

Special role of the two-phonon interaction in the problem of quantum tunneling with dissipation in a crystal

Yu. Kagan and N. V. Prokof'ev

I. V. Kurchatov Institute of Atomic Energy, Academy of Sciences of the USSR, Moscow
(Submitted 31 July 1989)

Zh. Eksp. Teor. Fiz. **96**, 2209–2228 (December 1989)

It is shown that in tunneling motion in a dielectric crystal the viscous (“ohmic”) regime of dissipation arises only when two-phonon (many-phonon) interactions are taken into account. One-phonon interactions in any order lead only to polaron narrowing of the band. It is found that two-phonon interactions lead to an exponential decrease of the coherent-transition amplitude even for $T \ll \theta_D$ and give rise to a transition from coherent quantum diffusion to sub-barrier incoherent diffusion. The latter, however, does not involve stimulated phonon transitions. In an analysis of crystals of lower dimensionality it is shown that the role of one-phonon processes in the kinetics is restored only in the case $d = 1$ under the additional condition that the “transport effect” is absent. The analysis is based on a direct determination of the overlap integral of the phonon wave functions that form during the finite time for which the particle can be found in an individual elementary cell. The special role of two-phonon processes in the determination of the effective action in the technique of functional integration is traced independently.

1. INTRODUCTION

The range of phenomena that has become known as “tunneling with dissipation” has been widely discussed recently (see, e.g., Refs. 1 and 2). We have in mind sub-barrier tunneling in conditions of interaction of the particle, or more complex object, with excitations of the medium. The Hamiltonian of the problem usually has the form

$$H = H_R + H_{ex} + H_{int}(\mathbf{R}), \quad H_R = M\mathbf{R}^2/2 + U(\mathbf{R}), \quad (1.1)$$

where H_R is the Hamiltonian of the particle in the fixed potential relief $U(\mathbf{R})$, H_{ex} is the Hamiltonian of the excitations of the medium, and $H_{int}(\mathbf{R})$ is the interaction of the particle with the excitations.

In the case of interaction with phonons H_{int} is chosen in the form

$$H_{int} = \sum_{\beta} c_{\beta}(\mathbf{R}) (b_{\beta} + b_{-\beta}^{\dagger}), \quad (1.2)$$

corresponding to one-phonon interaction (here, b_{β} and b_{β}^{\dagger} are phonon annihilation and creation operators). Important in the analysis of the problem is the assumption that the spectral function, of the form

$$f(\omega) = \sum_{\beta} \frac{|\bar{c}_{\beta}|^2}{2\omega_{\beta}} \delta(\omega - \omega_{\beta}), \quad (1.3)$$

$$\bar{c}_{\beta} = c_{\beta}(\mathbf{R}_1) - c_{\beta}(\mathbf{R}_2)$$

approaches a constant value as $\omega \rightarrow 0$, i.e.,

$$f(0) = \eta = \text{const.} \quad (1.4)$$

With this condition the extremum of the action constructed for the Hamiltonian (1.1) leads to the classical equation of motion of the particle in the form of Newton's equation with friction.^{1,2} At first glance, such a “viscous” (“ohmic”) regime of motion of a slow particle, especially when we go over to a crystal, appears natural. In addition, if we turn to (1.3) it is easy to understand that the result (1.4) requires a special assumption concerning the dependence of the density of

states of the phonon spectrum on the frequency for $\omega \rightarrow 0$. We note that in the case of interaction with conduction electrons in a metal the finiteness of the density of states at $\varepsilon = \varepsilon_F$ automatically ensures the validity of the relation (1.4) for the appropriately defined function $f_{el}(\omega)$. The same is true for the problem of tunneling in a Josephson junction, where the role of the particle coordinate in (1.1) is played by the phase of the superconducting wave function (see, e.g., Refs. 1–4). However, by considering the tunneling motion of a particle in a crystal of dimensionality d , it is not difficult to convince oneself that the frequency dependence of the function (1.3) as $\omega \rightarrow 0$ in the general case has the form⁵

$$f(\omega) \propto \omega^{d-1+(2)}. \quad (1.5)$$

The extra 2 in the power exponent appears whenever $c_{\alpha}(\mathbf{R}_1)$ and $c_{\beta}(\mathbf{R}_2)$ in the field of a phonon with wave vector \mathbf{q} differ only by the phase factor $\exp(i\mathbf{q} \cdot \mathbf{R}_i)$, which predetermines the appearance of a “transport effect”. It follows from (1.5) that the limit (1.4) is valid only in a one-dimensional crystal in the absence of the transport effect. In all other cases, one-phonon interaction does not lead to tunneling motion in the viscous regime, which is usually identified with the phenomenon of tunneling with dissipation. Therefore, in particular, analysis of tunneling motion in a three-dimensional crystal by the technique of functional integration with the use of the relation (1.4) has a doubly artificial character, leaving open both the question of the mechanism responsible for tunneling with dissipation and the character of the dependence on the temperature T and on the dimensionality d of the crystal.

The breakdown of the viscous regime of tunneling in a crystal makes it necessary, in the general case, to go beyond the framework of the one-phonon interaction. For this the Hamiltonian (1.1) should be supplemented, at least, by a term corresponding to the two-phonon interaction

$$H_{int}^{(2)} = 1/2 \sum_{\alpha\beta} B_{\alpha\beta}(\mathbf{R}) (b_{\alpha} + b_{-\alpha}^{\dagger}) (b_{\beta} + b_{-\beta}^{\dagger}). \quad (1.6)$$

Because of the small scale of the displacement of the atoms in the crystal at low temperatures, allowance for the many-

phonon interaction in (1.1) in the form (1.6) is sufficient. As will be shown below, the viscous regime of tunneling is then restored and it is the two-phonon interaction that turns out to be decisive for the quantum diffusion of particles in a regular crystal. We stress that we are speaking specifically of the interaction (1.6), and not of a two-phonon process that appears in second order with (1.2).

We remark that, even in an early stage of the study of quantum diffusion of particles in a crystal using the formalism of the kinetic equation for the density matrix,⁶⁻⁸ the important role of two-phonon processes was revealed. At the same time, there was no general approach permitting the determination of the amplitude of the tunneling transition between neighboring unit cells while simultaneously allowing for the one-phonon and two-phonon interactions, or, correspondingly, the determination of the coherent and incoherent diffusion and also the band regime of motion in the crystal. As is shown in the present paper, the solution of this problem can be found by means of a method based on the direct determination of the overlap integral of the wave functions of the medium that are formed during the finite time τ for which the particle is in an individual unit cell — a method that has been applied previously to the interaction with conduction electrons^{9,10} and to the one-phonon interaction.⁵ The analysis performed below is devoted primarily to this method. Independently, we shall examine how the effective action in the functional-integration technique is changed when (1.6) is taken into account, and how, at the same time, an infrared divergence appears in the action.

It should be noted that the question of how the role of two-phonon processes is worked out and how the results of Refs. 6 and 7 are regained can already be extracted, in part, from Kondo's paper¹¹ devoted to the diffusion of a μ^+ muon in a metal.

2. THE ADIABATIC APPROXIMATION

As the starting point we shall consider the problem of sub-barrier tunneling between wells in which the lowest level of one is shifted by an amount ξ from the lowest level of the other. Let the tunneling-transition amplitude Δ_0 (more precisely, the amplitude $\bar{\Delta}_0$ renormalized on account of the interaction with phonons) and the bias ξ be small in comparison with the spacing ω_0 to the next level and also in comparison with the characteristic frequency θ_D of the phonon spectrum of the crystal:

$$\xi, \bar{\Delta}_0 \ll \omega_0, \theta_D. \quad (2.1)$$

In addition, we assume that $T \ll \omega_0$ and consider transitions only along the lowest level. In these conditions the tunneling particle spends a long time $\tau \gg \theta_D^{-1}$ in an individual well. During this time, a many-particle wave function $\Psi_\nu^{(i)}(\mathbf{R}, \mathbf{x})$, incorporating all virtual excitations with $\omega > \tau^{-1}$, has time to be formed; here, \mathbf{x} are the collective coordinates of the medium and $i = 1, 2$ labels the well.

The excitations of the medium can be divided into "fast" excitations, with frequencies $\omega > \omega_0$, and "slow" excitations, with $\omega < \omega_0$. For barriers of ordinary shape the characteristic inverse (imaginary) time of the motion under the barrier has the same scale as ω_0 , and, for simplicity, we shall not distinguish these two characteristics. It is not difficult to show that the fast excitations adapt to the motion of the

particle both in a well and under the barrier, leading to renormalization of the potential relief and, to a small extent, of the mass M of the particle. The slow excitations, on the contrary, do not follow the particle, and the part corresponding to them in the wave function $\Psi_\nu^{(i)}$ is concentrated toward the center of the potential well. We note that in the case of the interaction of the tunneling particle with the electron subsystem this separation of the excitations has been traced explicitly in Ref. 9. Specifically, the interaction with the slow excitations predetermines the appearance of the polaron effect and the diffusion kinetics at low temperatures. Note that in both the limiting cases $\omega_0 \gg \theta_D$ and $\omega_0 \ll \theta_D$, which display qualitatively the entire physical picture, the actual division of the frequency intervals is simplified. In the former case, only slow excitations are present, and there is no preliminary renormalization of the potential relief. In the latter case, on the other hand, practically the entire spectrum takes part in the renormalization. Here the polaron effect in the three- and two-dimensional cases is small, and, when conditions (2.1) and $\omega_0 \gg T$ are fulfilled, the kinetics is determined by the phonons with frequencies $\omega \ll \omega_0$. Only in the one-dimensional case in the absence of the transport effect (see Ref. 5, and also below) do the results depend on the position of the boundary between the slow and the fast excitations. But this dependence is weak (logarithmic), and some degree of arbitrariness in the fixing of the boundary does not affect the qualitative results (cf. the discussion in Ref. 2). Henceforth, when considering the interaction with slow excitations, we shall use for the upper boundary of the spectrum the notation $\omega_c = (\omega_0, \theta_D)_{\min}$.

