since the effective action has a universal form with only one constant - the damping constant, which depends on integral characteristics of the thermostat. For this reason, we shall consider a simple model of the thermostat in the form of an infinite set of harmonic oscillators with coordinates y_k (Ref. 1):

$$H = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} + V(x) + \sum_k \left(-\frac{1}{2m_k}\frac{\partial^2}{\partial y_k^2} + \frac{m_k\omega_k^2}{2} y_k^2 \right) + x\sum_k C_k y_k. \quad (1)$$

An important characteristic of the interaction of the particle with the thermostat is the spectral density

 0038-5646/88/071486-06$04.00

$$J(\omega)=\frac{\pi}{2}\sum_k \frac{C_k^2}{m_k\omega_k}\delta(\omega-\omega_k). \quad (2)$$

For the case of a particle attached to an infinite elastic string, $J(\omega)=\eta\omega$ at all frequencies. The same approximation for the spectral density can be adopted in problems concerning Josephson junctions.[2,3]

The quantity η is the damping coefficient that appears in the classical limit in the equation of motion $m\ddot{x}+\eta\dot{x}+V'=0$. We shall assume that $V(x)$ corresponds to a quasiclassical symmetric two-well potential.

The partition function $\tilde{Z}$ of the multidimensional system (1) can be expressed in the form of a functional integral, over x and over all the y_k, of an exponential whose exponent contains the classical action (of the imaginary time i/T, where T is the temperature[15]) corresponding to the Hamiltonian (1). Performing the Gaussian integration over all the y_k, we obtain[1]

$$\tilde{Z}=Z\prod_k\left(2\,\mathrm{sh}\frac{\omega_k}{2T}\right)^{-1}, \quad (3a)$$

$$Z=\int Dx(\tau)e^{-A}, \quad (3b)$$

where the effective action

$$A=\int_0^{1/T} d\tau\left[\frac{m}{2}\left(\frac{\partial x}{\partial\tau}\right)^2+V(x)\right]$$
$$-\frac{\eta}{2\pi}\int_0^{1/T} d\tau\frac{\partial x}{\partial\tau}\int_0^{1/T} d\tau'\frac{\partial x}{\partial\tau'}\ln|\sin\pi T(\tau-\tau')|. \quad (4)$$

Here $x(\tau)$ is a periodic function with period $1/T$.

In the following we shall leave aside the contribution of the harmonic oscillators to the partition function $\tilde{Z}$ and assume that the partition function is simply the quantity Z.

3. EXPRESSION FOR THE PARTITION FUNCTION IN TERMS OF THE QUASI-ENERGIES

The second term in formula (4), quadratic in $\partial x/\partial\tau$, can be reduced to a linear term by the well known procedure of introducing an additional Gaussian integration over a new field $\mathscr{E}(\tau)$ that is periodic in τ with period $1/T$. After simple transformations we obtain

$$Z=\left\langle\int Dx(\tau)\exp\left\{-\int_0^{1/T} d\tau\left[\frac{m}{2}\left(\frac{\partial x}{\partial\tau}\right)^2+V(x)-ix\mathscr{E}(\tau)\right]\right\}\right\rangle, \quad (5)$$

where the angular brackets denote averaging

$$\langle\Phi[\mathscr{E}]\rangle=\frac{\int D\mathscr{E}(\tau)\exp(Q[\mathscr{E}])\Phi[\mathscr{E}]}{\int D\mathscr{E}(\tau)\exp(Q[\mathscr{E}])} \quad (6)$$

with the functional

$$Q[\mathscr{E}]=\frac{1}{2\pi\eta}\int_0^{1/T} d\tau\,\mathscr{E}(\tau)\int_0^{1/T} d\tau'\,\mathscr{E}(\tau')\ln|\sin\pi T(\tau-\tau')|. \quad (7)$$

The formulas (5)–(7) are easily obtained from (3b) and (4) by expanding in Fourier harmonics:

$$\mathscr{E}(\tau)=(2T)^{1/2}\sum_{n=1}^{\infty}(\mathscr{E}_n'\cos\omega_n\tau+\mathscr{E}_n''\sin\omega_n\tau), \qquad \omega_n=2\pi Tn. \quad (8)$$

