KINETIC THEORY OF SEMICONDUCTORS WITH LOW MOBILITY

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A low mobility theory for semiconductors with a narrow conductivity band (or valence band) is developed for strong coupling between the current carriers and lattice oscillations. At temperatures below the Debye temperature nonlocalized small-radius polarons are the current carriers. The scattering operator for these polarons is singled out and a transport equation is set up by which various kinetic coefficients can be calculated. It is demonstrated that at temperatures exceeding the Debye temperature the main mechanism of motion is classical superbarrier current-carrier jumps from site to site, in which the lattice actively participates. The temperature dependence of the mobility in this case is of an activation nature. The problem of the smallness parameters of the theory is considered. The results obtained are compared with the data of other authors.

1. INTRODUCTION

IT is known that in many semiconductors [1-3] the mobility u increases with the temperature as $\exp[-E_a/kT]$, starting near the Debye temperature and above (E_a is the activation energy). It is important to note that in such substances the mobility is very low ($u \ll 1$ cm^2/V-sec), and the Hall effect cannot be measured. It can be shown that these facts are closely related. Several papers [4-6] are devoted to an explanation of this temperature dependence of the mobility, and particular notice should be taken of the interesting paper by Holstein. Inasmuch as a dependence of the type $\exp[-E_a/kT]$ cannot be due to single-phonon or two-phonon carrier scattering processes, it is clear from the very outset that many phonons must participate simultaneously in the processes. But for this purpose the coupling between the carriers and the lattice vibrations should be strong. The criterion for the applicability of the kinetic equation is not satisfied in this case. Indeed, assuming the usual connection between the mobility and the relaxation time τ, we obtain

$$\frac{\hbar}{\tau kT} \approx 20 \frac{m}{m^*} \frac{500^\circ\mathrm{K}}{T} \frac{1\ \mathrm{cm^2/V\cdot sec}}{u}. \qquad (1)$$

Here m is the mass of the free electron and m* is the effective mass. Putting $T \approx 500^\circ$K, $m^* \approx m$, and $u \leq 1$ cm^2/V-sec, we find that $\hbar/\tau kT \gg 1$.

One could hope that the strong electron-phonon interaction would so renormalize the carrier mass (polaron) that the ratio m/m^* would become much smaller than unity. It may turn out then that the observed temperature dependence of the mobility is due only to the strong dependence of m* on the temperature. It will become clear from what follows that such an assumption is untrue. Therefore the activation character of the temperature dependence of the mobility indicates that even after the polarons are separated the transitions should remain multiphonon, and the interaction with the lattice remains strong. But this can lead to a situation wherein the uncertainty in the polaron energy $\hbar W_k$ (W_k is the total probability of scattering of a polaron with momentum $\hbar k$) exceeds the width of the polaron band ΔE_p, although it does remain much smaller than the dip in the polaron level. In this case one can speak of a localized polaron of small radius, but the concept of "polaron band" would seem to lose its meaning.

Following Yamashita and Kurosawa [4], Holstein proposed that in this case the principal role in the mobility mechanism is played by classical polaron jumps above the barrier from one lattice site to another [1]. The energy E_a sufficient to overcome the interatomic barrier is acquired by the polaron

[1] The concept of jumps from site to site is sometimes identified with the "motion mechanism after Fervey." It must be noted that the use of these ideas without any stipulations contradicts quantum mechanics. Indeed, by virtue of the translational invariance in the stationary state, the electron cannot be connected with some definite site, and no matter how narrow the band, an electron packet localized initially near some site will manage after a time on the order of $\hbar/\Delta E$ (where ΔE is the width of the band) to "smear out" over the entire lattice. Therefore the concepts of jumps from site to site can be used only when the electrons interact sufficiently strongly with the lattice vibrations. In other words, for the latter there is no motion mechanism after Fervey in the customary form.

from the lattice vibrations, with the ions vibrating about equilibrium positions that are shifted as a result of the polarization of the lattice by the electron. Such a jump over the barrier should occur more rapidly than the ordinary quantum-mechanical penetration through the barrier. The time of this penetration $\hbar/\Delta E_p$ (ΔE_p is the width of the polaron zone), and consequently the polaron effect (narrowing down of the zone and increase in the effective mass) decreases the probability of the tunnel penetration and thereby favors the occurrence of the jumps. According to Holstein, the condition under which the jumps predominate over the ordinary mobility mechanism, that is, $\hbar W(\mathbf{g}) > \Delta E_p$ (where $W(\mathbf{g})$ is the probability of the polaron jumping from site to site and $\mathbf{g}$ is the lattice vector drawn from the given site to the neighboring one) coincides exactly with the condition $\hbar W_{\mathbf{k}} > \Delta E_p$, and therefore the jumps actually come into play precisely when the concept of the polaron band loses its meaning. However, such a deduction is a consequence of the erroneous equation $W_{\mathbf{k}} = W(\mathbf{g})$. We shall show that in fact the inequality $W_{\mathbf{k}} \gg W(\mathbf{g})$ takes place, that is, there exists an intermediate region of temperatures in which the uncertainty in the polaron energy is already large ($\hbar W_{\mathbf{k}} \gtrsim \Delta E_p$), and jumps over the barrier still make a small contribution to the electric conductivity. It would be interesting to construct a theory for this temperature range, too.

In addition, the transition to the representation of an electron ascribed to a site, which was made by Yamashita and Kurosawa [4] and by Holstein [5] for temperatures on the order of the Debye temperature and above, needs a more rigorous substantiation. In the papers of Yamashita and Kurosawa [4] there is no proof whatever that the zeroth approximation employed (electron at the site) is the best. Holstein's estimates [5] are not complete and have a somewhat artificial character. By virtue of the considerations advanced above, it is desirable to develop a theory which makes it possible to separate judiciously the zeroth approximation and to estimate the discarded term [2]. It is desirable to start to learn how to calculate such kinetic coefficients as the thermal emf, the Hall coefficient, etc., for which the measures employed in [5] are generally not applicable. We must therefore develop a special technique for interpreting the Kubo formula [7] for electric conductivity in the case of strong electron-phonon interaction. The present article is devoted to these questions.

2. INITIAL HAMILTONIAN. CANONICAL TRANSFORMATION

Let us expand the quantized electronic $\hat{\psi}$ function in the orthonormalized system of functions φ_m, corresponding to the electron density concentrated near the m-th site, that is,

$$\hat{\psi}(\mathbf{r}) = \sum_m a_m \varphi_m(\mathbf{r}), \tag{2}$$

where $a_m (a_m^+)$ are the operators of annihilation (production) of electrons on the m-th site. No detailed information concerning these functions, except for the property

$$\varphi_m(\mathbf{r}) = \varphi(\mathbf{r} - \mathbf{R}_m) \tag{2a}$$

(where $\mathbf{R}_m$ is the radius vector characterizing the position of the site) will be necessary in what follows. For example, these may be Wannier functions [8]. The functions $\varphi_m(\mathbf{r})$ can be sought in the form of an expansion in the atomic functions $\psi^0(\mathbf{r} - \mathbf{R}_m)$ of the electron level corresponding to the investigated band, that is,

$$\varphi_m(\mathbf{r}) = \sum_n c_{nm} \psi^0(\mathbf{r} - \mathbf{R}_n) \tag{3}$$

(for simplicity we assume that the electron level is not degenerate). The coefficients c_{nm} must be obtained from the condition that the functions $\varphi_m(\mathbf{r})$ are orthonormal. For example, in the nearest-neighbor approximation ($\sum_{\mathbf{g}}$ is the sum over the nearest neighbors) we have

$$\varphi_m^{(1)}(\mathbf{r}) = \psi^0(\mathbf{r} - \mathbf{R}_m) - \tfrac{1}{2}\sum_{\mathbf{g}} L(\mathbf{g})\, \psi^0(\mathbf{r} - \mathbf{R}_m + \mathbf{g}), \tag{3a}$$

where $L(\mathbf{g})$ is the overlap of the integral wave functions between the nearest neighbors. Apparently the set of functions $\psi^0(\mathbf{r} - \mathbf{R}_m)$ is not complete, since (2) and (3) do not include the states corresponding to excited levels [3].

As a rule, in substances with small mobility there are several atoms in each elementary cell, and their degree of ionicity is high. Then the

[2] We note that the question of the smallness parameters is far from trivial here. Thus, the equation $W_{\mathbf{k}} = W(\mathbf{g})$ used in [5] is the consequence of an insufficiently rigorous analysis of the series for $W_{\mathbf{k}}$ and $W(\mathbf{g})$ (see Sec. 4).

[3] This approach corresponds to the known strong-coupling approximation in the calculation of bandwidths. It does not enable us to calculate the dielectric constant and determine the character of the electron-phonon interaction at large momentum transfers. However, this does not prevent us from finding all the temperature dependences, and the main parameters of the theory γ [see (10)] and J [see (6)], which are not calculated very accurately in this approximation, can be determined from experiment.

jumps occur over ions of the kind for which the affinity to a charge of a given sign is the largest, and therefore the vector $\mathbf{R_m}$ characterizes uniquely the required ion in the m-th elementary cell. In the self-consistent field approximation we write the electronic Hamiltonian in the form

$$H_e = -\frac{\hbar^2}{2m}\Delta + \sum_{n=1}^{N} U(\mathbf{r} - \mathbf{R}_m). \tag{4}$$

Here $U(\mathbf{r}-\mathbf{R_m})$ is the potential energy of the electron in the field of the m-th cell.

