

Ground state of a particle in a two-well potential

Yu. N. Ovchinnikov

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR

(Submitted 17 March 1988)

Zh. Eksp. Teor. Fiz. **94**, 346-352 (September 1988)

The ground state of a particle in a two-well symmetric potential and the rate of relaxation of the particle to the ground state are investigated. In the vicinity of the point $\alpha = \frac{1}{2}$ (α is the constant describing the interaction of the particle with the thermostat) a sharp change occurs in the behavior of the rate of relaxation and frequency of oscillation of the population of the wells in the two-well potential. At temperature T equal to zero the relaxation rate remains nonzero for arbitrary values of the coupling constant α . The temperature T_0 above which the temperature dependence of the relaxation rate becomes important is found.

1. INTRODUCTION

The behavior of a quantum particle in a two-well symmetric potential and interacting with a thermostat has been actively investigated in recent years. The principal results pertaining to this problem are described in the review Ref. 1.

In the absence of interaction with a thermostat the probability of finding the particle in the first (or in the second) well if at $t = 0$ it was localized in, e.g., the first well oscillates in time with a frequency Δ_0 equal to the magnitude of the splitting of the ground-state level in the two-well potential.² Interaction with a thermostat leads to a renormalization of the frequency of the oscillations and to the appearance of a nonzero relaxation rate γ . In addition, so-called incoherent terms, with a power-law decay, appear.¹ At large times $t \gg \gamma^{-1}$ the incoherent terms also decay exponentially. This picture remains valid in all cases so long as the effective coupling constant α of the interaction with the thermostat is less than $\frac{1}{2}$.

In Refs. 4-7 it was stated that at temperature $T = 0$ and with a thermostat-particle coupling constant $\alpha > 1$ the particle is localized in one of the wells. This statement is extremely important for an understanding of the dynamics of a quantum particle.

To check this statement, below we shall investigate the ground state of the system at $T = 0$ and find the rate of relaxation to the ground state. The ground state turns out to be nondegenerate for arbitrary values of the thermostat-particle coupling constant, and the relaxation rate is nonzero.

Hence, the conclusion that the particle is localized when $\alpha > 1$ appears to us to be erroneous.

2. DESCRIPTION OF THE MODEL

We replace the interaction of the quantum particle with the thermostat by interaction with an infinite set of oscillators¹ and write the Hamiltonian of the entire system in the form

$$\hat{H} = -\frac{1}{2M} \frac{\partial^2}{\partial x^2} + U(x) + \sum_k \left\{ -\frac{1}{2m_k} \frac{\partial^2}{\partial y_k^2} + \frac{m_k \omega_k^2 y_k^2}{2} + \frac{\alpha_k y_k x}{2} \right\}, \quad (1)$$

where M is the mass of the quantum particle, $U(x)$ is the two-well potential, and the quantities m_k , ω_k , and y_k are the mass, frequency, and coordinate of the k th oscillator. Henceforth we shall assume that the number of oscillators

tends to infinity while the coupling constant α_k of the interaction with each individual oscillator tends to zero.

As is well known,¹ in such a model the interaction with the set of oscillators is determined by a single function $J(\omega)$ of the frequency:

$$J(\omega) = \sum_h \frac{\pi \alpha_h^2 x_0^2}{2 m_h \omega_h} \delta(\omega_h - \omega), \quad (2)$$

where $\pm x_0$ are the positions of the minima of the potential $U(x)$. We shall assume that "viscous friction" is present in the system, i.e., that the function $J(\omega)$ is proportional to ω as $\omega \rightarrow 0$:

$$J(\omega)/2\pi = \alpha\omega \quad (3)$$

for $\omega \ll \Omega_p$, where Ω_p is the frequency of small oscillations about the minimum of $U(x)$:

$$M\Omega_p^2 = (\partial^2 U / \partial x^2)_{x=\pm x_0}. \quad (4)$$

We shall assume also that the interaction (3) is effectively cut off at a frequency ω_c of the order of Ω_p . A method of introducing the cutoff will be given below.

3. GROUND STATE OF THE SYSTEM AT $T=0$

When the coupling constant of the interaction with the thermostat is equal to zero the states of the system can be classified by their parity and by the excitation number n of each oscillator k (i.e., by the set $\{k, n\}$). The classification with respect to parity is preserved in an obvious manner in the presence of interaction with the thermostat. In addition, we shall assume that in accordance with the theorem that there can be no crossing of terms with the same symmetry,² upon change of the coupling constant from its value α to zero any eigenstate of the Hamiltonian (1) goes over into a state with the same, well defined set $\{k, n\}$, and the set $\{k, 0\}$ corresponds to the ground state.