The expression in the angular brackets in formula (5) can be written in terms of the one-particle Green function[15] of imaginary time:

$$Z=\left\langle\int G(x,x;1/T,0)\,dx\right\rangle. \quad (9)$$

This function can be represented in the form

$$G(x,x';\tau,\tau')=\sum_n\Psi_n(x,\tau)\,\bar{\Psi}_n(x',\tau'), \quad (10)$$

where $\Psi_n(x,\tau)$ is an eigenfunction of the Schrödinger equation

$$-\frac{\partial\Psi(x,\tau)}{\partial\tau}=-\frac{1}{2m}\frac{\partial^2\Psi}{\partial x^2}+[V(x)-ix\mathscr{E}(\tau)]\Psi. \quad (11)$$

The function $\bar{\Psi}(x,\tau)$ satisfies the same equation, but with a change of sign of the time derivative.

Since the potential in Eq. (11) is, according to formula (8), a periodic function of τ, the eigenfunctions $\Psi_n(x,\tau)$ can be written in the form[16]

$$\Psi_n(x,\tau)=e^{-\varepsilon_n\tau}u_n(x,\tau), \quad u_n(x,\tau+1/T)=u_n(x,\tau). \quad (12)$$

The quantities ε_n are the quasi-energies of the Schrödinger equation (11) with a periodic potential. The set of functions $\Psi_n(x,\tau)$ is analogous to the eigenfunctions for a time-independent potential.

When the formulas (9) and (10) are taken into account the partition function takes the form

$$Z=\left\langle\sum_n e^{-\varepsilon_n/T}\right\rangle. \quad (13)$$

Thus, the proposed method for calculating the partition function is as follows: For an arbitrary periodic electric field $\mathscr{E}(\tau)$ (8) find the quasi-energies $\varepsilon_n[\mathscr{E}]$ of the Schrödinger equation (11) and then, in formula (13), perform the averaging using the rule (6), (7).

Although, at first sight, this procedure does not appear to be more constructive than other methods, nevertheless it makes it possible to reduce the partition function (3b) systematically and rather simply to the form given below (formula (40)).

4. CASE OF TWO PARABOLIC WELLS

In this section we shall consider the situation when each part of the two-well potential is part of a parabola:

$$V(x)=\tfrac{1}{2}m\Omega^2(x-\tfrac{1}{2}d\,\mathrm{sgn}\,x)^2. \quad (14)$$

The advantage of choosing such a potential is that within each well Eq. (11) can be solved exactly.[16] The problem is then to match the solutions.

Using formulas from Ref. 16, we write the solution of Eq. (11) with the potential (14) to the left and right of the point $x=0$:

$$\Psi(z,\tau)=\exp\left\{-\int\frac{d\tau}{4\Omega z_0^2}\left[\left(\frac{\partial\xi}{\partial\tau}\right)^2+\frac{1}{\Omega^2}\left(\frac{\partial^2\xi}{\partial\tau^2}\right)^2\right]-\frac{iz}{2z_0\Omega^2}\frac{\partial^2\xi}{\partial\tau^2}\right\}$$

$$\times\begin{cases} e^{-i\xi/2}\int d\nu\,\gamma_\nu^- e^{-\nu\Omega\tau} D_\nu^{(1)}(z+z_-), & z<0 \\ e^{i\xi/2}\int d\nu\,\gamma_\nu^+ e^{-\nu\Omega\tau} D_\nu^{(2)}(z-z_+), & z>0 \end{cases}, \qquad (15)$$

where the functions $\gamma_\nu^\pm$ can be determined from the matching conditions and we have introduced the new notation

$$z=x(2m\Omega)^{1/2},\quad z_0=d(m\Omega/2)^{1/2},\quad z_\pm=z_0\pm(i/z_0\Omega)\partial\xi/\partial\tau. \qquad (16)$$

The function $\xi(\tau)$ is connected with the electric field $\mathscr{E}(\tau)$ by the relation

$$\frac{\partial\xi}{\partial\tau}-\frac{1}{\Omega^2}\frac{\partial^3\xi}{\partial\tau^3}=\mathscr{E}(\tau)d. \qquad (17)$$

