Intraband tunneling Umklapp of quasimomentum

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Processes of intraband tunneling Umklapp of quasimomentum that occur on account of interaction of a particle in an energy band with a thermostat are investigated. These processes are analogous to the tunneling of a particle through an energy barrier, with the role of the coordinate being played by the quasimomentum. Quasimomentum tunneling has a substantial influence on the dynamics of Josephson junctions of small capacitance.

1. INTRODUCTION

In this paper we shall investigate the motion of a particle in a periodic potential in the presence of dissipation.[1–7] This problem has a bearing on the dynamics of Josephson junctions of small capacitance,[1–3] and also on the electronic properties of a crystal in which the electron-electron interaction has a nonadiabatic character.[5] Interaction with the medium makes possible not only the usual scattering processes with small quasimomentum transfer but also tunneling Umklapp of quasimomentum within the same band, this being analogous to the tunneling of a particle through a potential barrier. Here the role of the coordinate is played by the quasimomentum.[8] Such quasiclassical processes are usually relatively improbable, since they are accompanied by the involvement of a large number of degrees of freedom of the medium. Nevertheless, owing to the large pre-exponential factor these processes can turn out to be important, even if the friction coefficient is still rather small. These processes are especially important in the description of the quantum dynamics of Josephson junctions, when, as shown below, they may be the only cause of the relaxation of certain components of the distribution function.

Below, we shall find the probability of intraband quasimomentum Umklapp. These processes give, first of all, an additional contribution to the relaxation of the distribution function of the particles in the band. In addition, in the presence of an infinitely large shunt resistance, i.e., in the absence of "Gaussian" dissipation, quasimomentum tunneling is the only cause of damping of single-particle oscillations in a Josephson junction.[9,10]

2. PROBABILITY OF TUNNELING UMKLAPP OF QUASIMOMENTUM

To calculate the probability of tunneling Umklapp of quasimomentum we shall analyze the partition function Z of a system consisting of a particle interacting with a medium[1,8]:

$$Z=\int Dp\,Dq\exp\left\{\int_0^{1/T}d\tau\left[-\varepsilon(p)+ip\frac{\partial q}{\partial\tau}\right.\right.$$
$$\left.\left.-\frac{\eta}{4\pi}\int_{-\infty}^{\infty}d\tau_1\left(\frac{q(\tau)-q(\tau_1)}{\tau-\tau_1}\right)^2\right]\right\},\tag{1}$$

where p is the quasimomentum of the particle, $\varepsilon(p)$ is the energy spectrum in the single-band approximation:

$$\varepsilon(p)=-{}^1/_2\delta\cos\pi p,\tag{2}$$

and the viscosity coefficient η determines the relaxation rate in the classical equation of motion for the coordinate q of the particle:

$$m\frac{\partial^2 q}{\partial t^2}+\eta\frac{\partial q}{\partial t}+\frac{\partial U}{\partial q}=0,\tag{3}$$

where $U(q)$ is the initial periodic potential.

The integration over one of the quasimomenta p in the formula (1) should be performed within the limits of the Brillouin zone $|p|<1$. Performing the integration over $q(\tau)$ in formula (1), we obtain for the partition function Z an expression that depends only on the variable p:

$$Z=\frac{1}{Z_0}\int Dp\exp\left\{-\int_0^{1/T}d\tau\left[\varepsilon(p)+\frac{1}{4\pi\eta}\right.\right.$$
$$\left.\left.\times\int_{-\infty}^{\infty}d\tau_1\left(\frac{p(\tau)-p(\tau_1)}{\tau-\tau_1}\right)^2\right]\right\},\tag{4}$$

where

$$Z_0=\int Dp\exp\left\{-\frac{1}{4\pi\eta}\int_{-\infty}^{\infty}d\tau_1\left(\frac{p(\tau)-p(\tau_1)}{\tau-\tau_1}\right)^2\right\}.\tag{5}$$

Below, we shall consider the case of small values of the viscosity coefficient η, when the quasimomentum p is a good quantum number. In this case the quantum fluctuations are small, and in the leading approximation the partition function is determined by the formula

$$Z=\frac{1}{2}\int_{-1}^{1}dp\exp\left[-\frac{\varepsilon(p)}{T}\right].\tag{6}$$

The partition function (4) coincides completely with the partition function of a massless particle moving in a potential $\varepsilon(p)$ and interacting strongly with a thermostat.[1–3] The role of the coordinate in this case is played by the momentum p. As is well known, in this case tunneling penetration of the particle through the potential barrier $\varepsilon(p)$ is possible (see the figure).