In the second-quantization representation, the total Hamiltonian of the system is written in the form

$$\begin{aligned}\hat{H} = &\sum_m \varepsilon a_m^+ a_m + \sum_{m,g} J(\mathbf{g})\, a_{m+g}^+ a_m + \sum_{\mathbf{q},j}\hbar\omega_{\mathbf{q},j}\left(b_{\mathbf{q}j}^+ b_{\mathbf{q}j} + \frac{1}{2}\right)\\ &- \sum_m a_m^+ a_m \sum_{\mathbf{q},j}\hbar\omega_{\mathbf{q},j}\,[u_{mj}^*(\mathbf{q})\, b_{\mathbf{q}} + u_{mj}(\mathbf{q})\, b_{\mathbf{q}}^+]\\ &- \sum_{m,g} a_{m+g}^+ a_m \sum_{\mathbf{q},j}\hbar\omega_{\mathbf{q}j}\,[I_j^*(\mathbf{g},\mathbf{q})\, u_{mj}^*(\mathbf{q})\, b_{\mathbf{q}j}\\ &+ I_j(\mathbf{g},\mathbf{q})\, u_{mj}(\mathbf{q})\, b_{\mathbf{q}j}^+],\end{aligned} \tag{5}$$

where $b_{\mathbf{q}}^+(b_{\mathbf{q}})$ are the phonon creation (annihilation) operators, j is the number of the oscillation branch, and $u_{mj}(\mathbf{q}) = -\gamma_{\mathbf{q}j}^*(2N)^{-1/2}\exp[-i\mathbf{q}\cdot\mathbf{R_m}]$ are dimensionless quantities that characterize the displacements that result from the polarization of the medium by the electron in the m-th site (here N is the number of cells in the crystal and $\gamma_{\mathbf{q}j}$ are coefficients which determine the interaction between the electrons and the phonons of the j-th branch). For the case of interaction with longitudinal optical oscillations of frequency ω_0 when $\mathbf{q}\cdot\mathbf{g} \ll 1$ we have in accordance with [9]

$$|\gamma_{\mathbf{q}}|^2 = \frac{4\pi e^2}{q^2\Omega\hbar\omega_0}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right),$$

where Ω is the volume of the elementary cell, while ϵ_0 and ϵ_∞ are the dielectric constants of the crystal with and without account of its ionic parts, respectively. $I_j(\mathbf{q}\cdot\mathbf{g})$ is the dimensionless quantity that characterizes the ratio of the electron-phonon interaction matrix element which is not diagonal in the functions $\varphi_m(\mathbf{r})$ to the diagonal element

$$\varepsilon = \int \varphi_m^*(\mathbf{r})\, H_e \varphi_m(\mathbf{r})\, d^3r;$$

$$J(\mathbf{g}) = \int \varphi_{m+g}^*(\mathbf{r})\, H_e \varphi_m(\mathbf{r})\, d^3r. \tag{6}$$

The fact that ϵ and $J(\mathbf{g})$ do not depend on the index m follows from property (2a) and reflects the translational invariance of the problem.

Let us leave in (5) the strongest interaction with the longitudinal polarization vibrations [4] and let us assume that for these vibrations

$$\sum_{\mathbf{q}} |u_m(\mathbf{q})|^2 = \frac{1}{2N}\sum_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 = \gamma \gg 1$$

(that is, strong coupling). To be able to retain in (5) only the linear terms in the displacements (that is, in $b_{\mathbf{q}}$ and $b_{\mathbf{q}}^+$) it is necessary that the fourth term be smaller than the first and the fifth smaller than the second. This means that the constant displacements that arise upon polarization of the surrounding medium by the electron should be small compared with the interatomic distances. But this requirement does not contradict the condition $\gamma \gg 1$, that is, the situation here is the same as in the case of large-radius polarons.

We assume further that $I(\mathbf{g}\cdot\mathbf{q}) \ll 1$. In any case, in the case of weak overlap of the functions φ_m and φ_{m+g} [that is, at small values of $J(\mathbf{g})$] this quantity is as small as the ratio $J(\mathbf{g})/\epsilon$. We leave out for the time being the last term of (5), which by virtue of the foregoing will be the smallest. We shall formulate later exact criteria which show when this can be done. Inasmuch as everything depends on the energy difference between the initial and final states, the constant ϵ drops out everywhere, that is, the first term of (5) can be left out, and since the ratio of the second to the fourth terms in (5) can be arbitrary, the fourth term in (5) cannot be regarded as perturbed.

Let us carry out the canonical transformation

$$\tilde{H} = e^{-S} H e^{S}, \tag{7}$$

where

$$S = \sum_{\mathbf{q},m} a_m^+ a_m\,(b_{\mathbf{q}}^+ u_m(\mathbf{q}) - b_{\mathbf{q}} u_m^*(\mathbf{q})). \tag{7a}$$

With such a choice of S, the following exact relations hold true:

$$\begin{aligned}\tilde{a}_m &= a_m \exp\left[\sum_{\mathbf{q}}(b_{\mathbf{q}}^+ u_m(\mathbf{q}) - b_{\mathbf{q}} u_m^*(\mathbf{q}))\right],\\ \tilde{a}_m^+ &= a_m^+ \exp\left[-\sum_{\mathbf{q}}(b_{\mathbf{q}}^+ u_m(\mathbf{q}) - b_{\mathbf{q}} u_m^*(\mathbf{q}))\right];\end{aligned} \tag{8}$$

$$\tilde{b}_{\mathbf{q}} = b_{\mathbf{q}} + \sum_{\mathbf{q}} u_m(\mathbf{q})\, a_m^+ a_m,$$

$$\tilde{b}_{\mathbf{q}}^+ = b_{\mathbf{q}}^+ + \sum_{\mathbf{q}} u_m^*(\mathbf{q})\, a_m^+ a_m; \tag{9}$$

[4] The problem can be solved also without this simplification, but the account of the additional interaction with the acoustical phonons would make the final expressions more cumbersome.

$$\tilde{H} = \sum_m a_m^+ a_m (\varepsilon - E_p) + \sum_q \hbar\omega_q \left(b_q^+ b_q + \tfrac{1}{2}\right) + \sum_{m,g} J(g)\, a_{m+g}^+ a_m \hat{\Phi}_{mg} - \sum_{m_1 \neq m_2} a_{m_1}^+ a_{m_1} a_{m_2}^+ a_{m_2} \sum_q \hbar\omega_q \mathrm{Re}\,(u_{m_1}^*(q)\, u_{m_2}(q)), \quad (10)$$

where

$$E_p = \frac{1}{2N}\sum_q \hbar\omega_q |\gamma_q|^2 = \hbar\bar{\omega}\gamma,$$

$$\Delta_q(m, m+g) = u_m(q) - u_{m+g}(q),$$

$$\hat{\Phi}_{mg} = \exp\left[\sum_q \left(b_q^+ \Delta_q(m, m+g) - b_q \Delta_q^*(m, m+g)\right)\right]. \quad (10a)$$

In the derivation of (10) and (10a) we used the identity $|\gamma_q|^2 = |\gamma - q|^2$, the consequence of which is

$$\frac{1}{N}\sum_q |\gamma_q|^2 \sin[q(R_m - R_{m_1})] = 0. \quad (11)$$

The fourth term in (10) characterizes the interaction between two electrons at the different sites by exchange of virtual phonons, but it is inconsistent to retain it, since it is smaller than the electron correlations that have been left out from (4). The pair interaction leads to screening at small momentum transfers [10,11], which overdetermines the constant γ of the theory, in view of the corrections that depend on the electron concentration n. These corrections are observable, since the carrier concentration can be varied in semiconductors. For example, the activation energy E_a, which will be shown later on to be proportional to γ, starts to depend with increasing n on the carrier concentration. It is possible that this explains the dependence of the slope of ln u (as a function of 1/T) on the concentration of Li observed in NiO [1] when $n > 10^{18} - 10^{19}$. Bearing in mind the low carrier concentrations, we leave out the last term in (10).

The value of E_p (the polaron atomic level shift) in the first term on (10) is the result of eliminating the term with $m_1 = m_2$ from the last sum in (10). In fact $(a_{m_1}^+ a_{m_1})^2$ has the same matrix elements as the operator $a_{m_1}^+ a_{m_1}$. We analogously obtain

$$I_x = e\sum_{mg} a_{m+g}^+ a_m \langle g|\hat{v}_x|0\rangle \hat{\Phi}_{mg}. \quad (12)$$

The diagonal elements of the velocity v_x are identically equal to zero by virtue of the symmetry with respect to time reversal.