The integration over ν in formula (15) must be understood as summation over the Matsubara frequencies ω_m and the quasi-energies ε_n:

$$\Omega\nu\to\varepsilon_n+i\omega_m. \qquad (18)$$

However, for convenience we shall keep the integral notation. In formula (15) we have used the parabolic cylinder functions,[17] with asymptotic forms

$$\begin{aligned} &D_\nu^{(1)}(z)\sim(-z)^\nu\exp(-z^2/4), \quad z\to-\infty, \\ &D_\nu^{(2)}(z)\sim z^\nu\exp(-z^2/4), \quad z\to+\infty. \end{aligned} \qquad (19)$$

Matching of the function $\Psi(z,\tau)$ and its derivative $\partial\Psi/\partial z$ at the point $z=0$ gives

$$\begin{aligned} &\int d\nu\,\gamma_\nu^- e^{-\nu\Omega\tau}\left[\nu D_{\nu-1}^{(1)}(z_-)+\frac{i}{2z_0\Omega}\frac{\partial\xi}{\partial\tau}D_\nu^{(1)}(z_-)\right] \\ &=e^{i\xi}\int d\nu\,\gamma_\nu^+ e^{-\nu\Omega\tau}\left[-D_{\nu+1}^{(2)}(-z_+)-\frac{i}{2z_0\Omega}\frac{\partial\xi}{\partial\tau}D_\nu^{(2)}(-z_+)\right], \\ &\int d\nu\,\gamma_\nu^+ e^{-\nu\Omega\tau}\left[-\nu D_{\nu-1}^{(2)}(-z_+)-\frac{i}{2z_0\Omega}\frac{\partial\xi}{\partial\tau}D_\nu^{(2)}(-z_+)\right] \\ &=e^{-i\xi}\int d\nu\,\gamma_\nu^- e^{-\nu\Omega\tau}\left[D_{\nu+1}^{(1)}(z_-)+\frac{i}{2z_0\Omega}\frac{\partial\xi}{\partial\tau}D_\nu^{(1)}(z_-)\right]. \end{aligned} \qquad (20)$$

The formulas (20) are exact. At this stage we must use the quasiclassicality condition, which is expressed in the inequality $z_0\gg1$ and in the smallness of the time derivative in comparison with Ω. In addition, we take into account only the ground state of the unperturbed harmonic oscillator, which is valid for $T\ll\Omega$. In this approximation, in formula (20), we must discard the terms with $\partial\xi/\partial\tau$ and use for the parabolic cylinder functions their asymptotic expression.[17] Then the functions

$$g^\mp(\tau)=\int d\nu\,\gamma^\mp e^{-\nu\Omega\tau}\frac{1}{z_0^\nu\Gamma(1-\nu)}, \qquad (21)$$

where $\Gamma(x)$ is the gamma-function, satisfy the equations

$$\frac{\partial g^-}{\partial\tau}=\frac{\Delta}{2}e^{i\xi}g^+,\qquad \frac{\partial g^+}{\partial\tau}=\frac{\Delta}{2}e^{-i\xi}g^-, \qquad (22)$$

where Δ is the amount by which the levels move apart in the absence of interaction with the thermostat:

$$\Delta=\Omega z_0(2/\pi)^{1/2}\exp(-z_0^2/2). \qquad (23)$$

Since $\xi(\tau)$ is a periodic function, the solutions of Eqs. (22) will have the form

$$g_{1,2}^-(\tau)=e^{-\varepsilon_{1,2}\tau}F_{1,2}(\tau), \qquad (24)$$

where $F_{1,2}(\tau+1/T)=F_{1,2}(\tau)$. The quantities $\varepsilon_{1,2}$ are the quasi-energies corresponding to the Schrödinger equation (11) when only the lowest split level is taken into account. Using this, we write the partition function (13) in the form

$$Z=\langle(e^{-\varepsilon_1/T}+e^{-\varepsilon_2/T})\rangle. \qquad (25)$$

The averaging in this formula

$$\langle\Phi[\xi]\rangle=\frac{\int D\xi(\tau)\exp(Q[\xi])\Phi[\xi]}{\int D\xi(\tau)\exp(Q[\xi])} \qquad (26)$$