Let $\psi_{\pm}(x)$ be the wave functions of a quantum particle in the absence of the interaction:

$$\left\{ -\frac{1}{2M} \frac{\partial^2}{\partial x^2} + U(x) \right\} \psi_{\pm}(x) = \frac{\Omega_p \mp \Delta_0}{2} \psi_{\pm}(x). \quad (5)$$

We write the wave function of the ground state of the system in the form

$$\bar{\Psi}_+ = \Phi\{y_k\} \frac{\psi_+ + \psi_-}{2^{1/2}} + \Phi\{-y_k\} \frac{\psi_+ - \psi_-}{2^{1/2}}. \quad (6)$$

Substituting the expression (6) into the eigenvalue equation for the operator \hat{H} , we obtain

$$E\Phi\{y_k\} = \left(\frac{\Omega_p}{2} + \hat{H}_{\Phi^+}\right)\Phi\{y_k\} - \frac{\Delta_0}{2}\Phi\{-y_k\} - \sum_k \frac{\alpha_k^2 x_0^2}{8m_k\omega_k^2}\Phi\{y_k\}, \quad (7)$$

where E is the eigenvalue of the operator \hat{H} :

$$\hat{H}_{\Phi^+} = \sum_k \left\{ -\frac{1}{2m_k} \frac{\partial^2}{\partial y_k^2} + \frac{m_k\omega_k^2}{2} \left(y_k + \frac{\alpha_k x_0}{2m_k\omega_k^2} \right)^2 \right\}. \quad (8)$$

Setting

$$E = \frac{\Omega_p}{2} + \sum_k \frac{\omega_k}{2} - \sum_k \frac{\alpha_k^2 x_0^2}{8m_k\omega_k^2} + \bar{E}_+, \quad (9)$$

$$z_k = y_k + \frac{\alpha_k x_0}{2m_k\omega_k^2},$$

we obtain from formula (7) an equation for the function $\Phi\{z_k\}$:

$$\Phi\{z_k\} = -\frac{\Delta_0}{2} \left[\bar{E}_+ - \left(\hat{H}_{\Phi^+} - \sum_k \frac{\omega_k}{2} \right) \right]^{-1} \Phi \left\{ -z_k + \frac{\alpha_k x_0}{m_k\omega_k^2} \right\}. \quad (10)$$

By direct calculation we can verify that the following formula is valid:

$$\begin{aligned} & \left[\bar{E}_+ - \left(\hat{H}_{\Phi^+} - \sum_k \frac{\omega_k}{2} \right) \right]^{-1} \Phi_0 \left\{ z_k - \frac{\alpha_k x_0}{2m_k\omega_k^2} \right\} \\ &= \prod_k \left(\frac{m_k\omega_k}{\pi} \right)^{1/4} \int_0^\infty dt \exp \left\{ t\bar{E}_+ - \frac{m_k\omega_k}{2} \left[z_k - \frac{\alpha_k x_0}{2m_k\omega_k^2} \exp(-t\omega_k) \right]^2 - \frac{\alpha_k^2 x_0^2}{16m_k\omega_k^3} (1 - \exp(-2t\omega_k)) \right\}, \quad (11) \end{aligned}$$

where

$$\Phi_0\{z_k\} = \prod_k \left(\frac{m_k\omega_k}{\pi} \right)^{1/4} \exp \left(-\frac{m_k\omega_k}{2} z_k^2 \right). \quad (12)$$

Taking into account the remarks made above, we shall seek the ground-state wave function by iterating Eq. (10), in which, as the zeroth approximation, we take the wave function (12).