We single out in the renormalized potential relief an individual well $U^{(i)}(\mathbf{R})$, extending its edges in the usual way. If we denote by $H_R^{(i)}$ the Hamiltonian of a particle in such a well, the general Hamiltonian of the one-well problem can be written in the form

$$H^i = H_R^{(i)} + H_{ph} + V^{(i)}(\mathbf{R}, \mathbf{x}), \quad (2.2)$$

where $V^{(i)}(\mathbf{R}, \mathbf{x})$ is the interaction of the particle with the slow phonon excitations. We denote by $H'(\mathbf{R})$ the difference between the true potential relief and the chosen "no-decay" well $U^{(i)}(\mathbf{R})$. Then for the matrix element of the transition from one well to the other we have

$$M_{\nu\nu'} = \langle \Psi_{\nu'}^{(2)}(\mathbf{R}, \mathbf{x}) | H'(\mathbf{R}) | \Psi_\nu^{(1)}(\mathbf{R}, \mathbf{x}) \rangle. \quad (2.3)$$

Knowledge of the matrix elements (2.3), both nondiagonal and diagonal in the state ν of the medium, fully determines, under the condition (2.1), the problem of tunneling with interaction with the medium. This also applies to the problem of a coherent transition with the formation of a band ($\nu' = \nu$) if we are concerned with a crystal.

The fact that only the interaction with the slow excitations appears in (2.9) means that it is possible to seek the eigenstates of this Hamiltonian in the adiabatic approximation

$$\Psi_\nu^{(i)}(\mathbf{R}, \mathbf{x}) = \varphi_0^{(i)}(\mathbf{R}, \mathbf{x}) \Phi_\nu^{(i)}(\mathbf{x}), \quad (2.4)$$

where the wave functions $\varphi_0^{(i)}$ and $\Phi_\nu^{(i)}$ are solutions of the equations

$$\begin{aligned} [H_R + V(\mathbf{R}, \mathbf{x})] \varphi_0(\mathbf{R}, \mathbf{x}) &= \varepsilon_0(\mathbf{x}) \varphi_0(\mathbf{R}, \mathbf{x}), \\ [H_{ph} + \varepsilon_0(\mathbf{x})] \Phi_\nu(\mathbf{x}) &= E_\nu \Phi_\nu(\mathbf{x}) \end{aligned} \quad (2.5)$$

(for simplicity we temporarily omit the index i). We expand the energy $\varepsilon_0(x)$ in powers of the displacement of the atoms from their equilibrium position:

$$\varepsilon_0(x) - \varepsilon_0(0) \approx \sum_{\beta} \gamma_{\beta} x_{\beta} + \frac{1}{2} \sum_{\beta\beta'} \gamma_{\beta\beta'} x_{\beta} x_{\beta'} + \dots, \quad (2.6)$$

where x_{β} are the normal phonon coordinates.

Up to now, in the determination of the restructuring of the phonon wave function $\Phi_{\nu}(x)$ only one-phonon processes [the first term in (2.6)] have been taken into account. However, as pointed out in the Introduction, the inclusion of two-phonon processes is fundamental for the description of quantum diffusion in crystals and, in general, for the determination of time correlation functions. At the same time, the inclusion of higher-order terms in (2.6) will not introduce any qualitative changes. Below, we shall confine ourselves to the first two terms in the expansion (2.6).

3. CONSTRUCTION OF THE SITE WAVE FUNCTION

In accordance with (2.5) and (2.6) the wave function $\Phi_{\nu}(x)$ is an eigenfunction of a Hamiltonian having, in second quantization, the form [cf. (1.2) and (1.6)]

$$H_{int} = \sum_{\beta} \omega_{\beta} (b_{\beta}^{+} b_{\beta} + \frac{1}{2}) + \sum_{\beta} c_{\beta}(\mathbf{R}) (b_{\beta} + b_{-\beta}^{+}) + \frac{1}{2} \sum_{\alpha\beta} B_{\alpha\beta}(\mathbf{R}) (b_{\alpha} + b_{-\alpha}^{+}) (b_{\beta} + b_{-\beta}^{+}). \quad (3.1)$$

Using the shift operator for normal oscillators, we can write out directly a unitary transformation that eliminates the one-phonon processes from the Hamiltonian (3.1):

$$\Phi_{\nu}(x) = \hat{S}_1 \Phi_{0\nu}(x), \quad \hat{S}_1 = \exp \left\{ \sum_{\alpha} \frac{A_{\alpha}}{\omega_{\alpha}} (b_{\alpha} - b_{-\alpha}^{+}) \right\} \equiv \prod_{\alpha} S_{1\alpha}, \quad (3.2)$$

$$\hat{H}_{ph} + \hat{H}_{int} = \sum_{\beta} \omega_{\beta} (\tilde{b}_{\beta}^{+} \tilde{b}_{\beta} + \frac{1}{2}) + \frac{1}{2} \sum_{\alpha\beta} B_{\alpha\beta}(\mathbf{R}) (\tilde{b}_{\alpha} + \tilde{b}_{-\alpha}^{+}) (\tilde{b}_{\beta} + \tilde{b}_{-\beta}^{+}). \quad (3.3)$$

Here, $\Phi_{0\nu}(x)$ is an unperturbed state of the phonon subsystem and $\tilde{b}_{\beta}^{+} = b_{\beta}^{+} - A_{\beta}/\omega_{\beta}$ are the creation operators of the shifted normal oscillators. By direct substitution it is easy to convince oneself that the coefficients A_{α} should satisfy the equation

$$A_{\alpha} = c_{\alpha} - 2 \sum_{\beta} A_{\beta} B_{\beta\alpha} / \omega_{\beta}, \quad (3.4)$$

which is easily solved if the coefficients $B_{\alpha\beta}$ can be represented in the form of a product $\sigma B_{\alpha} B_{\beta}$ (here $\sigma = \mp 1$).

We now consider the restructuring of the wave function on account of two-phonon processes in perturbation theory. The coefficients of the expansion of $\Phi_{\nu}(x)$ in the basis of the functions (3.2) are equal to

$$\xi_{\nu\nu'} = \frac{(H_{int}^{(2ph)})_{\nu\nu'}}{E_{\nu} - E_{\nu'}}. \quad (3.5)$$

Correspondingly, the total admixture of states in the initial state ν is characterized by the quantity

$$\gamma = \sum_{\nu'} \frac{|(H_{int}^{(2ph)})_{\nu\nu'}|^2}{(E_{\nu} - E_{\nu'})^2}. \quad (3.6)$$

Processes involving the direct creation or absorption of two phonons make a contribution to (3.6) equal to

$$\gamma' = \sum_{\alpha\beta} \frac{|B_{\alpha\beta}|^2}{(\omega_{\alpha} + \omega_{\beta})^2} [(N_{\alpha} + 1)(N_{\beta} + 1) + N_{\alpha} N_{\beta}], \quad (3.7)$$

where N_{α} are the occupation numbers in the state ν . The expression under the summation symbol in (3.7) has a singularity at $\omega_{\alpha} = \omega_{\beta} = 0$ (since $N_{\alpha} \propto 1/\omega_{\alpha}$), which, however, is removed when one takes into account the frequency dependence of the vertex $B_{\alpha\beta} \propto (\omega_{\alpha} \omega_{\beta})^{1/2}$ and of the density of states $g(\omega) \propto \omega^{d-1}$ in three-dimensional ($d = 3$) and two-dimensional ($d = 2$) crystals (we shall return specially to the one-dimensional case later).