is performed with the functional (7), in which the electric field must be expressed in terms of $\xi(\tau)$ in accordance with formula (17):

$$Q[\xi]=\frac{1}{4\pi^2\alpha}\int_0^{1/T}d\tau\left(\frac{\partial\xi}{\partial\tau}-\frac{1}{\Omega^2}\frac{\partial^3\xi}{\partial\tau^3}\right)\times\int_0^{1/T}d\tau_1\left(\frac{\partial\xi}{\partial\tau_1}-\frac{1}{\Omega^2}\frac{\partial^3\xi}{\partial\tau_1^3}\right)\ln|\sin\pi T(\tau-\tau_1)|. \qquad (27)$$

Here we have introduced the dimensionless quantity

$$\alpha=\eta d^2/2\pi, \qquad (28)$$

which is important for what follows.

Using the harmonic expansion

$$\xi(\tau)=(2T)^{1/2}\sum_{n=1}^{\infty}(\xi_n'\cos\omega_n\tau+\xi_n''\sin\omega_n\tau), \qquad (29)$$

we can represent the functional Q (27) in the form

$$Q=-\frac{1}{4\pi\alpha}\sum_{n=1}^{\infty}(\xi_n'^2+\xi_n''^2)\omega_n\left(1+\frac{\omega_n^2}{\Omega^2}\right)^2. \qquad (30)$$

We note that the specific form of the parabolic wells affects only the form of the averaging functional Q—namely, the terms $\partial^3\xi/\partial\tau^3$ in formula (27).

Thus, at low temperatures $T\ll\Omega$, in the quasiclassical approximation the problem of calculating the partition function reduces to averaging, by the rules (26), (27), of the expression (25), in which the quasi-energies $\varepsilon_{1,2}$ are obtained from the solution of Eqs. (22) with the periodic function (29).

5. SPLITTING OF THE LEVELS FOR SMALL FRICTION $\alpha\ll1$

In this section we shall find the amount by which the levels move apart in the presence of weak interaction with the thermostat ($\alpha\ll1$). Here we are concerned with the two lowest-energy states of the entire quantum system (1), of which one is even and the other is odd in x in the limit of small α. For $\alpha=0$, as follows from formula (27), $\xi=0$, and from the system (22) it follows that the quasi-energies $\varepsilon_{1,2}=\mp\Delta/2$, in agreement with the splitting Δ of the levels in the absence of friction. We shall find the linear (in α) correction to this splitting.

The system (22) can be reduced to the equation

$$\frac{\partial^2g^-}{\partial\tau^2}-i\frac{\partial\xi}{\partial\tau}\frac{\partial g^-}{\partial\tau}-\frac{\Delta^2}{4}g^-=0. \qquad (31)$$

We shall seek the function g^- in the form

$$g^-(\tau)=\exp[-\varepsilon\tau-\sigma(\tau)], \quad (32)$$

where $\sigma(\tau+1/T)=\sigma(\tau)$ is a periodic function. Then,

$$-\frac{\partial^2\sigma}{\partial\tau^2}+\left(\frac{\partial\sigma}{\partial\tau}\right)^2+\varepsilon^2+2\varepsilon\frac{\partial\sigma}{\partial\tau}+i\frac{\partial\xi}{\partial\tau}\left(\varepsilon+\frac{\partial\sigma}{\partial\tau}\right)=\frac{\Delta^2}{4}. \quad (33)$$

The quasi-energy ε is determined by this equation and the periodicity of $\sigma(\tau)$, and this is true for any value of α. The calculation is particularly simple in the limit $\alpha\ll 1$. To second order of perturbation theory in ξ we have from Eq. (33)

$$\varepsilon^2=\frac{\Delta^2}{4}+\overline{\left(\frac{\partial\sigma}{\partial\tau}\right)^2}, \qquad -\frac{\partial^2\sigma}{\partial\tau^2}+2\varepsilon\frac{\partial\sigma}{\partial\tau}=-i\varepsilon\frac{\partial\xi}{\partial\tau}. \quad (34)$$