The tunneling leads to the result that the lifetime of the particle in one of the potential wells $\varepsilon(p)$ is finite. We shall be interested in the probability of transition through the potential barrier for a given value of the initial quasimomentum.

To calculate this probability we shall make use of the above-noted analogy between the system under considera-

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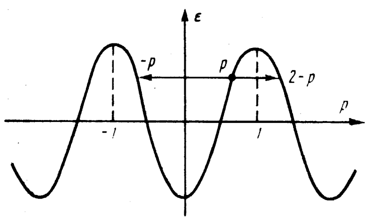

FIG. 1.

tion and a massless particle attached to an elastic string. The Lagrangian of such a system can be written in the form

$$\mathcal{L} = \frac{\rho}{2}\int_{-\infty}^{\infty} dy\left[\left(\frac{\partial R(y,t)}{\partial t}\right)^2 - s^2\left(\frac{\partial R(y,t)}{\partial y}\right)^2\right] - \varepsilon(R(0,t)), \tag{7}$$

where ρ is the density of the medium and s is the sound velocity. The particle is attached to the string at the point $y=0$.

First we shall find the quantum-mechanical probability of the tunneling of the system consisting of particle and string through a potential barrier. We shall then average the probability obtained over all the states of the string, assuming the position of the particle to be fixed. The resulting probability will be the probability of intraband breakdown with a given initial quasimomentum.

It is of special interest to investigate the case when the quasimomentum is close to the boundary of the Brillouin zone. Then the potential energy $\varepsilon(R(0,t))$ can be replaced by a quadratic dependence:

$$\varepsilon(R(0,t)) = \delta - {}^1/_4\pi^2\delta[1-R(0,t)]^2. \tag{8}$$

In this approximation the quantum-mechanical tunneling problem can be solved exactly by diagonalizing the Lagrangian (7) with allowance for the formula (8).

For this we go over to the normal coordinates R_n of the string:

$$R(y,t) = 1 + \sum_{n=-\infty}^{\infty} R_n(t)\exp\left(\frac{2\pi i}{L}ny\right). \tag{9}$$

In the coordinates R_n the Lagrangian (7) takes the form

$$\mathcal{L} = \frac{\rho L}{2}\sum_n\left[\left|\frac{\partial R_n}{\partial t}\right|^2 - \left(\frac{2\pi s}{L}n\right)^2|R_n|^2\right] + \frac{\pi^2\delta}{4}\left(\sum_n R_n\right)^2 - \delta \tag{10}$$

where L is the length of the string. The two quadratic forms in formula (10) can be brought simultaneously to diagonal form. Introducing the new variables

$$x_k = \rho^{1/2}\left[1+\left(\frac{\pi\alpha\delta}{sk}\right)^2\right]^{-1/2}\int_{-\infty}^{\infty} dy\left[\cos ky - \frac{\pi\alpha\delta}{sk}\sin(k|y|)\right][R(y)-1], \tag{11}$$

$$x_s = \frac{\pi\delta^{1/2}}{2s}\int_{-\infty}^{\infty} dy[R(y)-1]\exp\left(-\frac{\pi\alpha\delta}{s}|y|\right), \tag{12}$$

and $\alpha = \pi/4\rho s$, we obtain for the Lagrangian the expression

$$\mathcal{L} = \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{1}{2}\left[\left(\frac{\partial x_k}{\partial t}\right)^2 - (sk)^2x_k^2\right] + \frac{1}{2}\left(\frac{\partial x_s}{\partial t}\right)^2 + \frac{(\pi\alpha\delta)^2}{2}x_s^2 - \delta. \tag{13}$$