The situation is completely different with two-phonon processes of the scattering type, corresponding to terms of the form $b_{\alpha}^{+} b_{\beta}$ in (3.1). In this case,

$$\gamma'' = \sum_{\alpha\beta} \frac{|B_{\alpha\beta}|^2}{(\omega_{\alpha} - \omega_{\beta})^2} (N_{\alpha} + 1) N_{\beta}. \quad (3.8)$$

This expression has nonremovable singularity even at $\omega_{\alpha} = \omega_{\beta} \neq 0$. At low temperatures the contribution to (3.8) from the region $|\omega_{\alpha} - \omega_{\beta}| \gtrsim T$ is found to be proportional to $(T/\theta_D)^4 \ll 1$ and can be neglected. The region of frequencies $|\omega_{\alpha} - \omega_{\beta}| \ll T$ leads to a divergence of (3.8) that can be removed only by certain physical causes that introduce, effectively, a correction $\delta\omega_{\min}$. If we formally assume that the particle lives in an individual well for an infinite time, then in a macroscopic system we have $\delta\omega_{\min} \propto \theta_D/N$, i.e., on the order of the smallest spacing between the energy levels. In fact, the lifetime τ in the well is finite, though very large ($\tau \gg 1/\theta_D$). In the time τ an admixture of states with energies $\omega < \tau^{-1}$ does not have time to be formed. In (3.8) this corresponds effectively to the absence of terms with $|\omega_{\alpha} - \omega_{\beta}| < 1/\tau$ in the sum, and, thus, we now have $\delta\omega_{\min} \propto 1/\tau$. This is easily traced directly if we consider the evolution of the wave function $\Phi_{\nu}(x)$ over a finite time τ . For this it is sufficient to make use of time-dependent perturbation theory:

$$\gamma'' = \sum_{\alpha\beta} \frac{|B_{\alpha\beta}|^2}{(\omega_{\alpha} - \omega_{\beta})^2 + 1/\tau^2} (N_{\alpha} + 1) N_{\beta} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\omega^2 + 1/\tau^2} \Omega_1(\omega), \quad (3.9)$$

where

$$\Omega_1(\omega) = \pi \sum_{\alpha\beta} |B_{\alpha\beta}|^2 (N_{\alpha} + 1) N_{\beta} \delta(\omega - \omega_{\alpha} + \omega_{\beta}). \quad (3.10)$$

If the lifetime in an individual well is long enough, when $\tau T \gg 1$, the integral in (3.9) is built up over frequencies $\omega \ll T$, and in the argument of the δ -function we can set $\omega = 0$. Then

$$\gamma''(\tau) = \Omega_1 \tau, \quad \Omega_1 = \Omega_1(0). \quad (3.11)$$

The parameter γ'' can be arbitrarily large even when, in the usual sense, the two-phonon interaction is assumed to be weak:

$$B_{\alpha\beta}/(\omega_\alpha\omega_\beta)^{1/2} \ll 1, \quad (3.12)$$

and the temperature is assumed to be low.

Thus, the restructuring of the wave function as a result of the scattering processes in (3.1) is, in the general case, always strong, irrespective of the scale of the two-phonon interaction.

When higher orders of perturbation theory are taken into account the pattern of the restructuring of the wave function is qualitatively completely preserved. This can also be seen from the general solution, which can be obtained for $T \ll \theta_D$ without making assumptions about the quantity $B_{\alpha\beta}$ (see the Appendix). Effectively, everything reduces to a renormalization of the two-phonon interaction vertices, which corresponds physically to a change of the local interaction between the particle and the lattice.

To make the account as clear as possible, we shall assume henceforth that the inequality (3.12) is fulfilled. In this case $\gamma' \ll 1$, and in the determination of the wave function we shall take into account only the scattering processes in (3.1). For the same reason, it is possible simply to set $A_\alpha = c_\alpha$ in (3.4) and to make no distinction between the operators b_α and \tilde{b}_α . Then the general expression for $\Phi_\alpha(x)$ can be represented in the form

$$\Phi_\nu(x) = \tilde{s} \Phi_\nu^{(0)}(x), \quad \tilde{s} = \tilde{s}_2 S_1, \quad (3.13)$$

$$\tilde{s}_2 = T_i \exp \left\{ -i \int_{-\infty}^0 V(t) dt \right\} \quad (3.14)$$

where

$$V = \sum_{\alpha\beta} B_{\alpha\beta} b_{-\alpha}^+ b_\beta, \quad (3.15)$$

and T_i is the time-ordering operator.

Processes involving the creation or absorption of independent pair modes of excitation ($b_\alpha^+ b_\beta$) primarily determine (3.14). Rescattering processes, on the other hand, lead to a contribution that is small in the parameter (3.12). To convince ourselves of this, we consider the amplitude for creation of a mode $b_\alpha^+ b_\beta$ in second order with an intermediate rescattering:

$$\frac{1}{\omega_\alpha - \omega_\beta} \sum_s B_{-\alpha s} B_{s\beta} \left\{ \frac{1}{\omega_s - \omega_\beta} (1 + N_s) + \frac{1}{\omega_\alpha - \omega_s} N_s \right\}.$$

In view of the condition (3.12), this expression is small in comparison with (3.5). But if two independent modes are created in second order, their contribution to the formation of the wave function is characterized by the quantity $(\gamma'')^2$.

We rewrite (3.15) in the form

$$V = \sum_{\alpha\beta} V_{\alpha\beta}, \quad V_{\alpha\beta} = B_{\alpha\beta} b_{-\alpha}^+ b_\beta + B_{\alpha\beta} b_\alpha b_{-\beta}^+,$$

where the prime on the sum means that the summation is performed only over pair modes with different indices (α, β) . If we neglect rescattering processes, an arbitrary term in the series expansion of the matrix (3.14) will contain only commuting factors $V_{\alpha\beta}(t)$. This makes it possible in (3.14) to remove the time-ordering operator and perform the time integration directly in the argument of the exponential. Here, the noncommutativity of the operators $V_{\alpha\beta}(t)$ for

one and the same mode (α, β) at different times reduces to a phase factor $-i \int \Delta E dt$, where ΔE is the shift of the energy when the interaction is switched on. This phase factor cancels exactly the phase factor that was in fact omitted when we went over to (3.14).

If we take into account from the outset that the particle spends a large but finite time τ in an individual well, in a self-consistent approach we should substitute into (3.14) an interaction in the form $V(t) = V \exp(T/\tau)$:

$$\tilde{s}_2 = \exp \left\{ - \sum_{\alpha\beta}' B_{\alpha\beta} \left[\frac{1}{\omega_\alpha - \omega_\beta + i/\tau} b_{-\alpha}^+ b_\beta - \frac{1}{\omega_\alpha - \omega_\beta - i/\tau} b_\beta^+ b_{-\alpha} \right] \right\} = \prod_{\alpha\beta}' S_{2\alpha\beta}. \quad (3.16)$$

4. QUANTUM DIFFUSION IN A THREE-DIMENSIONAL CRYSTAL

When (2.4) is taken into account, the transition matrix element (2.3) takes the form

$$M_{\nu'\nu} = \langle \Phi_{\nu'}^{(2)}(x) | J(x) | \Phi_\nu^{(1)}(x) \rangle, \quad (4.1)$$

$$J(x) = \langle \Phi_0^{(2)}(\mathbf{R}, x) | H'(\mathbf{R}) | \Phi_0^{(1)}(\mathbf{R}, x) \rangle.$$

The expression (4.1) reflects the dependence of the transition amplitude on the extremal restructuring of the local potential relief when the motion of atoms of the crystal is taken into account. Here, both the relaxation of the surrounding atoms and the phenomenon of fluctuational preparation of the barrier¹² (an analogous result in the framework of the functional-integration technique was discussed in Ref. 13) turn out to be important. If we make use of the results of Ref. 12, we can show that for $T \ll \theta_D$ in the first nonvanishing approximation in the parameter (3.12)

$$M_{\nu'\nu} \approx \Delta_0 \langle \Phi_{\nu'}^{(2)}(x) | \Phi_\nu^{(1)}(x) \rangle, \quad (4.2)$$

$$\Delta_0 = \langle \Phi_0^{(2)}(x) | J(x) | \Phi_0^{(1)}(x) \rangle / \langle \Phi_0^{(2)}(x) | \Phi_0^{(1)}(x) \rangle.$$

The amplitude Δ_0 for $T \ll \theta_D$ depends only weakly on the temperature. Then, taking (3.13) into account, we have

$$M_{\nu'\nu} \approx \Delta_0 \langle \Phi_{0\nu'}(x) | (\tilde{s}^{(2)}) + S^{(1)} | \Phi_{0\nu}(x) \rangle = \Delta_0 \langle \nu' | \hat{\Lambda} | \nu \rangle. \quad (4.3)$$

[Here we have restored the well label omitted in (3.13).]

Taking into account the commutativity of individual modes in (3.2) and (3.16) and the fact that in the approximation under consideration the operators \hat{S}_1 and \hat{S}_2 commute, the definition of $\hat{\Lambda}$ reduces simply to the definition of \hat{S} from (3.13) with c_α and $B_{\alpha\beta}$ replaced by

$$\bar{c}_\alpha = c_\alpha^{(1)} - c_\alpha^{(2)}, \quad \bar{B}_{\alpha\beta} = B_{\alpha\beta}^{(1)} - B_{\alpha\beta}^{(2)}. \quad (4.4)$$

The amplitude Δ_c of the coherent transition between the wells is determined by the matrix element (4.1) with $\nu' = \nu$:

$$\Delta_c = \Delta_0 \langle \nu | \hat{\Lambda} | \nu \rangle = \Delta_0 \langle \hat{\Lambda} \rangle. \quad (4.5)$$

To determine (4.5) we make use of the relationship between $\hat{\Lambda}$ and \hat{S}_1 (3.2) and \hat{S}_2 (3.16). Expanding each term of the product in these operators in a series in powers of the argu-

ment of the exponential and retaining in each case the first three terms of the expansion (this corresponds to macroscopic accuracy), after transformations we find

$$\Delta_c = \Delta_0 \exp(-\phi(T)) \exp(-\frac{1}{2}\bar{\gamma}(T, \tau)). \quad (4.6)$$

The first exponential determines the usual polaron effect for purely one-phonon interaction. As is well known, the argument $\phi(T)$ of the polaron exponential remains finite as $T \rightarrow 0$ and varies on a scale of temperatures of the order of ω_c . The second factor already involves the role of two-phonon processes: γ is determined by the expressions (3.9) and (3.10), if in the latter we make the replacement $B \rightarrow \bar{B}$ (4.4). Again assuming $\tau T \gg 1$, we find

$$\Delta_c = \bar{\Delta}_0 e^{-\frac{1}{2}\alpha\tau}, \quad \bar{\Delta}_0 = \Delta_0 e^{-\phi(T)}. \quad (4.7)$$

It can be seen from this expression that the two-phonon interaction leads to an exponential decrease of the coherent transition amplitude, with an exponent proportional to the lifetime of the particle in the well. If we assume that the motion of the particle has a band (in the two-well case, coherent) character, then $\tau = (\xi \Delta_c)^{-1}$, where the numerical coefficient ξ depends on the type of lattice. Substituting this expression into (4.7), we obtain a self-consistent equation for Δ_c . It is easy to see that for $\Omega > \Omega_c = 2\xi/e\bar{\Delta}_0$ the coherent amplitude $\Delta_c = 0$, corresponding to complete suppression of the band (coherent) motion. For $\bar{\Delta}_0 \ll \theta_D$, this occurs for $\bar{\Delta} \ll T \ll \theta_D$. Indeed, from (3.10) we have

$$\Omega \propto 10^{4+(2)} \theta_D (T/\theta_D)^{7+(2)}, \quad (4.8)$$

where the 2 in the brackets corresponds to the case when the two wells are identical and $B^{(1)}$ and $B^{(2)}$ in (4.4) differ only by a phase factor.