Performing N interactions using the formula (11), we obtain

$$\begin{aligned} \Phi_N\{z_k\} &= \prod_k \left(\frac{m_k\omega_k}{\pi} \right)^{1/4} \int_0^\infty dt_1 \dots dt_N \exp \left(\bar{E} \sum_{L=1}^N t_L \right) \\ &\times \exp \left\{ -\frac{m_k\omega_k}{2} \left(z_k - \frac{\alpha_k x_0}{2m_k\omega_k^2} a_N(t_1 \dots t_N) \right)^2 - \frac{\alpha_k^2 x_0^2}{16m_k\omega_k^3} b_N(t_1 \dots t_N) \right\}. \quad (13) \end{aligned}$$

The functions a_N and b_N depend on N times t_1, \dots, t_N , and satisfy the recursion relations

$$\begin{aligned} a_{N+1} &= (2 - a_N) \exp(-\omega_k t_{N+1}), \\ b_{N+1} &= b_N + (2 - a_N)^2 [1 - \exp(-2\omega_k t_{N+1})]. \quad (14) \end{aligned}$$

Multiplying both sides of Eq. (10) by $\Phi_0\{z_k\}$ and integrating over the variables $\{z_k\}$, we obtain an expression for the quantity \bar{E}_+ :

$$\begin{aligned} & \prod_k \int_0^\infty dt_1 \dots dt_N \exp \left(\bar{E}_+ \sum_{L=1}^N t_L \right) \\ & \times \left\{ \bar{E}_+ + \frac{\Delta_0}{2} \exp \left[-\frac{\alpha_k^2 x_0^2}{4m_k\omega_k^3} (1 - a_N) \right] \right\} \\ & \times \exp \left\{ -\frac{\alpha_k^2 x_0^2}{16m_k\omega_k^3} (b_N + a_N^2 - 1) \right\} = 0. \quad (15) \end{aligned}$$

Using the recursion relations (14) we can rewrite Eq. (15) in the form

$$1 = \frac{\Delta_0}{2} \lim_{N \rightarrow \infty} \frac{I_N}{I_{N-1}}, \quad (16)$$

where

$$\begin{aligned} I_N &= \int_0^\infty dt_1 \dots dt_N \exp \left\{ \bar{E}_+ \sum_{L=1}^N t_L \right\} \\ & \times \exp \left\{ -\sum_k \frac{\alpha_k^2 x_0^2}{4m_k\omega_k^3} \sum_{L=1}^N (1 - a_L) \right\}. \quad (17) \end{aligned}$$

Equation (16) for the quantity \bar{E}_+ can be rewritten conveniently in the form

$$1 = \frac{\Delta_0^2}{4} \lim_{N \rightarrow \infty} \frac{I_{2N}}{I_{2N-2}}. \quad (18)$$

This equation determines not only the ground-state energy \bar{E}_+ but also the energy \bar{E}_- of the odd state without real excitations in the system of oscillators. In order to obtain the value of \bar{E}_- it is necessary in Eq. (18) to perform the analytic continuation in the energy \bar{E} in such a way that \bar{E} be positive for $\alpha = 0$.

To prove this statement we write the odd solution without real phonons in the form

$$\bar{\Psi}_- = \bar{\Phi}\{y_k\} \frac{\Psi_+ + \Psi_-}{2^{1/2}} - \bar{\Phi}\{-y_k\} \frac{\Psi_+ - \Psi_-}{2^{1/2}}. \quad (19)$$

By making use of the energy of this state in the form (9) with \bar{E}_+ replaced by \bar{E}_- we obtain for the quantity $\bar{\Phi}\{z_k\}$ an equation that differs from formula (10) by the replacement of the quantity Δ_0 by $-\Delta_0$:

$$\bar{\Phi}\{z_k\} = \frac{\Delta_0}{2} \left[\bar{E}_- - \left(\hat{H}_{\Phi^+} - \sum_k \frac{\omega_k}{2} \right) \right]^{-1} \Phi \left\{ -z_k + \frac{\alpha_k x_0}{m_k\omega_k^2} \right\}. \quad (20)$$

Using the formulas (11) and (20) and repeating the arguments that lead to the formula (18), we find that the energy \bar{E}_- satisfies the same equation (18). For the ground state of the system the quantity \bar{E}_+ is always negative and the integrals in formula (18) can be calculated without any complications. For the odd no-phonon state the quantity \bar{E}_- for $\alpha = 0$ is positive, and, as was noted above, in formula (18) it is necessary to perform analytic continuation in \bar{E} . When the discrete set of oscillators is replaced by a continuous distribution the energy of the odd state without real excitations of the oscillators is found to lie on the background of the continuous spectrum. As a result, the quantity

\tilde{E}_- acquires an imaginary part, the magnitude of which determines the rate of relaxation of the populations of the wells. We turn now to the calculation of the integrals in formula (18).