The bar denotes time averaging. Taking the expansion (29) into account, from this we easily find

$$\varepsilon_{1,2}=\mp\frac{\Delta}{2}\left[1-\frac{T\omega_n^2}{2(\Delta^2+\omega_n^2)}(\xi_n'^2+\xi_n''^2)\right]. \quad (35)$$

Performing the Gaussian integration in formula (25) with the aid of the relations (26) and (30), we find that $Z=2\cosh(\tilde\Delta/2T)$, where the renormalized splitting of the levels is

$$\tilde\Delta=\Delta-\alpha\Delta\,[\ln(\Omega/\Delta)-{}^1/_2]. \quad (36)$$

We note that, with logarithmic accuracy this formula is the well known result for the renormalized splitting of the levels in a two-well potential of general form.[5,12] The formula (36), which includes a number together with a large logarithm, is valid with this accuracy only for the potential (14) constructed from parabolic wells.

6. EXPRESSION FOR THE PARTITION FUNCTION

In this section we shall obtain for the partition function the expression that follows from the solution of Eqs. (22) with subsequent averaging. Iteration of the system (22) in the parameter Δ gives

$$g^-(\tau)=1+C\frac{\Delta}{2}\int_0^\tau d\tau_1\,e^{i\xi}+\frac{\Delta^2}{4}\int_0^\tau d\tau_1\,e^{i\xi}\int_0^{\tau_1} d\tau_2\,e^{-i\xi}+\dots. \quad (37)$$

The constant C appears as a coefficient in all the terms odd in Δ and fixes the value of $\partial g^-/\partial\tau$ at $\tau=0$. The solution (37) satisfies the condition $g^-=1$ at $\tau=0$. In the analogous series for g^+ the constant C appears as a coefficient of the even powers of Δ.

We shall find those solutions (24) in which $F_{1,2}(0)=1$. Then, from formula (25),

$$Z=\langle g_1^-(1/T)+g_2^-(1/T)\rangle. \quad (38)$$

Since Eq. (31) contains Δ^2, we have $\varepsilon_2(\Delta)=\varepsilon_1(-\Delta)$.

Since the Wronskian of Eq. (31) is proportional to $\exp(i\xi)$, the relation

$$F_1F_2\left(\varepsilon_1-\varepsilon_2+\frac{\partial}{\partial\tau}\ln\frac{F_2}{F_1}\right)e^{-\tau(\varepsilon_1+\varepsilon_2)}\sim e^{i\xi}$$

is valid for the solutions (24). From this and the periodicity in time we conclude that $\varepsilon_2=-\varepsilon_1$. For these reasons ε_1 and ε_2 are odd functions of Δ, and inside the averaging symbols in (38) is a quantity even in Δ. It follows from this that the conditions that $g_{1,2}^-(0)=1$ and that the quantity $g_1^-(1/T)+g_2^-(1/T)$ be even in Δ are necessary requirements on the solutions $g_{1,2}^-(\tau)$. These requirements are satisfied by two solutions of the type (37), with constants C of opposite signs. The sum in (38) will not depend on these constants, and we obtain

$$Z=2\left\langle\sum_{n=0}^{\infty}\left(\frac{\Delta}{2}\right)^{2n}\int_0^{1/T}d\tau_{2n}\int_0^{\tau_{2n}}d\tau_{2n-1}\dots\times\int_0^{\tau_2}d\tau_1\exp\left[i\sum_{k=1}^{2n}(-1)^k\xi(\tau_k)\right]\right\rangle. \quad (39)$$

The averaging in this formula by the rules (26), (27) reduces to a simple Gaussian integration, especially if we make use of the representations (29) and (30). As a result we obtain

$$Z=2\sum_{n=0}^{\infty}\left(\frac{\Delta}{2}\right)^{2n}\int_0^{1/T}d\tau_{2n}\int_0^{\tau_{2n}}d\tau_{2n-1}\dots\times\int_0^{\tau_2}d\tau_1\exp\left[\sum_{i>j}(-1)^{i+j}f(\tau_i-\tau_j)\right], \quad (40)$$

where the function $f(\tau)$ is determined by the relation

$$f(\tau)=4\pi\alpha T\sum_{n=1}^{\infty}\frac{1-\cos\omega_n\tau}{\omega_n}\left(1+\frac{\omega_n^2}{\Omega^2}\right)^{-2}, \qquad \omega_n=2\pi nT. \quad (41)$$

At zero temperature this gives

$$f(\tau)=2\alpha\int_0^\infty\frac{1-\cos q\Omega\tau}{q(1+q^2)^2}dq=\begin{cases}{}^1/_2\alpha(\Omega\tau)^2, & \Omega\tau\ll1\\ 2\alpha\ln(\gamma\Omega|\tau|e^{-1/2}), & 1\ll\Omega\tau\end{cases}. \quad (41a)$$

Here γ is the Euler constant.