Thus, the two-phonon interaction leads to narrowing, and, as a consequence, to the disappearance of the coherent band in that region of temperatures in which the one-phonon polaron effect practically does not change. For sufficiently small $\bar{\Delta}_0$ the result obtained has a universal character. It is analogous to the result found earlier for the case of tunneling in the presence of interaction with electrons.¹⁰ This circumstance is not accidental. In both cases it is associated with an infrared divergence of the reconstructed wave function of the excitations of the medium [see (3.8)], which, in the case of phonons, arises on account of scattering terms that are necessarily absent in the one-phonon interaction. We remark that for $T \ll \theta_D$ we certainly have $\Omega^{\text{ph}} \ll \Omega^{\text{el}}$ and the phonon destruction of the band occurs at a higher temperature.

The nature of the destruction of the coherent band becomes clear if we take into account that phonon fluctuations with a total energy of the order of τ^{-1} lead to relative fluctuations of the phase in neighboring cells. A consequence of this is the attenuation of the nondiagonal elements of the density matrix defined in the site representation. As was shown in Ref. 6, we have $\rho_{12} \propto \exp(-\Omega t)$, where the frequency Ω coincides with that found above. It is this distinctive loss of phase memory that causes the dynamical destruction of the coherence.

We shall make one remark. Since what replaces the coherent regime is an incoherent tunneling regime, for $\Omega > \Omega_c$ the lifetime of a particle in a unit cell remains finite, though very large (see below). Correspondingly, it is also the case

for $\Omega > \Omega_c$ that Δ_c is not identically equal to zero, but vanishes with exponential accuracy.

Thus, for $\Omega \gg \bar{\Delta}_0$ the tunneling motion of the particle acquires an incoherent character. In this case, the site representation is adequate for the problem. An analogous situation obtains for $\xi \gg \bar{\Delta}_0$ and arbitrary Ω . In both cases the probability of a transition from well to well can be represented in the following form:

$$W = \Delta_0^2 \int_{-\infty}^{+\infty} dt e^{i\omega t} \text{Sp} \{ \hat{\rho}_0 \hat{\Lambda}^{\dagger}(t) \hat{\Lambda} \}, \quad (4.9)$$

where ρ_0 is the equilibrium density matrix of the phonons. Using the same expansion of the operators \hat{S}_1 and \hat{S}_2 as in the calculation of (4.5), we have

$$W = \Delta_0^2 \int_{-\infty}^{+\infty} dt e^{i\omega t - \chi(t)}. \quad (4.10)$$

Here, $\chi(t) = \chi_1(t) + \chi_2(t)$, with

$$\chi_1(t) = \sum_{\alpha} \frac{|\bar{c}_{\alpha}|^2}{\omega_{\alpha}^2} [(1+N_{\alpha})(1-e^{-i\omega_{\alpha}t}) + N_{\alpha}(1-e^{i\omega_{\alpha}t})], \quad (4.11)$$

$$\chi_2(t) = \sum_{\alpha\beta} \frac{|\bar{B}_{\alpha\beta}|^2}{(\omega_{\alpha}-\omega_{\beta})^2 + 1/\tau^2} (1+N_{\alpha})N_{\beta}(1-e^{i(\omega_{\alpha}-\omega_{\beta})t}). \quad (4.12)$$

The expression for χ_2 does not in fact have a singularity as $|\omega_{\alpha} - \omega_{\beta}| \rightarrow 0$, because of the time dependence of the summand. The characteristic time scale is now dictated by the quantity Ω^{-1} (or ξ^{-1}). The smallest values of the difference $|\omega_{\alpha} - \omega_{\beta}|$ [those that are important in (4.12)] are determined by a quantity of the order of $(\Omega, \xi)_{\text{max}}$. But, as is clear physically and will be shown below, the lifetime of a particle in a unit cell satisfies $\tau \gg (\Omega^{-1}, \xi^{-1})_{\text{min}}$. Therefore, in the integration the term $1/\tau^2$ in the denominator plays no role. A simple transformation brings $\chi_2(t)$ to the form

$$\chi_2(t) = \sum_{\alpha\beta} \frac{|\bar{B}_{\alpha\beta}|^2}{(\omega_{\alpha}-\omega_{\beta})^2} (N_{\beta}-N_{\alpha}) [(1+2N(\omega_{\alpha}-\omega_{\beta})) \times (1 - \cos(\omega_{\alpha}-\omega_{\beta})t) + i \sin(\omega_{\alpha}-\omega_{\beta})t].$$

This makes it possible to represent the expression for $\chi(t)$ in the convenient form

$$\chi(t) = 2 \int_0^{\omega} \frac{d\omega}{\omega} f(\omega) \left[\text{cth} \frac{\omega}{2T} (1 - \cos \omega t) + i \sin \omega t \right]. \quad (4.13)$$

Here,

$$f(\omega) = A(\omega) + \Omega(\omega)/2\pi T, \quad (4.14)$$

$$A(\omega) = \sum_{\alpha} \frac{|\bar{c}_{\alpha}|^2}{2\omega_{\alpha}} \delta(\omega - \omega_{\alpha}), \quad (4.15)$$

$$\Omega(\omega) = \pi T \sum_{\alpha\beta} |\bar{B}_{\alpha\beta}|^2 \frac{N_{\beta}-N_{\alpha}}{\omega_{\alpha}-\omega_{\beta}} \delta(\omega_{\alpha}-\omega_{\beta}-\omega). \quad (4.16)$$

Generally speaking, the two-phonon term in (4.14) is small in comparison with the one-phonon term. However, the time behavior of the asymptotic form of $\chi(t)$ at large $t \gg 1/T$ for $d = 3$ is determined specifically by the two-phonon term, as dictated by its singular behavior in (4.13) at small $\omega \ll T$. In this region of frequencies we can certainly omit ω in the argument of the δ -function in (4.16). Then

$$\Omega(0) = \pi \sum_{\alpha\beta} |\bar{B}_{\alpha\beta}|^2 (1 + N_\alpha) N_\beta \delta(\omega_\alpha - \omega_\beta). \quad (4.16')$$

[This expression differs from (3.10) for $\omega = 0$ only in the replacement (4.4) of B by \bar{B} .] Rewriting the expression in the square brackets in (4.13) in the form

$$\frac{\text{ch}(\omega/2T) - \text{ch}(\omega(it-1/2T))}{\text{sh}(\omega/2T)}$$

and, in the integral (4.10), making the change of variables $t \rightarrow t - i/2T$ with a subsequent displacement of the integration contour onto the real axis, we obtain

$$W = \Delta_0^2 e^{i/2T} \int_{-\infty}^{+\infty} dt \cos \xi t \times \exp \left\{ -2 \int_0^{\omega} \frac{d\omega}{\omega} f(\omega) \frac{\text{ch}(\omega/2T) - \cos \omega t}{\text{sh}(\omega/2T)} \right\}. \quad (4.17)$$

In the calculation of the two-phonon contribution, in the integral over the frequencies we rewrite the numerator in the form

$$(\text{ch}(\omega/2T) - 1) + (1 - \cos \omega t). \quad (4.18)$$

Now neither term separately gives a divergence as $\omega \rightarrow 0$. The one-phonon contribution also has no divergence, since $A(\omega)$ behaves like (1.5). Then, omitting from in the argument of the exponential the time-independent term, we have

$$\phi = \int_0^{\infty} \frac{d\omega}{\omega \text{sh}(\omega/2T)} \left[A(\omega) \text{ch}(\omega/2T) + \frac{\Omega}{2\pi T} (\text{ch}(\omega/2T) - 1) \right]. \quad (4.19)$$

The second term in the square brackets is small in comparison with the first, which determines the usual polaron effect renormalizing the tunneling amplitude $\tilde{\Delta}_0$ (4.7). It can be seen that the quantity ϕ remains finite as $\omega \rightarrow 0$.