Using the recursion relation (14), for the quantity a_N we obtain the expression

$$a_N = (-)^{N-1} \exp\left(-\omega_k \sum_{L=1}^N t_L\right) \times \left[1 + 2 \sum_{p=1}^{N-1} (-)^p \exp\left(\omega_k \sum_{L=1}^p t_L\right)\right]. \quad (21)$$

The behavior of the system depends in an essential way on the quantity $J(\omega)$ given by formula (2). We shall assume that for small values of ω the relation (3) is fulfilled and the equality

$$\int_0^{\infty} \frac{d\omega J(\omega)}{2\pi\omega^2} [1 - \exp(-\omega t)] = \alpha \ln(1 + \omega_c t) \quad (22)$$

holds. Using the expressions (21) and (22), we find

$$\int_0^{\infty} \frac{d\omega J(\omega)}{2\pi\omega^2} [(1 - a_{2N}) + (1 - a_{2N-1})] = 2\alpha \ln(1 + \omega_c t_{2N}) + \alpha \ln \left[1 - \omega_c t_{2N} / \left(1 + \omega_c \sum_{L=1}^{2N} t_L\right)\right] + 2\alpha \ln \left\{ \prod_{h=1}^{N-1} \left[1 - \omega_c t_{2N} / \left(1 + \omega_c \sum_{L=2h+1}^{2N} t_L\right)\right]^{-1} \right\}. \quad (23)$$

It follows from this that in a narrow neighborhood of the point $\alpha = \frac{1}{2}$ a sharp change occurs in the dependence of the quantity \tilde{E} on the value of the coupling constant. In the region $\alpha < \frac{1}{2}$ the important values of all the times t are of the order of $|\tilde{E}|^{-1}$, and from the formulas (23) and (18) we obtain

$$E_+ = -\frac{\Delta_0}{2} \left(\frac{\Delta_0}{\omega_c}\right)^{\alpha/(1-\alpha)} \chi(\alpha), \quad (24)$$

$$\tilde{E}_- = \frac{\Delta_0}{2} \left(\frac{\Delta_0}{\omega_c}\right)^{\alpha/(1-\alpha)} \chi(\alpha) \exp\left(-\frac{i\pi\alpha}{1-\alpha}\right), \quad \alpha < 1/2.$$

The function $\chi(\alpha)$ is equal to 1 at $\alpha = 0$ and has a singularity $(1 - 2\alpha)^{-1}$ at values of α close to $\frac{1}{2}$. In the vicinity of the point $\alpha = \frac{1}{2}$ the expression (24) for the quantity \tilde{E}_+ ceases to be valid. In the region $|1 - 2\alpha| \ll 1$ the quantity \tilde{E}_+ can be found from the equation

$$1 = \frac{\Delta_0^2}{4} \frac{A}{\tilde{E}_+^2} \left(\frac{|\tilde{E}_+|}{\omega_c}\right)^{2\alpha} \frac{1 - (|\tilde{E}_+|/\omega_c)^{1-2\alpha}}{1 - 2\alpha}, \quad (25)$$

where the constant A is a number of order 1 and will be found below.

In the region $\alpha > \frac{1}{2}$, in the formula (23) for \tilde{E}_+ the important values of t_{2N} are $\sim |\tilde{E}_+|^{-1}$, and the important values of t_{2N-1} are $\sim \omega_c^{-1}$. Taking this remark into account, from the formulas (16), (18), and (23) we find

$$\tilde{E}_+ = -\frac{\Delta_0^2}{4\omega_c} \frac{1}{2\alpha - 1}, \quad \alpha > 1/2. \quad (26)$$

Comparing the values of \tilde{E}_+ obtained from formulas (25)

and (26) in the regions $\alpha > \frac{1}{2}$ and $\alpha - \frac{1}{2} \ll 1$, we obtain for the constant A the value

$$A = 1. \quad (27)$$

From the formulas (24) we find expressions for the splitting δE and relaxation rate γ in the region $\alpha < \frac{1}{2}$:

$$\delta E = \text{Re } \tilde{E}_- - \tilde{E}_+ = \frac{\Delta_0}{2} \left(\frac{\Delta_0}{\omega_c}\right)^{\alpha/(1-\alpha)} \chi(\alpha) \left[1 + \cos\left(\frac{\pi\alpha}{1-\alpha}\right)\right], \quad (28)$$

$$\gamma = -\text{Im } \tilde{E}_- = \frac{\Delta_0}{2} \left(\frac{\Delta_0}{\omega_c}\right)^{\alpha/(1-\alpha)} \chi(\alpha) \sin\left(\frac{\pi\alpha}{1-\alpha}\right).$$

From the formulas (28) it follows that

$$\gamma/\delta E = \text{tg}(\pi\alpha/2(1-\alpha)). \quad (29)$$

The formula (29) in the region $\alpha < \frac{1}{2}$ coincides with the result cited in the review Ref. 1.