Let us make the following transformation:

$$a_m = N^{-1/2}\sum_k a_k e^{ikR_m}. \quad (13)$$

We add and subtract in (10) the term

$$\sum_{mg} J(g)\, a_{m+g}^+ a_m \langle\Phi_g\rangle,$$

where (see Appendix I)

$$\langle\Phi_g\rangle = e^{-S_T(g)},\quad S_T(g) = \frac{1}{2N}\sum_q |\gamma_q|^2 (1 - \cos qg)\,\mathrm{cth}\frac{\hbar\omega_q\beta}{2}. \quad (14)^*$$

We then finally obtain $\tilde{H} = \tilde{H}_0 + \tilde{H}'$, where [5]

$$\tilde{H}_0 = \sum_k a_k^+ a_k \varepsilon(k) + \sum_q \hbar\omega_q (b_q^+ b_q + \tfrac{1}{2}),$$
$$\varepsilon(k) = \varepsilon - E_p + \sum_g J(g)\, e^{-ikg} e^{-S_T(g)}; \quad (15a)$$

$$\tilde{H}' = \sum_{kk'} a_{k'}^+ a_k \frac{1}{N}\sum_{mg} J(g)\,[\hat{\Phi}_{mg} - \langle\Phi_g\rangle] \times \exp\{i(k - k')R_m - ik'g\}. \quad (15b)$$

Carrying out an analogous procedure in (12), we obtain $\tilde{I}_x = I_x^0 + I_x'$ where

$$I_x^{(0)} = \frac{e}{\hbar}\sum_k a_k^+ a_k \frac{\partial}{\partial k_x}\varepsilon(k), \quad (16a)$$

$$I_x' = e\sum_{kk'} a_{k'}^+ a_k \frac{1}{N}\sum_{mg}\langle g|v_x|0\rangle\{\hat{\Phi}_{mg} - \langle\Phi_g\rangle\} \times \exp\{i(k - k')R_m - ik'g\}. \quad (16b)$$

We note that the operator $\hat{\Phi}_{mg}$ has translational invariance, that is, it is not changed by the substitution

$$R_m \to R_m + \Delta,\quad b_q \to b_q e^{-iq\Delta},$$

where Δ is some lattice vector. This operator describes processes which lead to a realignment of the lattice vibration relative to new equilibrium positions as the electron moves. If the phonon occupation numbers do not change (and such transitions are described by terms proportional to $\langle\Phi_g\rangle$), then the realignment is completed within the time of motion of the particle, and the particle drags as it were the entire "load of atomic displacements." This is indeed the polaron effect, which leads to mass renormalization, and $\epsilon(k)$ is the polaron energy (compare with [5]). The terms

*cth = coth

[5] Inclusion of terms proportional to I(q, g) in (5) would cause J to be replaced by

$$\tilde{J} = J - \frac{1}{N}\sum_q \hbar\omega_q |\gamma_q|^2 \mathrm{Re}\, I(q, g).$$

As noted earlier, $I \approx J/\epsilon$, and consequently the ratio of the correction to the main term is equal in order of magnitude to the ratio E_p/ϵ, which for substances of the type considered is usually much less than unity.

proportional to $\Delta\hat{\Phi}_{mg} = \hat{\Phi}_{mg} - \langle\Phi_{mg}\rangle$ describe transitions with change in the occupation number, that is, phonon emission and absorption processes resulting from the fact that the realignment of the lattice vibration relative to new equilibrium positions does not have time to run through its complete course. This is precisely why the second term I'_x in the current [see (16b)] plays the principal role in the kinetics of the jumps. In the high temperature region and in the absence of a magnetic field, the k- and m-representations [see (13)] lead in the lowest approximation to identical results, but in order to find the contribution to the electric conductivity resulting from the tunnel penetration, it is necessary to ascertain the role played by the continuity of the electronic spectrum. This is particularly important in the case of intermediate and low temperatures.

3. GENERAL TRANSPORT EQUATION AND JUMP PROCESSES

Let us use the Kubo formula for the electric conductivity in the form (compare with [12]):

$$\sigma_{xx} = \frac{\beta}{VZ}\,\mathrm{Re}\int_0^\infty \exp(-s\tau)\,\mathrm{Sp}\left\{\exp(-\beta H_0) \times T_C\left[\exp\left(-\frac{i}{\hbar}\int_C H'(z)\,dz\right) I_x(\tau)\, I_x(0)\right]\right\} d\tau. \quad (17)$$

Here $\beta = 1/kT$, V is the crystal volume, and Z is the partition function. The symbol T_C denotes ordering along the contour (Fig. 1). On the left of the trace symbol are the operators $H'(z)$ in which z is closer to the point $-i\hbar\beta$. $H'(z)$ and $I_X(\tau)$ are respectively the perturbation (15b) and the current operator in the interaction representation.

If we consider in the current operators corresponding to the zero and τ terminals only the terms I'_x which are nondiagonal in the phonons, then even in the zeroth approximation in H′ we obtain the following final result:

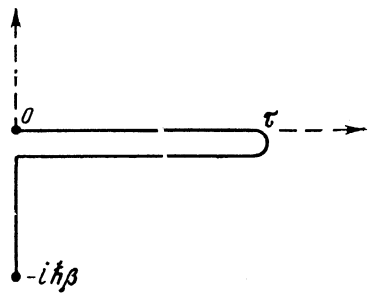

FIG. 1

$$\sigma_{xx}^{(0)} = \frac{ne^2\beta}{V}\,\mathrm{Re}\,\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{p}}\sum_{m_1,m_2}\sum_{g_1,g_2}\langle g_1|v_x|0\rangle\langle g_2|v_x|0\rangle \times \exp\{i[(\mathbf{k}-\mathbf{p})\mathbf{G} - \mathbf{k}g_1 - \mathbf{p}g_2]\}\, Z_0^{-1}e^{-\beta\varepsilon_k}\int_0^\infty \exp\left\{-s\tau + \frac{i}{\hbar}(\varepsilon_k - \varepsilon_p)\tau\right\} \times \{\langle\Phi_{m_1g_1}(\tau)\,\Phi_{m_2g_2}(0)\rangle - \langle\Phi_{g_1}\rangle\langle\Phi_{g_2}\rangle\}\,d\tau. \quad (18)$$

Here n is the electron concentration. It is the result of one "irregular" line (see, for example [12]) from the τ terminal to the zero terminal [6].

In the derivation of (18), account was taken of the fact that in Boltzmann statistics $\exp[\mu/kT] = n/Z_0$, where μ is the chemical potential and $Z_0 = V^{-1}\sum_{\mathbf{k}} \exp[-\beta\epsilon(\mathbf{k})]$. Using formula (AI.7) of the Appendix we find that the expression in the curly brackets of (18) is equal to

$$\exp[-S_T(g_1) - S_T(g_2)] \times \left\{\exp\left(\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2\,\frac{\cos[\omega_{\mathbf{q}}(\tau + i\hbar\beta/2)]}{\mathrm{sh}(\hbar\omega_{\mathbf{q}}\beta/2)}\,a_{1,2}(\mathbf{G}, g_1, g_2)\right) - 1\right\}, \quad (19)^*$$

where

$$\mathbf{G} = \mathbf{R}_{m_2} - \mathbf{R}_{m_1},$$

$$a_{1,2} = \tfrac{1}{2}[\cos\mathbf{q}(\mathbf{G} - g_1) + \cos\mathbf{q}(\mathbf{G} + g_2) - \cos\mathbf{q}\mathbf{G} - \cos\mathbf{q}(\mathbf{G} - g_1 + g_2)].$$

It can be shown that if the dispersion of the frequency of the longitudinal optical phonons is taken into account in the form $\omega(\mathbf{q}) = \omega_0 + \omega_1\cos\mathbf{q}\cdot\mathbf{g}$ or $\omega^2(\mathbf{q}) = \omega_0 + \omega_1\cos\mathbf{q}\cdot\mathbf{g}$ (see [5]), then the sum in the exponent of (19) oscillates and decreases as a function of τ. Consequently, only the contribution near the first saddle point is significant in the integral; at not too small a value of the dispersion the contribution from the next saddle point is exponentially small compared with the contribution from the first point (see, for example [5]).

The subtraction of unity in (19) denotes the elimination of the self-closing of the phonon lines in each of the terminals 0 and τ, that is, they are connected by at least one phonon line, and no divergences of the type 1/s, for which the "free" intersections are responsible, arise (the terminology is taken from [12]).

The saddle-point method is applicable so long as $\gamma/\sinh(\hbar\beta\omega/2) > 1$; this is indeed the criterion

[6] Inasmuch as we confine ourselves in terms linear to the concentration, we shall henceforth consider only graphs with a single irregular electron line.