The frequency integral of the remaining terms in (4.17) converges rapidly, and we can replace the upper limit of the integration by ∞ . The two-phonon contribution can then be integrated explicitly. As a result, we find

$$W = 2\tilde{\Delta}_0^2 e^{i/2T} \int_0^{+\infty} dt \cos \xi t \exp \left\{ -\frac{\Omega}{\pi T} \ln \text{ch}(\pi T t) + \bar{\Psi}(t) \right\}, \quad (4.20)$$

$$\bar{\Psi}(t) = 2 \int_0^{\infty} \frac{d\omega}{\omega} A(\omega) \frac{\cos \omega t}{\text{sh}(\omega/2T)}. \quad (4.21)$$

The expression obtained contains all phonon interaction channels in the case of incoherent tunneling of particles. We begin our analysis with the symmetric case $\xi = 0$. It is easy to

convince oneself that for $T \ll \theta_D$ we have $\bar{\Psi}(t) \ll 1$. In this case the probability (4.20) does not diverge, and remains finite only by virtue of the two-phonon interaction. Since we have $\Omega \ll T$, and the integral is built up over times $t \sim 1/\Omega$, for which $\text{cosh}(\pi T t) \gg 1$, we can represent the argument of the exponential in (4.20) immediately in the form $-\Omega t + \bar{\Psi}$. This asymptotic behavior reflects the tunneling process in the regime of ohmic dissipation. This links with the fact that the function $f(\omega)$ satisfies the criterion (1.4), only by virtue of two-phonon scattering. The important point is that allowance for only one-phonon processes, in any order in the interaction constant c_α (which, in the approximation under consideration, is $\sim \tilde{\Delta}_0^2$), does not give rise to ohmic dissipation.

It should be specially emphasized that allowance for two-phonon processes in tunneling, by removing the divergence in (4.20), makes it possible to avoid the procedure of replacing $\exp \bar{\Psi}$ by $\exp \bar{\Psi} - 1$ and simultaneously taking the coherent band motion into account together with (4.20) (see Refs. 14 and 15). In fact, from the results obtained above it follows that the expression (4.20) for the incoherent regime of motion is valid only when the coherent amplitude vanishes. In other words, we can say that the regimes of coherent and incoherent tunneling are exchanged.

The leading term in the incoherent-transition probability (4.20) arises even in zeroth order in $\bar{\Psi}$:

$$W = 2\tilde{\Delta}_0^2 / \Omega. \quad (4.22)$$

It corresponds to diffusive motion of the particle in the crystal, with diffusion coefficient

$$D = \frac{z a^2}{3} \frac{\tilde{\Delta}_0^2}{\Omega}, \quad (4.23)$$

where z is the number of equivalent sites at a distance a in the nearest coordination sphere in a cubic crystal. The expression (4.23) was first obtained in Refs. 6 and 7.

If we now make use of (4.22) and substitute $\tau = (zW)^{-1}$ into the expression (4.7), for Δ_c we obtain

$$\Delta_c = \tilde{\Delta}_0 \exp \left\{ -\Omega^2 / (4z\tilde{\Delta}_0^2) \right\}.$$

From this it can be seen immediately that for $\Omega \gg \tilde{\Delta}_0$ the coherent channel becomes negligibly small in comparison with the incoherent channel.

In Refs. 6 and 7, in the framework of the solution of the kinetic equation for the density matrix, it was found that in the consideration of macroscopic diffusion (small concentration gradient) the expression (4.23) also remains valid for $\Omega < \Delta_c$, under the condition $\Delta_c < T$; in other words, it also remains valid for coherent band motion in a comparatively wide range of temperatures [see (4.8) for Ω].

The next term in the expansion in $\bar{\Psi}(t)$ in the integrand of (4.20) determines the probability of a transition with the emission or absorption of one phonon:

$$W^{(1)} = 4\tilde{\Delta}_0^2 \int_0^{\infty} \frac{d\omega A(\omega)}{\omega \text{sh}(\omega/2T)} \times \int_0^{+\infty} dt \cos \omega t \exp \left\{ -\frac{\Omega}{\pi T} \ln \text{ch}(\pi T t) \right\}. \quad (4.24)$$

If the transition occurs between two crystallographically inequivalent isoenergetic positions, the $A(\omega) = g(\omega/\theta_D)^2$,

and the expression (4.24) has the finite value

$$W^{(1)} = 4\pi g \bar{\Delta}_0^2 T / \theta_D^2. \quad (4.25)$$

This result was first obtained in the paper of Teichler and Seeger.¹⁶ However, comparing (4.25) with (4.22) we see that at low temperatures the one-phonon transitions are always negligibly small in comparison with $W^{(0)}$. If, however, the transition occurs between crystallographically equivalent positions and $A(\omega) \propto (\omega/\theta_D)^4$ holds, the one-phonon processes vanish practically entirely. It is easy to verify that the next terms of the expansion in $\bar{\Psi}(t)$, which determine transitions of higher order in the one-phonon interaction, also lead to negligibly small corrections to $W^{(0)}$. Thus, when the phase correlation is dynamically destroyed, the band diffusion (4.22), (4.23) governs quantum diffusion in a crystal at low temperatures. An important point is that the dynamical breaking itself is induced specifically by the two-phonon processes, and it is these that determine the ohmic dissipation in tunneling.

Now let $\xi \neq 0$. Returning to the original expression (4.20), for $W^{(0)}$ we find

$$W^{(0)} = \frac{2\bar{\Delta}_0^2(T)\Omega}{\xi^2 + \Omega^2} e^{i/2\tau} \pi^{1/2} \frac{|\Gamma(1 + (\Omega + i\xi)/2\pi T)|^2}{\Gamma(1 + \Omega/2\pi T)\Gamma(1/2 + \Omega/2\pi T)}. \quad (4.26)$$

If we take into account that $\Omega \ll T$, we have

$$W^{(0)} \approx \frac{2\bar{\Delta}_0^2(T)\Omega}{\xi^2 + \Omega^2} \frac{\xi/T}{1 - e^{-\xi/\tau}}. \quad (4.26')$$

This result coincides with that found in Refs. 8 and 17 using the kinetic equation for the density matrix. For $\xi < \Omega$ all the preceding results remain unchanged. But for $\xi \gg \Omega$ we have $W^{(0)} \propto \xi^{-2}$, and in this case one-phonon processes can become important. In fact, under these conditions,

$$W^{(1)} = 2\bar{\Delta}_0^2 \frac{2\pi T A(\xi)}{\xi^2} \frac{\xi/T}{1 - e^{-\xi/\tau}}. \quad (4.27)$$

Comparing this expression with (4.26'), we see that for large biases, when we have

$$A(\xi) > \Omega/2\pi T,$$

one-phonon processes, and hence induced tunneling transitions, begin to play the leading role.

It is not difficult to convince oneself that the next terms of the expansion in $\bar{\Psi}$ again lead to small corrections, this time in relation to $W^{(1)}$ or, in the general case, in relation to the sum $W^{(0)} + W^{(1)}$. It is this sum that determines in all cases the probability of a tunneling transition in the presence of interaction with phonons. With high accuracy, it can be written in the form

$$W = W^{(0)} + W^{(1)} = \frac{2\bar{\Delta}_0^2(T)}{\xi^2 + \Omega^2} (\Omega + 2\pi T A(\xi)) \frac{\xi/T}{1 - e^{-\xi/\tau}}. \quad (4.28)$$

We have already noted that for $\xi = 0$ and $T \gg \bar{\Delta}_0$ the result (4.23) remains valid for $\omega < \bar{\Delta}_0$ as well. For $T < \bar{\Delta}_0$ it becomes necessary to solve the corresponding kinetic equation in the momentum representation. It is interesting that the answer for the diffusion coefficient in this case has the same form (4.23), but with $\Omega \propto T^7$ (see Ref. 18).

5. CRYSTALS OF DIMENSIONALITY $d=2$ AND $d=1$

When crystals of lower dimensionality are considered, the principle of the construction of the site wave functions of the phonon system remains entirely the same. If we are considering transitions between crystallographically equivalent positions, and the transport effect thereby remains present in the spectral function (1.5), all the general results obtained for the case $d=3$ remain unchanged. A new situation arises only when there is no transport effect. Below, we confine ourselves to examining precisely this case.

We start from an analysis of the case $d=2$. It is easily established that in this case the decisive channel in the restructuring of the site wave function on account of two-phonon processes is again the scattering channel. Therefore, the expression for the matrix \hat{S}_2 in the form (3.16) remains valid, and at the same time the expressions (4.6) for the coherent amplitude and (4.10) for the transition probability, with the function $\chi(t)$ in the form (4.13)–(4.16), also remain valid. However, in determining Δ_c we now come up against the fact that the formal calculation of the one-phonon polaron effect $\phi(T)$ [the first term in the function (4.19)] leads to a logarithmic divergence at $T \neq 0$. This divergence is removed only when the finiteness of the lifetime τ of the particle in a unit cell is taken into account. In fact, we ought to have introduced from the outset a cutoff associated with the finite value of τ in our consideration of one-phonon processes as well, but in the case $d=3$ there was no need for this. Formally, as in the case of the two-phonon interaction, this is equivalent to the replacement $\omega_\alpha \rightarrow \omega_\alpha + i/\tau$. Taking this into account, and introducing in explicit form $A(\omega) = g^{(2)} \omega/\theta_D$, instead of (4.7) we have, in the limit $\tau T \gg 1$,

$$\Delta_c = \Delta_0 \exp(-\phi(0)) \exp\{-1/2\Omega\tau - (g^{(2)}T/\theta_D) \ln(T\tau)\}, \quad (5.1)$$

$$\Omega \propto \theta_D (T/\theta_D)^5, \quad \phi(0) = \int d\omega A(\omega)/\omega, \quad (d=2). \quad (5.2)$$

Thus, in the case $d=2$ the dynamical destruction of the band is enhanced on account of the one-phonon interaction although the decisive role in this destruction is still played by two-phonon processes.