The partition function (40) has the same form as for the anisotropic Kondo model.[14] A formula of the same type has been obtained for the problem under consideration by the instanton technique in Refs. 4 and 5. In contrast to these papers, in formula (40) it is not necessary to introduce an artificial cutoff of the logarithmic dependence at small times, since this is taken into account automatically thanks to the function $f(\tau)$ (41).

A renormalization-group analysis of the partition function (40) shows[14,4,5] that for $\alpha>1$ the renormalized splitting $\tilde\Delta$ of the levels vanishes, corresponding to localization of the particle in one of the wells at zero temperature. The equality $\tilde\Delta=0$ corresponds, in the language of the Kondo model, to the vanishing of that part of the exchange constant which gives rise to a spin flip.

As can be seen from formula (40), the result obtained by the method of instantons for small values of α is also valid for large values of this parameter, e.g., for $\alpha\gg1$, provided that we write the exact function $f(\tau)$ in place of the logarithm.

The concrete form (41) of $f(\tau)$ obtains only for parabolic wells. The temperature should, in any case, be small in comparison with the spacing between the levels in each individual well, i.e., $T\ll\Omega$.

7. CASE OF A TWO-LEVEL SYSTEM

In this section we shall trace how the technique developed can be applied in the case of a two-level system.

The problem of the dynamics of a particle in a two-well potential is simplified substantially if from the outset, in the expansion of the wavefunction of the system in the eigenfunctions of the Schrödinger equation without the thermostat, we take into account only the first two states. These states correspond to the quasiclassical splitting of the ground state of a free particle in the two-well potential. Here it is not necessary to assume parabolicity of the wells (formula (14)), and the results are valid for a potential of general form.

We turn to Eq. (11), the solution of which can be represented, in accordance with the above account, in the form

$$\Psi(x,\tau)=\varphi_1(\tau)\frac{\Psi_1(x)+\Psi_2(x)}{\sqrt{2}}+\varphi_2(\tau)\frac{\Psi_1(x)-\Psi_2(x)}{\sqrt{2}}. \tag{42}$$

Here $\Psi_{1,2}(x)$ are the exact wave functions of the ground state and the state split off from it in a symmetric two-well potential $V(x)$. Substituting the solution (42) into Eq. (11) and using the orthogonality properties of the functions $\Psi_{1,2}(x)$, we obtain an equation for the spinor $\hat{\varphi}(\tau)$ with components φ_1 and φ_2:

$$-\frac{\partial\hat{\varphi}}{\partial\tau}=\left(-\frac{\Delta}{2}\sigma_x+\frac{id}{2}\mathscr{E}(\tau)\sigma_z\right)\hat{\varphi}. \tag{43}$$

From this equation we must determine the two quasi-energies, substitute them into formula (25), and average using the rules (6), (7). If in this situation we introduce, as above, the periodic quantity $\xi(\tau)$ by means of the formula $\partial\xi/\partial\tau=\mathscr{E}d$, then Eqs. (22), which give the same values of the quasi-energies as Eq. (43), will hold for the functions $g^{+}=\exp(\pm i\xi/2)\varphi_{1,2}$.

In an analogous way the Hamiltonian (1) in the two-level approximation is reduced to the form

$$H'=-\frac{\Delta}{2}\sigma_x+\sum_k\left(-\frac{1}{2m_k}\frac{\partial^2}{\partial y_k^2}+\frac{m_k\omega_k^2}{2}y_k^2\right)+\frac{d}{2}\sigma_z\sum_k C_k y_k, \tag{44}$$

and is called a spin-boson Hamiltonian.[11]

To obtain the formula (44) it is necessary to use the expansion (42), in which the functions $\varphi_{1,2}$ also depend on all the phonon coordinates. Equation (43) is related to the Hamiltonian (44) to the same extent that Eq. (11) is related to the Hamiltonian (1).