For the analytic continuation in formulas (17) and (18) we first of all replace $\tilde{E}t$ by $-t$. After this the analytic continuation reduces, in a very simple integral, to the replacement

$$\int_0^{\infty} \frac{dte^{-t}}{(1 - \omega_c t/E)^{2\alpha}} \rightarrow \int_{\Gamma} \frac{dte^{-t}}{(1 - \omega_c t/E)^{2\alpha}}. \quad (30)$$

The contour Γ is shown in the figure, and the quantity $(1 - \omega_c t/E)^{2\alpha}$ is defined so that it is equal to 1 at $t = 0$.

In the region $\alpha > \frac{1}{2}$, in the leading approximation we obtain for the quantity \tilde{E}_- the same value (26) as for the quantity \tilde{E}_+ . Allowance for the correction leads to the appearance of splitting and of an imaginary part of the energy \tilde{E}_- :

$$1 = \frac{\Delta_0^2}{4} \left\{ -\frac{1}{2\alpha - 1} \frac{1}{\omega_c \tilde{E}_-} - \frac{1}{\omega_c \tilde{E}_-} \left(-\frac{\tilde{E}_-}{\omega_c}\right)^{2\alpha - 1} \times (\psi_1(\alpha) + i\psi_2(\alpha)) \right\}. \quad (31)$$

The functions ψ_1 and ψ_2 arise as a result of the integration over the contour Γ . In order of magnitude,

$$\psi_1, \psi_2 \sim \Gamma^{-1}(2\alpha), \quad (32)$$

where $\Gamma(x)$ is the gamma function.

For sufficiently large values of the parameter α and not very low temperatures, when coherent processes are unimportant, the relaxation rate γ is given by the expression^{1,3,8}

$$\gamma = \frac{\Delta_0^2}{4T(\pi\alpha)^{1/2}} \exp\left\{-2\alpha \ln\left(\frac{\omega_c}{\pi T}\right)\right\}. \quad (33)$$

Comparing the expressions (31) and (33), we find the temperature T_0 below which the relaxation rate does not depend

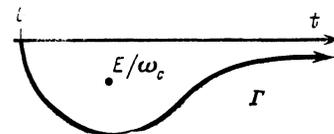


FIG. 1.

on the temperature:

$$T_0 = \frac{|\tilde{E}_+|}{2\pi\alpha} \exp(1) = \frac{\Delta_0^2}{16\pi\alpha^2\omega_c} \exp(1), \quad \alpha \gg 1.$$

The expression for the general energy shift (26) coincides with the result obtained by Ivlev in Ref. 9.

4. CONCLUSION

We have obtained an expression for the quantity δE —the difference of the levels in the odd state and the even state without real excitations of the system of oscillators in the entire range of values of the coupling constant α . In the region $\alpha < \frac{1}{2}$ all important values of the times are of the order of $|\tilde{E}|^{-1}$ and increase with increase of the parameter α . However, in a narrow neighborhood of the point $\alpha = \frac{1}{2}$ the behavior of the system changes sharply: The important values of some of the times begin to decrease rapidly and, as the coupling constant passes through the point $\alpha = \frac{1}{2}$, become of the order of ω_c^{-1} , i.e., of the order of the inverse cutoff frequency. Thus, for a complete description of the system in the region $\alpha > \frac{1}{2}$ it is necessary to take into account higher excited states in the potential $U(x)$.

For an arbitrary value of the coupling constant α the ground state is found to be nondegenerate and the relaxation rate nonzero.

We note once again that the frequency cutoff at ω_c becomes important at values $\alpha > \frac{1}{2}$. Neglect of unity alongside the term ωt in formula (22) would lead to a widening of the region of applicability of formula (24) for \tilde{E}_+ to values $\alpha < 1$ and to the appearance of a singularity at the point $\alpha = 1$.

In conclusion the author expresses his gratitude to A. I. Larkin, B. I. Ivlev, and S. A. Bulgadaev for a useful discussion of the results obtained.

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Translated by P. J. Shepherd