In this language, the tunneling of the system consisting of a particle and a string corresponds to sub-barrier motion along the coordinate x_s. As is well known,[11] the transmission coefficient is determined by the formula

$$D = \exp\left\{-\alpha\left[\frac{\pi^2\delta}{s}\int_0^{\infty} dy(R(y)-1)\exp\left(-\frac{\pi\alpha\delta}{s}y\right)\right]^2\right\}. \tag{14}$$

The expression (14) must be averaged over the states of the string for a fixed value $R(0)$. We shall assume that the string is at temperature T. Then the expression (14) for the transmission coefficient must be averaged with weight

$$\exp\left[-\frac{\rho s^2}{2T}\int_{-\infty}^{\infty} dy\left(\frac{\partial R}{\partial y}\right)^2\right]. \tag{15}$$

With exponential accuracy, the quantity $\langle D\rangle$ is determined by an extremal trajectory $R(y)$ that is even in y and is found from the condition for the minimum of the sum A of the exponents from formulas (14) and (15):

$$A[R(y)] = \alpha\left[\frac{\pi^2\delta}{2s}\int_{-\infty}^{\infty} dy(R(y)-1)\exp\left(-\frac{\pi\alpha\delta}{s}|y|\right)\right]^2 + \frac{\rho s^2}{2T}\int_{-\infty}^{\infty} dy\left(\frac{\partial R}{\partial y}\right)^2 \tag{16}$$

Varying the quantity A with respect to the function $R(y)$, we obtain for the latter the equation

$$-\frac{\partial^2 R}{\partial\xi^2} + \frac{2T}{T_0}e^{-\xi}\int_0^{\infty} d\xi_1[R(\xi_1)-1]e^{-\xi_1} = 0, \quad \xi\geqslant 0, \tag{17}$$

where $\xi = \pi\alpha\delta y/s$ and $T_0 = \alpha\delta/2$.

The solution of Eq. (17) with a specified value $R(0)$ is the function

$$R_0(y) = 1 + \frac{2}{\pi}\left[1-\frac{\varepsilon(p)}{\delta}\right]^{1/2} \times \frac{1}{T_0+T}\left[2T\exp\left(-\frac{\pi\alpha\delta}{s}y\right) + T_0 - T\right], \tag{18}$$

where the function $\varepsilon(p)$ is determined by formula (2).

Substituting the expression (18) for the function $R(y)$ into formula (16), we obtain

$$A[R_0(y)] = w(\varepsilon(p),T) = \frac{\delta-\varepsilon(p)}{\alpha\delta}\frac{4T_0}{T_0+T}. \tag{19}$$

The quantity $w(\varepsilon, T)$ determines, with exponential accuracy, the probability $\Gamma(p, T)$ of tunneling Umklapp of quasimomentum:

$$\Gamma(p,T) = B\exp[-w(\varepsilon(p),T)]. \tag{20}$$

It is simplest to find the pre-exponential factor B at a temperature T close to T_0 for quasimomentum values close to the boundary of the Brillouin zone.

In the state of thermal equilibrium the total probability $\gamma(T)$ of intraband tunneling Umklapp can be found by averaging the quantity $\Gamma(p, T)$ over the equilibrium distribution function:

$$\gamma(T)=\left(\frac{\pi\delta}{4T}\right)^{1/2}\int_{-1}^{1} dp\Gamma(p,T)\exp\left[-\frac{\varepsilon(p)}{T}\right]. \tag{21}$$

On the other hand, at a temperature T close to T_0 the quantity $\gamma(T)$ can be found by the well known technique of Refs. 1–3 using trajectories in imaginary time:

$$\gamma(T)=(8\pi\delta T)^{1/2}\exp\left(-\frac{\delta}{T}\right)\left(\frac{\omega_c}{2\pi T_0}\right)^{\alpha\delta/T} \times\exp\left[\frac{\delta}{2T_0}\left(1-\frac{T}{T_0}\right)^2\right]. \tag{22}$$

In deriving the formula (22) we have used for the partition function the expression (4), corresponding to a large viscosity. The coefficient η is connected with the parameter α by the relation

$$\alpha=\pi\eta/2. \tag{23}$$

The frequency cutoff ω_c is equal in order of magnitude to the spacing between the bands.