The spin-boson Hamiltonian (44) serves as a good model for many problems—in particular, for the analysis of the hopping motion of a small polaron.[13] As shown in this paper, the exact partition function corresponding to the Hamiltonian (44) is expressed by formula (40).

We see that the formulation of the problem of the dynamics of a two-level system interacting with a thermostat is equivalent to specifying either the Hamiltonian (44) or the simulating equation (43) with the corresponding averaging rules. By specifying the Hamiltonian (44) we thereby also specify the spectral function $J(\Omega)$ (2). The expression (40) for the partition function in this case follows exactly from this, in contrast to the situation in the preceding section, when we had to neglect small parameters. To calculate the function $f(\tau)$ appearing in formula (40) we note that, for an arbitrary spectral density, in the expression (4) for the action it is necessary to make the formal substitution[1]

$$-\frac{\eta}{2\pi}\ln|\sin\pi T\tau|\rightarrow\sum_k\frac{C_k^2}{4m_k\omega_k^3}\frac{\mathrm{ch}(\omega_k|\tau|-\omega_k/2T)}{\mathrm{sh}(\omega_k/2T)}. \tag{45}$$

The kernel Q in the functional average (6) also changes correspondingly. As a result, after averaging the expression (39) we obtain

$$f(\tau)=\frac{d^2}{\pi}\int_0^\infty\frac{J(\omega)}{\omega^2}\frac{\mathrm{ch}(\omega/2T)-\mathrm{ch}(\omega/2T-\omega|\tau|)}{\mathrm{sh}(\omega/2T)}d\omega. \tag{46}$$

Thus, we see that for a two-level system the method described in the preceding sections, like that in Ref. 13, leads to an exact expression (40) for the partition function, with the function $f(\tau)$ given by formula (46). The requirement that the density $J(\omega)$ have the linear dependence $J=\eta\omega$ at small frequencies leads to logarithmic behavior of $f(\tau)$ at large times, and, consequently, to localization for $\alpha>1$. In contrast to the situation in the preceding section, for a two-level system the assumption that $J(\omega)$ is linear at all frequencies does not give a cutoff of the function $f(\tau)$ at small times. Therefore, in the case under consideration $J(\omega)$ should increase more slowly than ω at large frequencies.[11]

We shall consider the term of order $2n$ in the series (40) for the partition function. For $n=2$ and for large values of $\tau_i-\tau_j$ the exponential factor can be represented in the form

$$\frac{1}{[(\tau_1-\tau_2)(\tau_3-\tau_4)]^{2\alpha}}\left\{\frac{(\tau_1-\tau_3)(\tau_2-\tau_4)}{(\tau_1-\tau_4)(\tau_2-\tau_3)}\right\}^{2\alpha}. \tag{47}$$

For large α in the limit of low T, the corresponding term in formula (40) is proportional to T^{-2}. This occurs because the integrals over $\tau_1-\tau_2$ and $\tau_3-\tau_4$ are concentrated at the inverse cutoff frequency, while the remaining two integrations occur at times T^{-1}, since with this choice of scales the factor in the curly brackets in formula (47) becomes equal to unity.

An arbitrary term of order $2n$ in formula (40) is proportional to T^{-n} for the same reason, since all neighboring instantons $(\tau_1-\tau_2)$, $(\tau_3-\tau_4)$, $(\tau_5-\tau_6)$, ... turn out to be bound in pairs, and the motion of each pair will be free. As a result, the partition function (40) acquires the form

$$Z=2\sum_{n=0}^{\infty}(-\delta E)^n\int_0^{1/T}d\tau_{2n}\int_0^{\tau_{2n}}d\tau_{2n-2}\ldots\int_0^{\tau_4}d\tau_2, \tag{48}$$

where, when formula (46) is taken into account,

$$\delta E=-\frac{\Delta^2}{4}\int_0^\infty d\tau\exp\left[-\frac{d^2}{\pi}\int_0^\infty\frac{J(\omega)}{\omega^2}(1-e^{-\omega\tau})d\omega\right]. \tag{49}$$

The partition function (48) $Z=2\exp(-\delta E/T)$, and the quantity δE is a correction to the ground-state energy. The same result for this correction is obtained in second order of perturbation theory in Δ for the Hamiltonian (44). The applicability of perturbation theory in the magnitude of the bare separation of the levels is associated with a situation of the zero-charge type, since the renormalized $\tilde{\Delta}$ is equal to zero. Allowance for four-instanton correlations corresponds to a term of order Δ^4 in δE, and so on.