*sh = sinh.

that indicates when multiphonon processes are significant. The greatest contribution to (18) is made by the term in which $\mathbf{G} = \mathbf{g}_1 = -\mathbf{g}_2$. The remaining terms are small like $\exp[-S_T]$. Putting $\epsilon(\mathbf{k}) = \epsilon(\mathbf{p}) = 0$ and summing in (18) with respect to p and k, we again obtain the condition $\mathbf{G} = \mathbf{g}_1 = -\mathbf{g}_2$. Here $Z_0 \to N/V$. Changing over in (18) to a new variable $t = \tau + i\hbar\beta/2$, taking the real part of the integral with respect to t (that is, integrating within the limits from 0 to ∞), and expanding $\cos \omega_q t$ in a series near $t = 0$ (that is, near the first saddle point), we see that the time within which the integrand decreases sharply (we call this the jump-over time t_0) is

$$t_0^{-1} = \left[\frac{1}{2N}\sum_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 \frac{\omega_{\mathbf{q}}^2}{\mathrm{sh}\,(\hbar\omega_{\mathbf{q}}\beta/2)}(1-\cos \mathbf{qg})\right]^{1/2}$$

$$\approx \omega_0 \left(\frac{\gamma}{\mathrm{sh}\,(\hbar\omega_0\beta/2)}\right)^{1/2} \gg \omega_0. \qquad (20)$$

The difference $\epsilon(\mathbf{k}) - \epsilon(\mathbf{p})$ in (18) can be neglected if the following conditions are satisfied [7]:

$$\frac{\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{p})}{\hbar} t_0 \ll 1, \text{ i.e., } \frac{Je^{-S_T}}{\hbar\omega_0}\left(\frac{\mathrm{sh}\,(\hbar\omega_0\beta/2)}{\gamma}\right)^{1/2} \ll 1, \qquad (21a)$$

$$[\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{p})]\beta \ll 1, \text{ i.e., } Je^{-S_T}/kT \ll 1. \qquad (21b)$$

For the process to be irreversible, that is, for the appearance of a finite resistance, it is necessary that the energy spectrum of the system be continuous. If conditions (21a) and (21b) are satisfied, the continuous spectrum of the polarization-oscillation frequencies plays a more important role than the polaron band. Thus, neglecting the dispersion in the polaron band we obtain [8]

$$\sigma_{xx}^{(0)} = ne^2\beta\frac{\pi^{1/2}}{2}\sum_{g} |\langle g|v_x|0\rangle|^2 e^{-E_a/kT}$$

$$\times \left\{\frac{1}{N}\sum_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 \frac{\omega_{\mathbf{q}}^2}{2}(1-\cos \mathbf{qg})\,\mathrm{cosec}\,\frac{\hbar\omega_{\mathbf{q}}\beta}{2}\right\}^{-1/2}, \qquad (22)^*$$

where

$$E_a = \frac{1}{N\beta}\sum_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 (1-\cos \mathbf{gq})\,\mathrm{th}\,\frac{\hbar\omega_{\mathbf{q}}\beta}{4}.$$

At high temperatures ($\hbar\omega\beta/4 \ll 1$) we have $E_a \leq E_p/2$, that is, when $E_p/2 - E_a \gg aT$, the increase in electric conductivity with temperature like $\exp[-E_a/kT]$ is not connected at all with the increase in the number of carriers in the electronic conductivity band due to the dissociation of the localized polarons.

In the nearest-neighbor approximation, when $\langle g|v_x|0\rangle - iJ(\mathbf{g})g_x/\hbar$, we obtain for $\sigma_{xx}^{(0)}$ an expression which coincides, apart from numerical factors (the number of nearest neighbors), with the result of Holstein:

$$\sigma_{xx}^{(0)} \approx \frac{1}{2} ne^2\beta \sum_{g} W_H(\mathbf{g})\, g_x^2, \qquad (23)$$

$$W_H(\mathbf{g}) = J^2\sqrt{\pi}e^{-E_a/kT}\Big/\hbar^2$$

$$\times \left[\frac{1}{N}\sum_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 \frac{\omega_{\mathbf{q}}^2}{2}(1-\cos \mathbf{gq})\,\mathrm{cosec}\,\frac{\hbar\omega_{\mathbf{q}}\beta}{2}\right]^{1/2}. \qquad (23a)$$

Actually, Holstein's computational procedure was to calculate the jump-over probability $W_H(\mathbf{g})$ in the first Born approximation, assuming H′ to be the perturbation. He then determined the diffusion coefficient as $g^2W_H(\mathbf{g})$ and calculated the electric conductivity from the Einstein relation. The results coincide, since the operators H′ and I′ have an identical structure.

It is known that when the integrand of (17) is expanded in powers of H′, diverging terms arise, proportional to arbitrary powers of 1/s, starting with the first. In our case, however, because of the terms I_x' in the current, an additional set of finite terms independent of s arises. We call these terms of the Holstein type and replace their subscripts xx by the subscript H. The superscript m is the number of points on the contour (with the exception of the two terminals). The first term of this set, $\sigma_H^{(0)}$, was just calculated [see (22)]. The term $\sigma_H^{(1)}$ corresponds to a set of three diagrams, for each of which the operator I_x' is at the terminal 0 and τ, while the third point can be on the upper or lower part of the time contour or on the imaginary axis (from 0 to $-i\hbar\beta$) [9]. Using formula (AI.11) with $kT > \hbar\omega_0/2$ we obtain in the nearest-neighbor approximation [10]

a) $\sigma_H^{(1)}/\sigma_H^{(0)} = \eta_1 = J/E_a \ll 1$, if $\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 = 0$,

b) $\sigma_H^{(1)}/\sigma_H^{(0)}$ proportional to e^{-S_T}, if $\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 \neq 0$. (24)

[7] It follows from the sequel that there are more stringent criteria for the applicability of the theory than (21a) and (21b), that is, the latter are automatically satisfied.

[8] If terms proportional to $I(\mathbf{g}, \mathbf{q})$ are taken into account in (5), a correction appears in (22); the ratio of this correction to the principal term is $(E_a\hbar\omega_0/\epsilon^2)(\sinh[\hbar\omega_0\beta/2])^{-1} \ll 1$.

*th = tanh.

[9] The diagrams with the current I_x^0 in the left terminal and without free intersections also make a contribution to σ_H, but this contribution is small since it is proportional to $\exp[-S_T]$.

[10] The summation of the diagrams and the integration by the saddle-point method is straightforward but cumbersome. We therefore present only the final results. By way of an example we give in Appendix III a scheme for calculating the second-order probability (block with four points).

For hexagonal and trigonal crystals cases a) and b) are possible, while for cubic crystals only b) is possible. The smallness of the parameter η_1 corresponds to a polaron of small radius (see [5]). The dip in the polaron level E_p exceeds here the width of the electronic band J. Then, owing to the narrowness of the polaron band ($\Delta E_p \approx J \exp[-S_T] \ll J$) it does not overlap the initial band, and all its states are energetically more favored. In the opposite case ($\eta_1 > 1$) the problem becomes more complicated and corresponds to the case of polarons with medium and large radii.

The term $\sigma_H^{(2)}$ (two terminals with operators I_x' and two points on the contour) corresponds to seven diagrams. If at least one of the points lies on the horizontal portions of the contour and each of the terminals is connected by phonon lines only with the point nearest to it, a free intersection arises. This case of closure of the phonon lines will be singled out and included among the diagrams that diverge as 1/s. For example, if the point 1 lies on the lower part of the time contour and point 2 on the upper part, and if 1 is closer to the terminal τ than 2, then the expression under the sign of triple integration with respect to τ, z_1, and z_2 is

$$\langle \Delta\Phi_{m_1g_1}(z_1)\,\Delta\Phi_{mg}(\tau)\,\Delta\Phi_{m_2g_2}(z_2)\,\Delta\Phi_{m'g'}(0)\rangle - \langle \Delta\Phi_{m_1g_1}(z_1)\,\Delta\Phi_{mg}(\tau)\rangle \langle \Delta\Phi_{m_2g_2}(z_2)\,\Delta\Phi_{m'g'}(0)\rangle,$$

$$\Delta\Phi_{mg}(z) = \hat{\Phi}_{mg}(z) - \langle \Phi_g \rangle. \qquad (25)$$

The subtraction procedure must be carried out also for diagrams with a large number of points, and this gives rise to terms proportional to arbitrary powers of 1/s. These must be combined with diagrams with the same order in 1/s, arising when the current $I_x^{(0)}$ is inserted in one or both terminals. The procedure for summing diagrams of the type $(1/s)^n$ will be described below.

For $kT > \hbar\omega_0/2$ we obtain

$$\sigma_H^{(2)}/\sigma_H^{(0)} \approx \eta_2 = J^2/(E_a kT)^{1/2}\hbar\omega_0,$$

a) $\sigma_H^{(2)}/\sigma_H^{(1)} = (J/\hbar\omega_0)(E_a/kT)^{1/2} \gtrsim 1$, if $g_1 + g_2 + g_3 = 0$,

b) $\sigma_H^{(2)}/\sigma_H^{(1)}$ proportional to $e^{S_T} \gg 1$, if $g_1 + g_2 + g_3 \neq 0$. (26)

However, the inequality $\sigma_H^{(2)} > \sigma_H^{(1)}$ still does not mean that the series diverges. From an analysis of the next terms of the expansion it follows that

$$\sigma_H^{(3)}/\sigma_H^{(1)} \sim \cdots \sim \sigma_H^{(2n+1)}/\sigma_H^{(2n-1)} \sim \cdots \sim \eta_2,$$
$$\sigma_H^{(2)}/\sigma_H^{(0)} \sim \cdots \sim \sigma_H^{(2n+2)}/\sigma_H^{(2n)} \sim \cdots \sim \eta_2, \qquad (27)$$

and the ratio $\sigma_H^{(2n+1)}/\sigma_H^{(2n)}$ is determined by relations of the type (24).

Thus, the series for the even and odd terms of the Holstein type contain a single parameter η_2, but the first term of the odd series is smaller than the first term of the even series at least in a ratio η_1:1.

Let us proceed to the summation of diagrams containing free intersections. The simplest diagram containing one free intersection is obtained if there are no points on the contour except the terminals 0 and τ, and the latter contain $I_x^{(0)}$. The next diagram of the type 1/s is obtained if there is at least one point z_1 on the contour. In one of the terminals, say in 0, we insert I_x' and we close it with point z_1, while in terminal τ we insert $I_x^{(0)}$. Then a free gap arises between z_1 and τ, and on the left between the points 0 and z_1 lies a multiphonon two-point block. We have already explained how a diagram of the type 1/s arises for four points (two terminals and two points on the contour), etc.