Assuming that the pre-exponential factor B depends only weakly on the temperature, comparing the formulas (21) and (22) we obtain

$$B=\frac{\omega_c^2}{\pi\alpha\delta}\left[\frac{\delta-\varepsilon(p)}{\pi\alpha\delta}\right]^{1/2}. \tag{24}$$

Thus, the formulas (19), (20), and (24) determine the probability of intraband quasimomentum tunneling near the boundary of the Brillouin zone.

We note that, with quasiclassical accuracy, owing to the symmetry of the $\varepsilon(p)$ spectrum, energy is conserved in the intraband tunneling, and the quasimomentum p in the given band is replaced by $-p$, as shown in the figure.

3. DYNAMICS OF A PARTICLE IN A SLOPING PERIODIC POTENTIAL

As is well known,[1] the dynamics of a Josephson junction of small capacitance is analogous to the dynamics of a quantum particle moving in a sloping periodic potential and interacting with a medium. The potential in this case is the quantity

$$U(\varphi)=-E_J\cos 2\varphi-F\varphi, \tag{25}$$

where $E_J = I_c/2e$, $F= I/e$, I_c is the critical current for the junction, and I is the current flowing across the junction. The role of the mass is played by the quantity $m = C/e^2$, where C is the capacitance of the junction.

In the absence of a current I the motion has a band character. We shall take into account the lowest Brillouin zone, with spectrum determined by formula (2). Short circuits of normal metal, shunting the Josephson junction, lead to a dissipation mechanism of the Gaussian type, corresponding to formulas (1) and (4). The state of the particle can be described using the distribution function $n(p, t)$. In the quasiclassical approximation, in a limited interval of time $t\gg\gamma_2^{-1}$, in which $\gamma_2\sim\alpha\delta^2/T$ at high temperatures $T\gg\delta$ (Ref. 7), the distribution function satisfies the Fokker-Planck equation[9,10]

$$\left(\frac{\partial}{\partial t}+F\frac{\partial}{\partial p}\right)n(p,t)=\eta\frac{\partial}{\partial p}\left[\frac{\partial\varepsilon(p)}{\partial p}n\right]+\eta T\frac{\partial^2 n}{\partial p^2}, \tag{26}$$

from which it follows that the characteristic relaxation time is of the order of $(\eta T)^{-1}$.

The intraband-tunneling processes considered above are not taken into account by the quasiclassical equation (26). Although the probability of such processes, as follows from formula (20), is exponentially small, to the large pre-exponential factor can make these processes important. They can be taken into account by adding to the right-hand side of formula (26) the term

$$-\Gamma(p, T)\,[n(p)-n(-p)], \tag{27}$$

where the quantity $\Gamma(p, T)$ is determined by the formulas (19), (20), and (24).

In the limit of small viscosity ($\eta\ll1$), the quasiclassical intraband-tunneling processes give a small contribution to the relaxation rate in (26). However, in real Josephson junctions the parameter η, as a rule, is not very small, and intraband-tunneling processes make a substantial contribution to the relaxation rate.

Intraband tunneling leads to a qualitatively new phenomenon in Josephson junctions, in which dissipation arises because of tunneling of normal electrons between impregnations of normal phase in the edges of the tunnel junction. Dissipation of this type leads to replacement of the quantity $[q(\tau)-q(\tau_1)]^2$ in formula (1) by $4\sin^2\{[q(\tau)-q(\tau_1)]/2\}$. With this dissipation mechanism an exact calculation of the intraband-tunneling probability Γ is difficult. The important point, however, is that such a process exists.