The analysis of the common shift δE of the levels is not fundamental in the phenomenon of localization. Nevertheless, the arguments given make it possible to interpret the transition to the localized state as the formation, from a plasma of instantons, of a gas of their neutral atoms, which interact weakly with each other.

In kinetic problems as well, the applicability of perturbation theory in the bare quantity Δ for $\alpha > 1$ makes it possible to confine oneself to second order in Δ in the calculation of the relaxation rate Γ. The probability of finding the particle in the left (right) well is

$$W_{1,2}={}^1/_2(1\pm e^{-\Gamma t}), \tag{50}$$

where, for $\alpha \gg 1$,[11,12]

$$\Gamma=\frac{\Delta^2}{4\Omega(\pi\alpha)^{1/2}}\left(\frac{\pi e^{1/2}}{\gamma}\right)^{2\alpha}\left(\frac{T}{\Omega}\right)^{2\alpha-1}. \tag{51}$$

8. CONCLUSION

The partition function of a system consisting of a particle interacting with a thermostat reduces to the same form as in the anisotropic Kondo model. The properties of this model are well known and tell us that for a sufficiently strong interaction with the thermostat ($\alpha > 1$) the particle will be found to be localized in one of the wells at zero temperature. This corresponds to a relaxation rate $\Gamma \propto T^{2\alpha-1}$.

It is essential for this conclusion that the spectral density $J(\omega)$ be linear in the frequency at small ω. This property is inherent in models describing the quantum properties of Josephson junctions. Such a phenomenon as localization is qualitatively reflected in the quantum dynamics of the phase difference at a low-capacitance Josephson junction.[18]

I am grateful to S. A. Bulgadaev, P. B. Wiegmann, A. I. Larkin, Yu. N. Ovchinnikov, and A. M. Finkel'shteĭn for valuable discussions.

[1]A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. **46**, 211 (1981).
[2]V. Ambegaokar, U. Eckern, and G. Schön, Phys. Rev. Lett. **48**, 1745 (1982).
[3]A. I. Larkin and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **85**, 1510 (1983) [Sov. Phys. JETP **58**, 876 (1983)].
[4]S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982).
[5]A. J. Bray and M. A. Moore, Phys. Rev. Lett. **49**, 1545 (1982).
[6]A. Schmid, Phys. Rev. Lett. **51**, 1506 (1983).
[7]S. A. Bulgadaev, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 264 (1984) [JETP Lett. **39**, 315 (1984)].
[8]Yu. Kagan and N. V. Prokof'ev, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 70 (1987) [JETP Lett. **45**, 115 (1987)].
[9]F. Guinea, V. Hakim, and A. Muramatsu, Phys. Rev. B **32**, 4410 (1985).
[10]K. Hida, Z. Phys. B **61**, 223 (1985).
[11]A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[12]Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **94**, No. 5 365 (1988) [Sov. Phys. JETP **67**, No. 5 (1988)].
[13]N. Rivier and T. J. Coe, J. Phys. C **10**, 4471 (1977).
[14]P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B **1**, 4464 (1970).
[15]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York (1965) [Russ. transl., Mir, Moscow (1968)].
[16]A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, *Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics*, Israel Programme for Scientific Translations (1969) [Russ. original, Nauka, Moscow (1971)].
[17]A. Erdélyi (ed.), *Higher Transcendental Functions* (California Institute of Technology H. Bateman MS Project), 3 vols., McGraw-Hill, New York (1953, 1955).
[18]K. K. Likharev and A. B. Zorin, J. Low Temp. Phys. **59**, 347 (1985).

Translated by P. J. Shepherd