When examining the incoherent tunneling we can use the expression (4.17), which is valid in the general case, introducing the identical transformation (4.18) for the one-phonon contribution as well. Calculating the time-independent term in the argument of the exponential in (4.17), we obtain $2\phi(0)$. The second term, however, gives rise to a somewhat modified expression for $\bar{\Psi}$ in (4.20):

$$\bar{\Psi}(t) = 2 \int_0^\infty \frac{d\omega}{\omega} A(\omega) \frac{1 - \cos \omega t}{\text{sh}(\omega/2T)}. \quad (5.3)$$

In contrast to the case $d=3$, at large times $\bar{\Psi}(t)$ increases logarithmically:

$$\bar{\Psi}(t) = 4g^{(2)}(T/\theta_D) \ln(T\tau), \quad (T\tau \gg 1), \quad (5.4)$$

and, generally speaking, it is not a correct operation to expand $\exp(-\bar{\Psi}(t))$ in a series in the integrand of (4.20).

We now calculate the transition probability (4.20) for $\xi = 0$, using the asymptotic form found for $\bar{\Psi}(t)$ (the integral is built up over large times $T\tau \gg 1$)

$$W = 2\bar{\Delta}_0^2 \int_0^{+\infty} dt e^{-\alpha t} (1/Tt)^{4g^{(1)}\tau/\theta_D} \approx \frac{2\bar{\Delta}_0^2}{\Omega} (\Omega/T)^{4g^{(1)}\tau/\theta_D}. \quad (5.5)$$

For $T/\theta_D \gg 1$ the result obtained differs little from that found for the case $d = 3$. This circumstance is connected with the fact that the main contribution to the integral comes from times $t \sim 1/\Omega$, at which $\bar{\Psi}(t)$ is small. For $\xi \neq 0$ the characteristic times can only become smaller, and, therefore, we can expand $\exp(-\bar{\Psi}(t))$ in a series from the outset. If we return to the original expression (5.3), it is easy to see that the answer will coincide with the general expression (4.28), where $A(\omega)$ and Ω should be taken in the form corresponding to $d = 2$.

In the case $d = 1$, the pattern is radically altered. Now, the phonon function of the system undergoes an anomalously strong rearrangement on account of the one-phonon interaction. To see this, as in Sec. 3 we make use of perturbation theory and calculate the correction to the wave function of the initial state, replacing $H_{int}^{(2ph)}$ by $H_{int}^{(1ph)}$ in (3.5) and (3.6):

$$\gamma = \sum_{\alpha} \frac{|c_{\alpha}|^2}{\omega_{\alpha}^2 + 1/\tau^2} (2N_{\alpha} + 1) = 2\pi g^{(1)} T \tau, \quad (5.6)$$

[$A(\omega) = g^{(1)} = \text{const}$]. The expression given is written in the limit $T\tau \gg 1$. The quantities γ' (3.7) and γ'' (3.11) found earlier, which characterize the restructuring on account of two-phonon processes, take in the case $d = 1$, in the same limit $T\tau \gg 1$, the values

$$\gamma' \sim (\Omega/T) \ln(T\tau), \quad \gamma'' \sim \Omega\tau. \quad (5.7)$$

In the one-dimensional case under consideration,

$$\Omega^{(1)} \propto \theta_D (T/\theta_D)^3. \quad (5.8)$$

Comparing the expression (5.6) with (5.7), (5.8), we see that for $T \ll \theta_D$ the most important role in the restructuring of the wave function is played by one-phonon processes. The character of the dependence of γ on the lifetime τ in a unit cell is the same as in the case of two-phonon processes. But precisely this circumstance played a decisive role in the appearance of ohmic dissipation in the presence of tunneling. Thus it is now the one-phonon interaction that is responsible for this tunneling regime. The general expression for the spectral function in formula (4.13) in the case under consideration takes the form

$$f(\omega) = \Omega_{\tau}/2\pi T, \quad \Omega_{\tau} = 2\pi T g^{(1)} + \Omega \quad (5.9)$$

and satisfies the criterion (1.4) even at $T = 0$. At low temperatures the two-phonon contribution to $f(\omega)$ is small, and for all kinetic problems we can confine ourselves to considering one-phonon processes. Thus, the role of the one-phonon interaction in tunneling for $d = 1$ turns out to be exactly the same as the role of two-phonon scattering for $d = 3$ and $d = 2$. This makes it possible to make use of the results of the previous sections for the purely two-phonon interaction.

Calculating the coherent transition amplitude (4.5) in the one-dimensional case, we find

$$\begin{aligned} \Delta_c &= \Delta_0 \exp \left\{ - \int_0^{+\infty} \frac{d\omega \omega g^{(1)}}{\omega^2 + 1/\tau^2} \text{cth} \frac{\omega}{2T} \right\} \\ &= \Delta_0 \exp \left\{ -g^{(1)} \left[\ln \frac{\omega_c}{2\pi T} - \Psi \left(1 + \frac{1}{2\pi T\tau} \right) + \pi T\tau \right] \right\}. \end{aligned} \quad (5.10)$$

Here the function $\Psi(z)$ is the logarithmic derivative of the Γ -function. In the limit $T \rightarrow 0$ this expression is transformed to the form

$$\Delta_c = \Delta_0 (1/\omega_c \tau)^{g^{(1)}}. \quad (5.11)$$

Substituting $\tau = (2\Delta_c)^{-1}$ and solving the resulting self-consistent equation, we have

$$\Delta_c = \Delta_0 \left(\frac{2\Delta_0}{\omega_c} \right)^{g^{(1)/(1-g^{(1)})}}. \quad (5.12)$$

This result is well known in the theory of tunneling with dissipation (see, e.g., Ref. 2 and the references therein). For $T\tau > 1$,

$$\begin{aligned} \Delta_c &= \bar{\Delta}_0(T) e^{-1/2\Omega\tau}, \\ \bar{\Delta}_0(T) &= \Delta_0 \left(\frac{2\pi T}{\gamma \omega_c} \right)^{g^{(1)}}. \end{aligned} \quad (5.13)$$

(here γ is the Euler constant). Dynamical destruction of the band now sets in at the simple level $T \gg \Delta_c$. This result was first obtained in Ref. 10 in connection with an analysis of coherent tunneling in a metal, in which the constancy of the density of states at the Fermi level causes the condition (1.4) to be satisfied for the interaction with the electrons. For $(T, \xi)_{\max} \gg \Delta_c$ the transition probability in the incoherent regime is determined by the expression (4.26) with Ω replaced by Ω_{τ} . This result was first found in Refs. 19 and 20, and, for the case of interaction with electrons, in Ref. 9.

6. THE EFFECTIVE ACTION

It is of interest to trace how the special role of two-phonon processes is manifested in the analysis of tunneling motion in the functional-integration technique. With this aim, we determine the effective action for the problem under consideration, taking into account in the Hamiltonian (1.1) both the one-phonon interaction (1.2) and the two-phonon interaction (1.6). We consider the partition function $Z = \text{Sp} \exp(-H/T)$ of the system [$\text{Sp} \equiv \text{Tr}$]. In this expression we go over to a mixed representation, introducing functional integration only over the particle variables:

$$\begin{aligned} Z &= \int D\mathbf{R} \exp \left\{ - \int_{-1/2T}^{+1/2T} d\tau \left[\frac{M\dot{\mathbf{R}}^2(\tau)}{2} + U(\mathbf{R}(\tau)) \right] \right\} \\ &\times \text{Sp}_{ph} \left\{ \exp(-H_{ph}/T) T_{\tau} \exp \left\{ - \int_{-1/2T}^{+1/2T} d\tau H_{int}(\mathbf{R}(\tau)) \right\} \right\}. \end{aligned} \quad (6.1)$$

It follows immediately from this that the effective action for the particle can be written in the form

$$S_{eff} = \int_{-1/2T}^{+1/2T} d\tau L_{\mathbf{R}} - \ln \left\langle T_{\tau} \exp \left\{ - \int_{-1/2T}^{+1/2T} d\tau H_{int}(\mathbf{R}(\tau)) \right\} \right\rangle_{ph}. \quad (6.2)$$

We assume for simplicity, as in Sec. 3, that the two-phonon interaction vertex in (1.6) is small and the relation (3.12) is fulfilled. In this case, all the arguments that were used in the calculation of the S -matrix (3.14) remain valid. Again neglecting rescattering of individual excitation modes, i.e., considering two-phonon excitations with noncoinciding pairs of indices that commute with each other, we can represent the exponential in (6.2) in the form of a product of exponentials pertaining to different one-phonon and two-phonon modes. Expanding then each of the exponentials to the second-order terms and gathering the result back into the argument of the exponential, we find

$$S_{eff} = \int_{-1/2T}^{+1/2T} d\tau L_R^0 - \iint_{-1/2T}^{+1/2T} d\tau d\tau' \int_0^\infty d\omega \omega \frac{\text{ch}[\omega(1/2T - |\tau - \tau'|)]}{\text{sh}(\omega/2T)} \cdot \alpha(\omega, \mathbf{R}(\tau), \mathbf{R}(\tau')). \quad (6.3)$$

Here $\alpha = \alpha_1 + \alpha_2$, with

$$\alpha_1(\omega, \mathbf{R}, \mathbf{R}') = \sum_{\beta} \frac{c_{\beta}(\mathbf{R}) c_{-\beta}(\mathbf{R}')}{2\omega_{\beta}} \delta(\omega - \omega_{\beta}), \quad (6.4)$$

$\alpha_2(\omega, \mathbf{R}, \mathbf{R}')$

$$= \frac{1}{2} \sum_{\alpha\beta} B_{\alpha\beta}(\mathbf{R}) B_{-\alpha-\beta}(\mathbf{R}') \frac{1 + N_{\beta} + N_{\alpha}}{2(\omega_{\alpha} + \omega_{\beta})} \delta(\omega_{\alpha} + \omega_{\beta} - \omega) + \sum_{\alpha\beta} B_{\alpha-\beta}(\mathbf{R}) B_{-\alpha\beta}(\mathbf{R}') \frac{N_{\beta} - N_{\alpha}}{2(\omega_{\alpha} - \omega_{\beta})} \delta(\omega_{\alpha} - \omega_{\beta} - \omega). \quad (6.5)$$

In the absence of the two-phonon interaction the result obtained is well known (see Ref. 21).