In the general case the factor of the first power of 1/s is a product of two "vertices": the left vertex $r_{1,k}^x$ and the right vertex $r_{2,k}^x$, each of which is a sum of multi-point blocks which contain no free intersections (see Appendix III). The left "vertex" is not equal to the right vertex, since it contains blocks with points on the vertical portion of the contour. Diagrams containing more than one free intersection other than verticles include "horizontal irreducible parts" (see [12]). The sum of all the horizontal irreducible parts (containing no free intersections) will be called the probability W_{pk}. In the aggregate of all the diagrams containing at least one intersection, we separate the right-hand vertex, and the free intersection ahead of it will be included in the left part. For the left part F_k^x we obtain the equation

$$F_k^x = r_{1,k}^x \frac{1}{s} + \frac{1}{s}\sum_p F_p^x W_{pk}. \qquad (28)$$

Multiplying (28) by s and letting s approach zero, we obtain ultimately

$$r_{1,k}^x + \sum_p F_p^x W_{pk} = 0. \qquad (29)$$

Equation (29) is analogous to the Boltzmann kinetic equation. Therefore we denote the contribution to the electric conductivity associated with it by σ_B. In (29) it is possible to segregate the "departure" and "arrival" terms [12]; the former correspond to the probability $W_{pk}^{(d)} = -W_k\delta_{kp}/N$. On the diagrams corresponding to these "departure probabilities," in contradiction to those corresponding to "arrival probabilities" $W_{kp}^{(ar)}$, there are no phonon lines joining the upper and lower portions of the contour. In the region of low and intermediate temperatures ($kT < \hbar\omega_0\xi/2$, where

$\xi \leq 1$), this equation determines the entire kinetics for arbitrary coupling between the electrons and the phonons. When $kT > \hbar\omega_0/2$, it enables us to estimate the contribution made to the electric conductivity by the tunnel penetration, but we shall show that for such temperatures the principal role is played by the jump-over processes.

When $kT > \hbar\omega_0/2$, Eq. (29) can be readily solved, for by virtue of inequalities of the type (21a) and (21b) the probabilities are practically independent of $\mathbf{k}$ and $\mathbf{p}$ ($W_{\mathbf{pk}} \approx W + W'_{\mathbf{pk}} \exp[-S_T]$). Therefore the arrival terms in (29) vanish (accurate to terms of order $\exp[-S_T]$)

$$\sum_{\mathbf{p}} F^x_{\mathbf{p}} W^{(ar)}_{\mathbf{pk}} \approx W \sum_{\mathbf{p}} F^x_{\mathbf{p}} = 0. \tag{30}$$

Equation (30) is satisfied by virtue of the condition $\sum_{\mathbf{p}} F^x_{\mathbf{p}} = 0$. Consequently

$$F^x_{\mathbf{k}} = r^x_{1\mathbf{k}}/W_{\mathbf{k}} \approx r^x_{1\mathbf{k}}/W. \tag{31}$$

It can be shown that the probability $W_{\mathbf{k}}$ is real, inasmuch as one can set any block, in which l_1 points lie on the upper part of the contour and l_2 points on the lower, in correspondence with a complex-conjugate block with l_2 points on top and l_1 points on the bottom. We ultimately obtain

$$\sigma_B \approx ne^2\beta W^{-1} \frac{1}{N} \sum_{\mathbf{k}} \mathrm{Re}\,(r^x_{1\mathbf{k}} r^x_{2\mathbf{k}}). \tag{32}$$

We present the results of an analysis of the terms of the series for the departure probability $W_{\mathbf{k}}$. The first term $W^{(0)}$ coincides with $W_H(\mathbf{g})$ [see (23)]. For $W^{(1)}$ we obtain

$$W^{(1)}/W^{(0)} \approx J/E_a < 1, \quad \text{if} \quad \mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 = 0,$$
$$W^{(1)}/W^{(0)} \text{ proportional to } \exp(-S_T\gamma_1 - E_a\delta_1/kT) \ll 1, \tag{33}$$

where $\gamma_1 < 1$ and $\delta_1 \geq 1$ if $\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 \neq 0$.

However, for the term $W^{(2)}$ (the sum of two blocks P_4 and P_4^* with four points lying either only on the upper part of the contour or only on the lower one) we find (see Appendix III) that when $\hbar\omega_0\beta/2 \ll 1$

$$W^{(2)} \approx \left(\frac{J}{E_a}\right)^4 \frac{(kT)^2}{\hbar^2\omega_0}, \qquad \frac{W^{(2)}}{W^{(0)}} \approx \frac{J^2}{\hbar\omega_0} \frac{(kT)^{5/2}}{E_a^{7/2}} e^{E_a/kT} \gg 1, \tag{34}$$

that is, $W^{(2)}$, in contradistinction to the Holstein-type term $\sigma_H^{(2)}$, does not contain the factor $\exp[-E_a/kT]$. This difference is connected with the fact that in the calculation of $\sigma_H^{(2)}$ we summed seven diagrams (depending on the location of the two additional points on the contour) and in the sum the large terms of the type (34) cancelled out.

We note that the imaginary part of the two-point block lying on the upper part of the contour, which is equal to $J^2/4\hbar E_a$, likewise contains no exponential smallness, but it makes no contribution to the probability $W^{(0)} = W_H(\mathbf{g}) = P_2 + P_2^*$.

The calculations show that starting with $W^{(2)}$ all the even terms of the series $W^{(2n)}$ contain no exponential smallness of the type $\exp[-E_a/kT]$ and $W^{(2n+2)}/W^{(2n)} \approx \eta_2$. For the odd terms of the series, starting with $W^{(3)}$, we obtain $W^{(2n+1)}/W^{(2n-1)} \sim \eta_2$, and the ratio $W^{(3)}/W^{(2)}$ is small at least as η_1. Thus, we must substitute $W^{(2)}$ for W in (32).[11]

In the region of high temperatures ($kT > \hbar\omega_0/2$), the properties of the series for the vertices are as follows. In the lowest order

$$r^{x(0)}_{1\mathbf{k}} = r^{x(0)}_{2\mathbf{k}} = v_x(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial}{\partial k_x}\varepsilon(\mathbf{k})$$
$$= -\frac{i}{\hbar}\sum_{g} J(g)\, g_x e^{-i\mathbf{kg}} e^{-S_T(\mathbf{g})}. \tag{35}$$

In the next order (two-point blocks, one of the points is a terminal) we have

$$r^{x(1)}_{2\mathbf{k}}/r^{x(0)}_{2\mathbf{k}} \sim e^{-S_T\gamma} \ll 1,$$
$$r^{x(1)}_{1k}/r^{x(0)}_{1k} \approx J/E_a \text{ for } \mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 = 0,$$
$$r^{x(1)}_{1k}/r^{x(0)}_{1k} \sim e^{-S_T\gamma} \text{ for } \mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 \neq 0, \tag{36}$$

where $0 < \gamma < 1$. The series of the odd terms $r^{x(2n+1)}_{1\mathbf{k}}$ and $r^{x(2n+1)}_{2\mathbf{k}}$ contain as before the parameter η_2, but the saddle points $t_1^0, t_2^0, \ldots, t_{2n}^0$ for all the variables do not lie at zero ($\bar{\omega}t_1^0, \bar{\omega}t_2^0, \ldots, \bar{\omega}t_{2n}^0 \approx 1$) in the series of the even terms (starting with two points apart from the terminal). Consequently there is no total cancellation of the factors outside the integrals signs, of the type $\exp[-S_T(\mathbf{g}_1) \ldots - S_T(\mathbf{g}_{2n+1})]$, that is, the even terms are proportional to $\exp(-S_T\gamma_{2n})$, where $0 < \gamma_{2n} < 1$. In addition, near the new saddle points, by virtue of the condition $t_0\omega_0 \ll 1$ [see (20)], we can integrate over all the variables from $-\infty$ to ∞, which yields $(Jt_0/\hbar)^{2n} \exp(-E_a\delta_{2n}/kT)$, where $\delta_{2n} > 1$.

We thus have for a vertex with 2n points

$$r^{x(2n)}_{1\mathbf{k}} \approx r^{x(2n)}_{2\mathbf{k}} \sim v_x(\mathbf{k})\, \eta_3^n e^{-E_a\delta_{2n}/kT} e^{S_T(1-\gamma_{2n})}, \tag{37}$$

where

$$\eta_3 = \left(\frac{Jt_0}{\hbar}\right)^3 = \frac{J^2}{E_a kT} = \eta_2 \frac{\hbar\omega}{(E_a kT)^{1/2}} \ll \eta_2. \tag{37a}$$

It is difficult to obtain the exact values of the

[11] In [4] we actually used for W the zeroth term of the expansion $W^{(0)}$. However, inasmuch as the inequality $W^{(2)} \gg W^{(0)}$ holds true for all temperatures, the results of [4] are incorrect in the region $kT \leq \hbar\omega_0/2$.

numbers δ_{2n} and γ_{2n}, for they depend on the form and magnitude of the phonon frequency dispersion and on the form of the dependence of γ_q on q. It can be stated, however, that owing to the increase in the number of integration variables $(t_1, \ldots, t_{2n})$, the following relation holds true

$$1 < \delta_2 \leqslant \delta_4 \cdots \leqslant \delta_{2n} \cdots \qquad (38)$$

Taking the largest (say the 2n-th) terms in the series for the vertices, we obtain

$$\frac{\sigma_B^{(2n)}}{\sigma_H^{(0)}} \approx \eta_3^{2n}\eta_2^{-1}\eta_1^{-2}\left(\frac{E_a}{kT}\right)^2 e^{-E_a(2\delta_{2n}-1)/kT} e^{-2S_T\gamma_{2n}} \ll 1, \qquad (39)$$

that is, when $E_a > kT > \hbar\omega_0/2$ this ratio is exponentially small for any term in the series.