At high temperatures $T\gg\delta$, for times $t\ll\gamma_2^{-1}$ (Ref. 7), the equation for the distribution function has the form[10,12]

$$\left(\frac{\partial}{\partial t}+F\frac{\partial}{\partial p}\right)n(p)=2\eta\{-\varepsilon(p)\,[n(p-\operatorname{sgn}p)+n(p)] +T[n(p-\operatorname{sgn}p)-n(p)]\}-\Gamma[n(p)-n(-p)]. \tag{28}$$

With neglect of the intraband tunneling the symmetrized part of the distribution function, i.e.,

$$W(p,t)=n(p)+n(p-\operatorname{sgn}p), \tag{29}$$

satisfies Eq. (28) without the right-hand side. The solution of this equation has the form

$$W(p,t)=W(p-Ft) \tag{30}$$

for an arbitrary periodic function W,

$$W(p+1)=W(p). \tag{31}$$

We remark that when intraband tunneling and dissipation of the Gaussian type are disregarded the solution (30) for the symmetrized part (29) of the distribution function is valid for arbitrary times. The restriction on the applicability of Eq. (28) by the inequality $t\ll\gamma_2^{-1}$ pertains in this case to the antisymmetric part $n(p)-n(p-\operatorname{sgn}p)$ of the distribution function.

It follows from formula (31) that the quasimomentum depends linearly on the time, and at the moment when $\varepsilon(p)$

approaches its maximum value the Umklapp process occurs. As a result the function W relaxes rapidly to a constant value. Single-particle voltage oscillations with frequencies equal to multiples of $2\pi F$ (Refs. 10, 7, 12) are thereby damped even in the presence of an infinitely large shunt resistance, i.e., in the absence of dissipation of the Gaussian type.

4. CONCLUSION

Above, we have found the probability of intraband tunneling Umklapp of quasimomentum. The probability of this quasiclassical process is exponentially small in the inverse coupling constant describing the interaction with the thermostat [formula (19)]. However, the large pre-exponential factor compensates for this exponential smallness to a considerable degree. As has been shown, such processes exert a substantial influence on the dynamics of Josephson junctions.

Tunneling Umklapp of quasimomentum also exists in real crystals. In crystals the analog of the dissipation mechanism considered above is the nonadiabatic part of the electron-electron interaction.[5] This interaction is analogous in many respects to the dissipative mechanism that operates in Josephson junctions in the tunneling of normal electrons. In narrow-band crystals the nonadiabatic part of the electron-electron interaction can lead to a substantial rearrangement of the electron spectrum, leading to a still greater narrowing of the band of allowed energies.

[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. **86**, 719 (1984) [Sov. Phys. JETP **59**, 420 (1984)].
[4] S. Chakravarty, Phys. Rev. Lett. **49**, 681 (1982).
[5] Yu. Kagan and N. V. Prokof'ev, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 91 (1987) [JETP Lett. **45**, 115 (1987)].
[6] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[7] B. I. Ivlev and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **95**, 2065 (1989) [Sov. Phys. JETP **68**, 1194 (1989)].
[8] B. I. Ivlev and Yu. N. Ovchinnikov, Pis'ma Zh. Eksp. Teor. Fiz. **48**, 630 (1988) [JETP Lett. **48**, 682 (1988)].
[9] K. K. Likharev and A. B. Zorin, J. Low Temp. Phys. **59**, 347 (1985).
[10] D. V. Averin and K. K. Likharev, Zh. Eksp. Teor. Fiz. **90**, 733 (1986) [Sov. Phys. JETP **63**, 427 (1986)]; D. V. Averin, Fiz. Nizk. Temp. **13**, 364 (1987) [Sov. J. Low Temp. Phys. **13**, 208 (1987)].
[11] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, 3rd ed., Pergamon Press, Oxford (1977) [Russ. original, Nauka, Moscow (1974)].
[12] Yu. N. Ovchinnikov and B. I. Ivlev, Preprint, Instituto di Cibernetica, C.N.R., Italy (1988).

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