We shall extract in (6.3) the adiabatic renormalization of the potential relief, by making the identical replacement (see, e.g., Ref. 1)

$$c_{\beta}(\mathbf{R}) c_{-\beta}(\mathbf{R}') \equiv \frac{1}{2} [|c_{\beta}(\mathbf{R})|^2 + |c_{\beta}(\mathbf{R}')|^2] - \frac{1}{2} |c_{\beta}(\mathbf{R}) - c_{\beta}(\mathbf{R}')|^2, \quad (6.6)$$

and analogously for the product $B_{\alpha\beta}(\mathbf{R}) B_{-\alpha-\beta}(\mathbf{R}')$. The first terms in these transformations lead to the replacement of $U(\mathbf{R})$ by the renormalized potential $\tilde{U}(\mathbf{R})$. Here, α is replaced by a function $\tilde{\alpha}$, which differs from (6.4), (6.5) by the replacement of the product of coefficients by the square of the modulus of their difference.

A special role in the problem under consideration is played by trajectories connecting the minima \mathbf{R}_1 and \mathbf{R}_2 of the potential. We shall calculate the contribution made to the action by the simplest one-instanton trajectory. The principal contribution to S_{eff} is associated with the region of $\mathbf{R}(\tau) = \mathbf{R}_1$, $\mathbf{R}(\tau') = \mathbf{R}_2$ and, vice versa, $\mathbf{R}(\tau) = \mathbf{R}_2$, $\mathbf{R}(\tau') = \mathbf{R}_1$, and also with the narrow transitional regions $|\Delta\tau_1|, |\Delta\tau_2| \sim \omega_0^{-1}$. In the former case the corresponding contribution to the action has the form

$$\delta S_{eff} = \int_0^{\omega_0} \frac{d\omega (\text{ch}(\omega/2T) - 1)}{\omega \text{sh}(\omega/2T)} \alpha(\omega, \mathbf{R}_1, \mathbf{R}_2). \quad (6.7)$$

The expression for $\alpha(\omega, \mathbf{R}_1, \mathbf{R}_2)$ coincides with the definition of the spectral function $f(\omega)$ (4.14)–(4.16). From this it follows immediately that the infrared singularity in the action, which is essential for tunneling with dissipation, will be connected, in the cases $d = 2$ and $d = 3$, with the two-phonon processes only. This means that, in the functional-integration technique too, it is essential to use a Hamiltonian that takes the two-phonon interaction into account.

7. CONCLUDING REMARKS

The results obtained in the paper show that tunneling motion in a crystal in the presence of interaction with phonons has a viscous (or ohmic) character only because of the two-phonon (many-phonon) interaction. The only exception to this rule is a one-dimensional crystal in which neighboring positions that are equivalent in energy are crystallographically inequivalent. In all other cases, quantum diffusion in a crystal is determined specifically by the two-phonon processes. This applies both to the coherent band motion and to the distinctive dynamical destruction of the coherent transport and the purely incoherent motion that arises as a consequence of this with increase of temperature. The role of the one-phonon interaction, however large it may be in relation to the two-phonon interaction, reduces at low temperatures merely to a finite renormalization of the band. It should be specially emphasized that many-phonon processes associated with allowance for the one-phonon interaction in higher orders lead neither to a viscous regime of tunneling nor to appreciable corrections in the corresponding kinetic coefficients.

Thus, when considering tunneling with dissipation in real crystals it is necessary to take the two-phonon interaction into account in the Hamiltonian of the system from the outset.

APPENDIX

We consider the problem of the construction of the wave function of a phonon system described by a Hamiltonian of the form

$$H = H_0 + H_{int} = \sum_{\beta} \omega_{\beta} (\tilde{\nu}_{\beta}^+ \tilde{\nu}_{\beta} + \frac{1}{2}) + \frac{1}{2} \sum_{\alpha\beta} B_{\alpha\beta} (\tilde{\nu}_{\alpha} + \tilde{\nu}_{-\alpha}^+) (\tilde{\nu}_{\beta} + \tilde{\nu}_{-\beta}^+). \quad (A1)$$

We seek Φ_{ν} in the form of an expansion in states of the unperturbed Hamiltonian H_0 :

$$\Phi_{\nu} = \hat{S}_{2\nu} \Phi_{0\nu} \equiv \sum_{\alpha} (\hat{S}_{2\nu})_{\alpha\nu} \Phi_{0\alpha}. \quad (A2)$$

In the region of low temperatures the problem of constructing the operator $\hat{S}_{2\nu}$ can be solved exactly in the parameter $T/\theta_D \ll 1$. The following circumstance plays a decisive role. By virtue of the small density of phonon states at $\omega \ll \theta_D$, all virtual processes of rescattering of phonons are important only in the region of high frequencies $\omega \propto \theta_D$, i.e., in a region in which the initial wave function $\Phi_{0\nu}$ contains practically no phonons.

The operator \hat{S} can be represented in a form which ex-

licitly contains the amplitudes of the expansion of Φ_ν in states that differ from $\Phi_{0\nu}$ by the creation (annihilation) of two phonons or by the rescattering of one phonon:

$$\begin{aligned} \hat{S}_2 = R \exp \left\{ +\frac{1}{2} \sum_{\alpha\beta}^{\nu} \frac{\eta_{\alpha\beta}}{\omega_\alpha + \omega_\beta} (\tilde{b}_\alpha \tilde{b}_\beta - \tilde{b}_{-\alpha}^+ \tilde{b}_{-\beta}^+) \right. \\ \left. + \sum_{\alpha\beta}^{\nu} \frac{\eta_{\alpha\beta}}{\omega_\alpha - \omega_\beta} \tilde{b}_\alpha \tilde{b}_{-\beta}^+ \right\}, \end{aligned} \quad (\text{A3})$$

where R is a normalization factor. In this expression it is assumed that the annihilation operators in the argument of the exponential act only on states with nonzero occupation numbers in $\Phi_{0\nu}$. This circumstance is indicated by the symbol ν on the summation symbol in (A3). It is easy to see that all the operators in (A3) can be regarded as independent and mutually commuting, to within terms $\propto (T/\theta_D)^3$. For example, the result of commutation of the first and third terms gives

$$\begin{aligned} \left[\frac{1}{2} \sum_{\alpha\beta}^{\nu} \frac{\eta_{\alpha\beta}}{\omega_\alpha + \omega_\beta} \tilde{b}_\alpha \tilde{b}_\beta \sum_{\alpha'\beta'}^{\nu} \frac{\eta_{\alpha'\beta'}}{\omega_{\alpha'} - \omega_{\beta'}} \tilde{b}_{\alpha'} \tilde{b}_{-\beta'}^+ \right] \\ = \sum_{\alpha\alpha'}^{\nu} \frac{\tilde{b}_{\alpha'} \tilde{b}_\alpha}{\omega_\alpha + \omega_{\alpha'}} \left\{ \sum_{\beta\beta'}^{\nu} \eta_{\alpha'-\beta} \eta_{\beta'\alpha} \left(\frac{1}{\omega_{\alpha'} - \omega_{\beta'}} + \frac{1}{\omega_\alpha + \omega_{\beta'}} \right) \right\}. \end{aligned} \quad (\text{A4})$$

The expression in curly brackets is equal in order of magnitude to $\eta^2 (T/\theta_D)^3$, and so can be discarded in comparison with the first term in (A3).