Thus, if $\eta_2 \ll 1$, then the main contribution to the electric conductivity is determined by the equivalent formulas (22) or (23).

4. DISCUSSION OF RESULTS

Let us present an illustrative physical picture of the phenomena considered above. At sufficiently high temperatures $\sinh(\hbar\omega_0/2kT) < \gamma$ $(\gamma \gg 1)$, all the processes are essentially multiphonon. When $kT > \hbar\omega_0/4$ the principal mechanism of motion is by jumps from site to site, and the time Δt between jumps is smaller than the time t_p of tunnel penetration, but much larger than the jump time t_0. Since the jump (collision) time t_0 [see (20)] is much shorter than ω_0^{-1}, the jump occurs so rapidly that the electron jumps out of the polarization well produced by it, shakes off the "heavy load of atomic displacements" (that is, the process is essentially multiphonon), and ceases to exist as a polaron. But inasmuch as the time between jumps Δt is much longer than ω_0^{-1}, then, on landing on a new site, the electron again has time to produce a polarization well and sink in it (that is, it goes into the polaron state) before it jumps over to a second site, and this jump will occur before the electron can tunnel through the barrier.

Thus, the following inequalities hold true:

$$t_p \gg \Delta t \gg t_0, \qquad t_0 < \omega_0^{-1}, \qquad \Delta t \gg \omega_0^{-1},$$

where

$$t_p = \frac{\hbar}{\Delta E_p} \sim \frac{\hbar}{J} e^{S_T}, \qquad t_0 \sim \frac{\hbar}{(E_a kT)^{1/2}},$$

$$\Delta t \approx \frac{1}{W_H} = \frac{\hbar^2}{J^2 t_0} e^{E_a/kT}. \qquad (40)$$

At first glance it is necessary to add to these inequalities still another one, $t_e \approx \hbar/J > \omega_0^{-1}$, which requires that the electron wave packet spread out more slowly than the time of transition of the electron to the polaron state. It follows from our work, however, that in order for (22) to be valid a weaker condition is necessary:

$$\eta_2 = J^2/(E_a kT)^{1/2}\hbar\omega_0 \ll 1, \text{ i.e., } t_e > (t_0/\omega_0)^{1/2}. \qquad (41)$$

Condition (41) requires that the initial electron band (of width J) be sufficiently narrow. Incidently, for substances such as NiO, in which it is formed as a result of levels belonging to the unfilled d-shell, the interatomic distances are large; apparently this is precisely the case that is realized.

We note that for arbitrary values of η_2 it is necessary to sum all terms of the series for σ_H, for the probability and for the vertices. From the structure of the terms of the series for σ_H it follows that they are all proportional to $\exp(-E_a/kT)$, so that we can hope that even in the case of wider bands the contribution to the electric conductivity due to jumps (σ_H) will increase with temperature like $\exp(-E_a/kT)$, provided the factor preceding the exponential $F(\eta_2)$ will be a weaker function of the temperature $(\eta_2 \sim T^{-1/2})$. If in addition it turns out that the contribution to the electric conductivity due to the jumps is the largest, that is, $\sigma_B < \sigma_H$, then the temperature dependence of the mobility will carry as before an activation character [12]. The analysis of electric conductivity at low and intermediate temperatures and the calculation of the high frequency conductivity and the hole effect will be the subject of a separate communication.

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[12] In a recently published article[6] Klinger also investigated the question of low mobility, using the van Hove procedure.[13] However, we strongly disagree with him in many respects, including the question of the limits of validity of the theory (smallness parameters). Klinger states that the main criteria for the applicability of the theory are the conditions (6) in [6], that is, $\Delta t \gg \omega_0^{-1}$ and $t_p \gg \Delta t$. It follows from our work, however, that in order for (22)–(23a) to be valid [compare with (9) and (10) in [6]) it is necessary to satisfy the more stringent requirements $\eta_1 \ll 1$ and $\eta_2 \ll 1$, that is, the initial electron band should be narrow, and the carriers must be polarons of small radius. In [6] no separation is made in the contributions to the mobility made by the transport processes of the ordinary type and made by the jumps, which may lead to an incorrect estimate of the next approximations. Apparently, these are precisely the reasons for the discrepancies.

APPENDIX I

AVERAGING OF PRODUCTS OF THE TYPE $\hat{\Phi}_{m_1 g_1}(z_1) \ldots \hat{\Phi}_{m_n g_n}(z_n)$ OVER THE PHONONS

We consider a block with two points. Representing $\Phi_{m_l g_l}(z_l)$ in the form $\prod_{\mathbf{q}} \exp[H_l(\mathbf{q})]$, where

$$H_l(\mathbf{q}) = \Delta_{\mathbf{q}}(m_l, m_l + g_l)\, b_{\mathbf{q}}^{+} e^{i\omega_{\mathbf{q}} z_l} - \Delta_{\mathbf{q}}^{*}(m_l, m_l + g_l)\, b_{\mathbf{q}} e^{-i\omega_{\mathbf{q}} z_l}, \quad \text{(AI.1)}$$

we obtain

$$Q_2 = \langle \Phi_{m_1 g_1}(z_1)\, \Phi_{m_2 g_2}(z_2) \rangle = \prod_{\mathbf{q}} F_{\mathbf{q}} = \prod_{\mathbf{q}} 2 \operatorname{sh} \frac{\hbar\omega_{\mathbf{q}}\beta}{2} \langle e^{-\hbar\omega_{\mathbf{q}}\beta(b_{\mathbf{q}}^{+} b_{\mathbf{q}} + 1/2)} e^{H_1(\mathbf{q})} e^{H_2(\mathbf{q})} \rangle. \quad \text{(AI.2)}$$

Inasmuch as the commutator $[H_2, H_1]$ is a number, the following formula holds

$$e^{H_1 + H_2} = e^{H_1} e^{H_2} e^{1/2\,[H_2, H_1]}. \quad \text{(AI.3)}$$

Using twice the formula (AI.3), we reduce $F_{\mathbf{q}}$ to the form

$$F_{\mathbf{q}} = (1 - e^{-\hbar\omega_{\mathbf{q}}\beta})\, e^{-1/2\,[H_2, H_1] - 1/2\,|\delta_{\mathbf{q}}|^2} \times \mathrm{Sp}\{e^{-\hbar\omega_{\mathbf{q}}\beta b_{\mathbf{q}}^{+} b_{\mathbf{q}}} e^{\delta_{\mathbf{q}} b_{\mathbf{q}}^{+}} e^{-\delta_{\mathbf{q}}^{*} b_{\mathbf{q}}}\}, \quad \text{(AI.4)}$$

where

$$\delta_{\mathbf{q}} = \Delta_{\mathbf{q}}(m_1, m_1 + g_1)\, e^{i\omega_{\mathbf{q}} z_1} + \Delta_{\mathbf{q}}(m_2, m_2 + g_2)\, e^{i\omega_{\mathbf{q}} z_2} \quad \text{(AI.5)}$$

Putting $\exp[-\hbar\omega_{\mathbf{q}}\beta] = \alpha_{\mathbf{q}}$, we write the trace of the curly bracket in (AI.4) in the form

$$\sum_{N,\, n<N} \alpha_{\mathbf{q}}^{N} (-1)^n \frac{|\delta_{\mathbf{q}}|^{2n}}{(n!)^2} N(N-1)\ldots(N-n+1) = \sum_{n=0}^{\infty} (-1)^n \frac{|\delta_{\mathbf{q}}|^{2n}}{(n!)^2} \alpha_{\mathbf{q}}^{n} \frac{d^n}{d\alpha_{\mathbf{q}}^{n}} \sum_{N=0}^{\infty} \alpha_{\mathbf{q}}^{N}. \quad \text{(AI.6)}$$

Taking the sum over N and differentiating it n times, we obtain n in the numerator, after which the series over n adds up to an exponential, that is, (AI.6) turns out equal to $\exp[-|\delta_{\mathbf{q}}|^2 N_{\mathbf{q}}]/(1-\alpha_{\mathbf{q}})$, where $N_{\mathbf{q}}$ is the Planck function. We ultimately get

$$Q_2 = \langle \hat{\Phi}_{m_1 g_1}(z_1)\, \hat{\Phi}_{m_2 g_2}(z_2) \rangle = e^{-S_T(g_1) - S_T(g_2)} \times \exp\left[\frac{1}{N} \sum_{\mathbf{q}} \frac{|\gamma_{\mathbf{q}}|^2}{\operatorname{sh}(\hbar\omega_{\mathbf{q}}\beta/2)} a_{1,2}(\mathbf{G}, \mathbf{g}_1, \mathbf{g}_2) \cos\omega_{\mathbf{q}}\left(z_1 - z_2 + \frac{i\hbar\beta}{2}\right)\right], \quad \text{(AI.7)}$$

where

$$a_{1,2}(\mathbf{G}, \mathbf{g}_1, \mathbf{g}_2) = \tfrac{1}{2}[\cos\mathbf{q}(\mathbf{G} - \mathbf{g}_1) + \cos\mathbf{q}(\mathbf{G} + \mathbf{g}_2) - \cos\mathbf{q}\,\mathbf{G} - \cos\mathbf{q}(\mathbf{G} - \mathbf{g}_1 + \mathbf{g}_2)], \quad \text{(AI.8)}^*$$

$$S_T(\mathbf{g}) = \frac{1}{2N} \sum_{\mathbf{q}} |\gamma_{\mathbf{q}}|^2 \operatorname{cth} \frac{\hbar\omega_{\mathbf{q}}\beta}{2} (1 - \cos\mathbf{q}\mathbf{g}),\ \mathbf{G} = \mathbf{R}_{m_2} - \mathbf{R}_{m_1}.$$

*cth = coth.