To the indicated accuracy, we can represent the exponential (A3) in the form of a product

$$\hat{S}_{2\nu} = R \prod_{\alpha\beta}^{\nu} (S_2)_{\alpha\beta}. \quad (\text{A5})$$

That (A2) and (A3) are the solution of the problem is verified directly by substituting Φ_ν into the Schrödinger equation:

$$\begin{aligned} (H_0 + H_{int}) \Phi_\nu = E_\nu \Phi_\nu, \\ (\hat{S}_{2\nu}^{-1} (H_0 + H_{int}) \hat{S}_{2\nu})_{\alpha\beta} = E_\alpha \delta_{\alpha\beta}. \end{aligned} \quad (\text{A6})$$

Since the operator $\hat{S}_{2\nu}$ (like $\hat{S}_{2\nu}^{-1}$) independently creates and annihilates excitations, by simple but rather cumbersome calculations it is possible to obtain an explicit expression for the coefficients $\eta_{\alpha\beta}$ and the state energy E_ν (in the calculations it is convenient to transform the operator S in the right-hand side of (A6) by means of the well known relation $\exp(cb^+) (b) \exp(-cb^+) \equiv b - c$:

$$E_\nu - E_\nu^0 = \frac{1}{2} \sum_{\alpha} B_{\alpha-\alpha} - \frac{1}{2} \sum_{\alpha\beta} \frac{B_{\alpha\beta} \eta_{-\alpha-\beta}}{\omega_\alpha + \omega_\beta}, \quad (\text{A7})$$

$$\begin{aligned} \eta_{\alpha\beta} = B_{\alpha\beta} - \sum_{\nu} \frac{B_{\alpha-\nu} \eta_{\nu\beta}}{\omega_\nu + \omega_\beta} - \sum_{\mu} \frac{B_{\beta-\mu} \eta_{\mu\alpha}}{\omega_\mu + \omega_\alpha} \\ + \sum_{\nu\mu} \frac{B_{-\mu-\nu} \eta_{\nu\beta} \eta_{\mu\alpha}}{(\omega_\nu + \omega_\beta)(\omega_\mu + \omega_\alpha)}. \end{aligned} \quad (\text{A8})$$

We note that the relations obtained do not contain occupation numbers. As already noted above, this is connected with the fact that for virtual excitations the region of frequencies $\omega < T \ll \theta_D$ is unimportant. The equations obtained can be regarded as ordinary perturbation-theory equations for the coefficients of the expansion (A2):

$$(E_\nu - E_\alpha^0) (S_2)_{\alpha\nu} = \sum_{\beta} (H_{int})_{\alpha\beta} (S_2)_{\beta\nu}.$$

A final state that differs from $\Phi_{0\nu}$ by two phonons can be obtained by direct creation of them in $\Phi_{0\nu}$, rescattering of the first or second phonon, and also absorption of an excess pair of phonons from a state with two pairs of phonons. The sequence of terms in (A8) corresponds to this. The fact that the four-phonon amplitude decomposes into a product of pair amplitudes is true with macroscopic accuracy.

For the case when the function $B_{\alpha\beta}$ can be represented in the form

$$B_{\alpha\beta} = \sigma B_\beta B_\alpha, \quad \sigma = \mp 1, \quad (\text{A9})$$

the solution of (A8) is found directly: $\eta_{\alpha\beta} = B_{\alpha\beta} \eta_\alpha \eta_\beta$;

$$E_\nu - E_\nu^0 = \frac{1}{2} \sum_{\beta} |B_\beta|^2 \eta_\beta, \quad (\text{A10})$$

$$\eta(\omega) = 1 - \sigma \sum_{\beta} \frac{|B_\beta|^2 \eta(\omega_\beta)}{\omega + \omega_\beta} \eta(\omega). \quad (\text{A11})$$

The latter equation is conveniently transformed to a form linear in $\eta(\omega)$. For this, we substitute in the right-hand side of (A11) the function $\eta(\omega_\beta)$ expressed in terms of the same equation:

$$\begin{aligned} \eta(\omega) = 1 - \sigma \sum_{\beta} \frac{|B_\beta|^2}{\omega + \omega_\beta} \eta(\omega) \\ + \sigma^2 \sum_{\alpha\beta} \frac{|B_\alpha|^2 |B_\beta|^2}{\omega_\beta - \omega} \eta(\omega_\alpha) \eta(\omega_\beta) \eta(\omega) \left\{ \frac{1}{\omega_\alpha + \omega} - \frac{1}{\omega_\alpha + \omega_\beta} \right\}. \end{aligned} \quad (\text{A12})$$

Now, having regrouped the terms, we again express the sums over α in terms of Eq. (A11). As a result, we find

$$\eta(\omega) = 1 - 2\sigma \sum_{\beta} \frac{\omega_\beta |B_\beta|^2}{\omega_\beta^2 - \omega^2} \eta(\omega) + \sigma \sum_{\beta} \frac{|B_\beta|^2 \eta(\omega_\beta)}{\omega_\beta - \omega}. \quad (\text{A13})$$

The equation obtained is well known in the theory of singular integral equations, and admits an exact solution in quadratures.²² We shall not do this here, however, since by means of (A11) and (A13) it is easy to establish the general properties of the solution and the value $\eta(0)$. In fact, it follows immediately from (A11) that $\eta(\omega)$ is a monotonic function of the frequency, increasing or decreasing, depending on the sign of σ . For $\omega = 0$, Eqs. (A11) and (A13) give the system

$$\eta(0) \left(1 + \sigma \sum_{\beta} \frac{|B_{\beta}|^2}{\omega_{\beta}} \eta(\omega_{\beta}) \right) = 1,$$

$$(1 + 2\sigma D) \eta(0) = 1 + \sigma \sum_{\beta} \frac{|B_{\beta}|^2}{\omega_{\beta}} \eta(\omega_{\beta}), \quad D = \sum_{\beta} \frac{|B_{\beta}|^2}{\omega_{\beta}}, \quad (\text{A14})$$

from which it follows that

$$\eta(0) = (1 + 2\sigma D)^{-1/2}. \quad (\text{A15})$$

Taking into account the definition of the quantity D and the fact that the sum is built up over frequencies $\omega_{\beta} \propto \theta_D$, from the second equation (A14) we obtain the approximate estimate

$$\eta(\theta_D) \propto \frac{(1 + 2\sigma D)^{1/2} - 1}{\sigma D}. \quad (\text{A16})$$

Thus, solving Eq. (13) makes it possible to obtain the operator \hat{S}_2 explicitly. On the other hand, as can be seen from (A15) and (A16), the difference from perturbation theory reduces only to a quantitative renormalization of the solution.

¹A. O. Caldeira and A. J. Leggett, *Ann. Phys. (N.Y.)* **149**, 374 (1983); **153**, 445 (1984).

²A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P.A. Fisher, A. Garg,

and W. Zwerger, *Rev. Mod. Phys.* **59**, 1 (1987).

³U. Eckern, G. Schön, and V. Ambegaokar, *Phys. Rev. B* **30**, 6419 (1984).

⁴A. I. Larkin and Yu. N. Ovchinnikov, *Zh. Eksp. Teor. Fiz.* **86**, 719 (1984) [*Sov. Phys. JETP* **59**, 520 (1984)].

⁵Yu. Kagan and N. V. Prokof'ev, *Pis'ma Zh. Eksp. Teor. Fiz.* **43**, 434 (1986) [*JETP Lett.* **43**, 558 (1986)].

⁶Yu. Kagan and L. A. Maksimov, *Zh. Eksp. Teor. Fiz.* **65**, 622 (1973) [*Sov. Phys. JETP* **38**, 307 (1974)].

⁷Yu. Kagan and M. I. Klinger, *J. Phys. C* **7**, 2791 (1974).

⁸Yu. Kagan and L. A. Maksimov, *Zh. Eksp. Teor. Fiz.* **84**, 792 (1983) [*Sov. Phys. JETP* **57**, 459 (1983)].

⁹Yu. Kagan and N. V. Prokof'ev, *Zh. Eksp. Teor. Fiz.* **90**, 2176 (1986) [*Sov. Phys. JETP* **63**, 1276 (1986)].

¹⁰Yu. Kagan and N. V. Prokof'ev, *Pis'ma Zh. Eksp. Teor. Fiz.* **45**, 91 (1987) [*JETP Lett.* **45**, 114 (1987)].

¹¹J. Kondo, *Hyperfine Interact.* **31**, 117 (1986).

¹²Yu. Kagan and M. I. Klinger, *Zh. Eksp. Teor. Fiz.* **70**, 225 (1976) [*Sov. Phys. JETP* **43**, 132 (1976)].

¹³J. P. Sethna, *Phys. Rev. B* **24**, 698 (1981); *Phys. Rev. B* **25**, 5050 (1982).

¹⁴T. Holstein, *Ann. Phys. (N.Y.)* **8**, 343 (1959).

¹⁵C. P. Flynn and A. M. Stoneham, *Phys. Rev. B* **1**, 3966 (1970).

¹⁶H. Teichler and A. Seeger, *Phys. Lett.* **82A**, 91 (1981).

¹⁷Yu. Kagan, in *Defects in Insulating Crystals* (Proceedings of an International Conference, Riga, May 1981; Springer-Verlag, Berlin, Heidelberg, New York, 1982).

¹⁸A. A. Gogolin, *Pis'ma Zh. Eksp. Teor. Fiz.* **32**, 30 (1980) [*JETP Lett.* **32**, 28 (1980)].

¹⁹H. Grabert and U. Weiss, *Phys. Rev. Lett.* **54**, 1605 (1985).

²⁰M. P. A. Fisher and A. T. Dorsey, *Phys. Rev. Lett.* **54**, 1609 (1985).

²¹R. P. Feynman and F. L. Vernon, *Ann. Phys. (N.Y.)* **24**, 118 (1963); R. P. Feynman, *Statistical Mechanics* (Benjamin, New York, 1972).

²²N. I. Muskhelishvili, *Singular Integral Equations* (Noordhoff, Groningen, 1953) [Russ. original (2nd edition), Fizmatgiz, Moscow, 1962].

Translated by P. J. Shepherd