In order to calculate $\langle \hat{\Phi}_{m_1 q_1}(z_1) \rangle$, we use (AI.3) and (AI.6). Putting

$$H_1(\mathbf{q}) = b_{\mathbf{q}}^{+} e^{i\omega_{\mathbf{q}} z_1} \delta_{\mathbf{q}},\ H_2(\mathbf{q}) = b_{\mathbf{q}} e^{-i\omega_{\mathbf{q}} z_1} \delta_{\mathbf{q}}^{*},\ \delta_{\mathbf{q}} = \Delta_{\mathbf{q}}(m_1, m_1 + g_1), \quad \text{(AI.9)}$$

we obtain

$$Q_1 = \langle \Phi_{m_1 g_1}(z_1) \rangle = e^{-S_T(g_1)}. \quad \text{(AI.10)}$$

The expression for the case of three points has the form

$$Q_3 = e^{-S_T(g_1) - S_T(g_2) - S_T(g_3)} \times \exp\left\{\frac{1}{N} \sum_{\mathbf{q}} \frac{|\gamma_{\mathbf{q}}|^2}{\operatorname{sh}(\hbar\omega_{\mathbf{q}}\beta/2)} (a_{12} f_{12} + a_{13} f_{13} + a_{23} f_{23})\right\}, \quad \text{(AI.11)}$$

where $f_{ik} = \cos\omega_{\mathbf{q}}(z_i - z_k + i\hbar\beta/2)$, a_{ik} coincides in form with $a_{1,2}$ in (AI.8), but in this case $\mathbf{G} = \mathbf{R}_{m_k} - \mathbf{R}_{m_i}$. The generalization to include the case of an arbitrary number of points $z_1, z_2, \ldots, z_n$ is obvious.

APPENDIX II

THE 1/s RULE FOR FREE INTERSECTIONS

This rule was proved earlier [12] for weak electron-phonon interaction. Let us prove it for our case. If a free intersection exists between z_n and z_{n+1} (see Fig. 2), then in expressions of the type (AI.11) the time arguments with $m_1 \geq n+1$ and $m_2 \leq n$ are not coupled. We assume that

$$l_{nm}(z) = \exp\left[\frac{1}{N} \sum_{\mathbf{q}} \frac{|\gamma_{\mathbf{q}}|^2}{\operatorname{sh}(\hbar\omega_{\mathbf{q}}\beta/2)} a_{nm} f_{nm}(z)\right],$$

and then the expression corresponding to Fig. 2 is written in the form

$$\lim_{\substack{T\to\infty \\ s\to 0}} \int_0^T dz_n \int_{z_n}^{T} d\tau \int_{z_n}^{\tau} dz_1 \ldots \int_{z_n}^{z_{n-2}} dz_{n-1} e^{-s\tau} l_{0,1}(\tau - z_1)\, l_{0,2} \times (\tau - z_2) \ldots l_{0,n}(\tau - z_n) \times l_{1,2}(z_1 - z_2) \ldots l_{1,n}(z_1 - z_n) \ldots l_{n-1,n} \times (z_{n-1} - z_n)\, \varphi(z_n), \quad \text{(AII.1)}$$

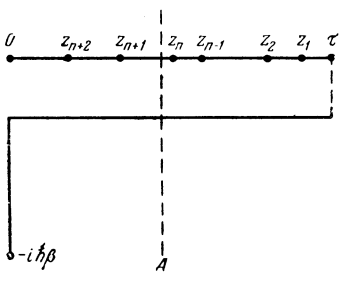

FIG. 2

where $\varphi(z_n)$ is an expression corresponding to the part to the left of the intersection A:

$$\varphi(z_n) = \int_0^{z_n} dz_{n+1} \int_0^{z_{n+1}} dz_{n+2}\, l_{n+1,\,n+2}(z_{n+1} - z_{n+2}) \ldots = \int_0^{z_n} dz_{n+1} F(z_{n+1}). \quad \text{(AII.2)}$$

The expression $F(z_{n+1})$ contains in principle arbitrarily many free intersections, but is independent of z_n. In the Kubo formula it is necessary first to let $T \to \infty$, and then $s \to 0$. Let us make the change of variables

$$\tau = \tau' + z_n, \qquad z_1 = z_1' + z_n, \qquad z_{n-1} = z_{n-1}' + z_n. \quad \text{(AII.3)}$$

Then expression (AII.1) assumes the form

$$\lim_{\substack{T\to\infty\\ s\to 0}} \int_0^T e^{isz_n}\, {}^n\varphi(z_n)\, dz_n \int_0^{T-z_n} e^{-s\tau} d\tau \int_0^{\tau} dz_1 \ldots \int_0^{z_{n-2}} dz_{n-1} l_{0,1}(\tau - z_1) l_{0,2}(\tau - z_2) \ldots l_{0,n}(\tau)\, l_{1,2}(z_1 - z_2) \ldots l_{1,n}(z_1) \ldots l_{n-1,n}(z_{n-1}). \quad \text{(AII.4)}$$

Making the transitions to the limit in the proper sequence, we replace the limit $T - z_n$ in the second integral by T and the entire remaining multiple integral, which does not depend on z_n, we denote by $r^{x(n)}_{2,\mathbf{k}}$ —this is the right vertex of n-th order. Using expression (AII.2) for $\varphi(z_n)$, we integrate with respect to z_n by parts. We ultimately obtain

$$\frac{1}{s}\int_0^{\infty} e^{-sz_{n+1}} F_{\mathbf{pk}}(z_{n+1})\, dz_{n+1}\, r^{x\,(n)}_{2,\,\mathbf{k}}. \quad \text{(AII.5)}$$

If free intersections are still contained in $F(z_{n+1})$, then, using analogous procedure and denoting again the block separated on the right by $W_{\mathbf{p'k}}$, we obtain

$$\int_0^{\infty} e^{-sz} F_{\mathbf{pp'}}(z)\, \frac{1}{s}\, W_{\mathbf{p'k}}\, \frac{1}{s}\, r^{x\,(n)}_{2,\,\mathbf{k}} dz \quad \text{(AII.6)}$$

etc. This property enables us to write down equations (28) and (29).

APPENDIX III

CALCULATIONS OF THE "DEPARTURE PROBABILITY" $W^{(2)}_{\mathbf{k}}$

The quantity $W^{(2)}_{\mathbf{k}}$ taken with the opposite sign is equal to twice the real part of P_4, corresponding to the diagram on Fig. 3. The contribution

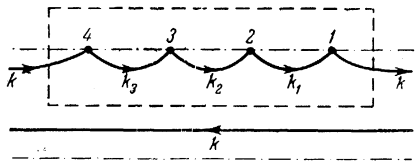

FIG. 3

from diagrams with two overlapping blocks (one in the upper part of the contour, the other under it on the lower part) is omitted, since it is proportional to $\exp[-E_a/kT]$. We put

$$\Phi_i = \Phi_{m_i g_i}(z_i),\ \omega_{kp} = (\varepsilon_k - \varepsilon_p)/\hbar,\ z_4 = 0.$$

then

$$W^{(2)}_{\mathbf{k}} = -2\,\mathrm{Re}\left(\frac{iJ}{\hbar}\right)^4 \frac{1}{N^4} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3} \sum_{m_1m_2m_3m_4} \exp\{i\,[\mathbf{k}(\mathbf{m}_4 - \mathbf{m}_1 - \mathbf{g}_1) + \mathbf{k}_1(\mathbf{m}_1 - \mathbf{m}_2 - \mathbf{g}_2) + \mathbf{k}_2(\mathbf{m}_2 - \mathbf{m}_3 - \mathbf{g}_3) + \mathbf{k}_3(\mathbf{m}_3 - \mathbf{m}_4 - \mathbf{g}_4)]\} \int_0^{\infty} dz_1 \int_0^{z_1} dz_2 \int_0^{z_2} dz_3 \exp\{i\,(\omega_{\mathbf{kk}_1} z_1 + \omega_{\mathbf{k}_1\mathbf{k}_2} z_2 + \omega_{\mathbf{k}_2\mathbf{k}_3} z_3)\}\{\langle\Phi_1\Phi_2\Phi_3\Phi_4\rangle - \langle\Phi_1\Phi_2\rangle\langle\Phi_3\Phi_4\rangle - \langle\Phi_1\rangle\langle\Phi_2\Phi_3\Phi_4\rangle - \ldots + \langle\Phi_2\rangle\langle\Phi_3\rangle\langle\Phi_1\Phi_4\rangle + \ldots - 2\langle\Phi_1\rangle\langle\Phi_2\rangle\langle\Phi_3\rangle\langle\Phi_4\rangle\}. \quad \text{(AIII.1)}$$

The third and following terms in the curly bracket in (AIII.1) are small compared with the first two in a ratio $\exp(-S_T\gamma)$, where $\gamma \gtrsim 1$. We replace quantities of the type $\exp(i\omega_{\mathbf{kk}_1} z_1)$ by unity by virtue of (21a) and (21b). Summing over $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$ we obtain

$$\mathbf{m}_1 - \mathbf{m}_2 = \mathbf{g}_2,\ \mathbf{m}_2 - \mathbf{m}_3 = \mathbf{g}_3,\ \mathbf{m}_3 - \mathbf{m}_4 = \mathbf{g}_4.$$

The largest result that does not depend on $\mathbf{k}$ is obtained under the condition $\mathbf{g}_1 + \mathbf{g}_2 + \mathbf{g}_3 + \mathbf{g}_4 = 0$. The sum over $\mathbf{m}_1$ is equal to N. Let us put $\mathbf{g}_1 = -\mathbf{g}_2 = \mathbf{g}_3 = -\mathbf{g}_4 = \mathbf{g}$. Then

$$a_{1,2} = a_{2,3} = a_{3,4} = a_{\mathbf{q}},\quad a_{1,3} = a_{2,4} = -a_{\mathbf{q}},$$

where $a_{\mathbf{q}} = 1 - \cos \mathbf{q}\cdot\mathbf{g}$ (see AI.8). Making the change of variables $z_1 = t_1 + t_2 + t_3$, $z_2 = t_2 + t_3$, and $z_3 = t_3$ and putting

$$\cos\omega_{\mathbf{q}}(u + i\hbar\beta/2) = f_{\mathbf{q}}(u),$$

we get

$$W^{(2)}_{\mathbf{k}} = -2\,\mathrm{Re}\left(\frac{J}{\hbar}\right)^4 \int_0^{\infty} dt_1 \int_0^{\infty} dt_2 \int_0^{\infty} dt_3 \left\{\exp\left[\frac{1}{N}\sum_{\mathbf{q}} \Gamma_{\mathbf{q}}\,(f_{\mathbf{q}}(t_1) + f_{\mathbf{q}}(t_2) + f_{\mathbf{q}}(t_3) + f_{\mathbf{q}}(t_1 + t_2 + t_3) - f_{\mathbf{q}}(t_1 + t_2) - f_{\mathbf{q}}(t_2 + t_3)) - 4S_T\right] - \exp\left[\frac{1}{N}\sum_{\mathbf{q}} \Gamma_{\mathbf{q}}\,(f_{\mathbf{q}}(t_1) + f_{\mathbf{q}}(t_3)) - 4S_T\right]\right\},$$

$$\Gamma_{\mathbf{q}} = |\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}} \Big/ \mathrm{sh}\,\frac{\hbar\omega_{\mathbf{q}}\beta}{2}. \quad \text{(AIII.2)}$$

Let us put $t_1' = t_1 + i\hbar\beta/2$, and let us break up the integral with respect to t_1' into two parts, with limits from $i\hbar\beta/2$ to 0 and from 0 to ∞. The second part is exponentially small, since both exponents in (AIII.2) have for $t_1' = t_2 = t_3 = 0$ a value

$$\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}\left(\operatorname{cosec}\frac{\hbar\omega_{\mathbf{q}}\beta}{2}+\operatorname{cth}\frac{\hbar\omega_{\mathbf{q}}\beta}{2}\right)-4S_T\approx -E_a/kT,$$

that is, the second part can be discarded. In the first part the essential contribution is near $t_1' = i\hbar\beta/2$, where the exponents vanish. Let us put $t_2' = t_2 + i\hbar\beta/2$ and break up the integral with respect to t_2' into two, with limits from $it\beta/2$ to 0 and from 0 to ∞. We introduce $t_1' = i\hbar\beta/2 - iv_1$ and $t_2' = iv_2$, and transform the first exponent in the first integral to the form

$$\frac{1}{N}\sum_{\mathbf{q}}\Gamma_{\mathbf{q}}\left[\operatorname{ch}\left(\frac{\hbar\omega_{\mathbf{q}}\beta}{2}-\omega_{\mathbf{q}}v_1\right)-\operatorname{ch}\omega_{\mathbf{q}}(v_2-v_1)+\operatorname{ch}\omega_{\mathbf{q}}v_2\right.$$

$$\left.+\sqrt{F_1^2(\mathbf{q})-F_2^2(\mathbf{q})}\cos\omega_{\mathbf{q}}(t_2+iz)\right]-4S_T,$$

$$F_1(\mathbf{q})=\operatorname{ch}\omega_{\mathbf{q}}(v_2-v_1)+\operatorname{ch}\frac{\hbar\omega_{\mathbf{q}}\beta}{2}-\operatorname{ch}\omega_{\mathbf{q}}v_2,$$

$$F_2(\mathbf{q})=\operatorname{sh}\omega_{\mathbf{q}}(v_2-v_1)+\operatorname{sh}\frac{\hbar\omega_{\mathbf{q}}\beta}{2}-\operatorname{sh}\omega_{\mathbf{q}}v_3, \qquad \text{(AIII.3)*}$$

where $\tanh\omega_{\mathbf{q}}z = F_2/F_1$.

Putting $u_3 = t_3 + iz$ and leaving the limits of integration with respect to v_3 from 0 to ∞ (since we are taking the real part), we obtain that near $v_3 = 0$ (the first saddle point) the exponent does not exceed

$$-\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}\operatorname{th}\frac{\hbar\omega_{\mathbf{q}}\beta}{4}\approx -\frac{E_a}{kT},$$

no matter what the value of v_1 or v_2, that is, the contribution is exponentially small.

Thus, the first integral can be discarded. In the second integral (from 0 to ∞ with respect to t_2') we put $t_1' = i\hbar\beta/2 - iv_1$ and expand both exponents (see AIII.2) in powers of v_1, retaining the first term on the expansion. Integrating with respect to v_1 we obtain

$$W^{(2)} = -2\left(\frac{J}{\hbar}\right)^4 e^{-2S_T}\operatorname{Im}\int_0^\infty dt_2'\int_0^\infty dt_3\exp\left[\frac{1}{N}\sum_{\mathbf{q}}\frac{|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}}{\operatorname{sh}(\hbar\omega_{\mathbf{q}}\beta/2)}\right.$$

$$\left.\times\cos\omega_{\mathbf{q}}\left(t_3+\frac{i\hbar\beta}{2}\right)\right]R(t_2', t_3), \qquad \text{(AIII.4)}$$

where

$$R(t_2', t_3)=\left\{\frac{1}{N}\sum_{\mathbf{q}}\Gamma_{\mathbf{q}}\omega_{\mathbf{q}}\left[\operatorname{sh}\frac{\hbar\omega_{\mathbf{q}}\beta}{2}-i(\sin\omega_{\mathbf{q}}(t_2'+t_3)\right.\right.$$

$$\left.\left.-\sin\omega_{\mathbf{q}}t_2')\right]\right\}^{-1}-\left\{\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}\omega_{\mathbf{q}}\right\}^{-1}.$$

*ch = cosh.

Having made the substitution $t_3' = t_3 + i\hbar\beta/2$, we discard the integral with respect to t_3' from 0 to ∞, which contains the small factor $\exp[-E_a/kT]$. In the remaining integral we put $t_3' = i\hbar\beta/2 - iv_3$, in which the essential region is near $v_3 = 0$. We expand the exponent and the factor $R(t_2', t_3)$ in (AIII.3) in powers of v_3, retaining the first term in the exponent, and the first and second terms in $R(t_2', t_3)$. Integrating with respect to v_3, we obtain

$$W^{(2)}=2\left(\frac{J}{\hbar}\right)^4\int_0^\infty dt_2\left\{\frac{1}{N}\sum_{\mathbf{q}}\Gamma_{\mathbf{q}}\cos\omega_{\mathbf{q}}t_2\Big/\left(\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}\omega_{\mathbf{q}}\right)^4\right.$$

$$\left.+2\left(\frac{1}{N}\sum_{\mathbf{q}}\Gamma_{\mathbf{q}}\omega_{\mathbf{q}}^2\cos\omega_{\mathbf{q}}t_2\right)^2\Big/\left(\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}\omega_{\mathbf{q}}\right)^6\right\}. \qquad \text{(AIII.5)}$$

Integrating with respect to t_2, we find that the first term contains a delta function of $\omega_{\mathbf{q}}$ and is equal to zero ($\omega_{\mathbf{q}} \neq 0$). The second term contains the sum $\delta(\omega_{\mathbf{q}_1} + \omega_{\mathbf{q}_2}) + \delta(\omega_{\mathbf{q}_1} - \omega_{\mathbf{q}_2})$. In the isotropic case we obtain finally

$$W^{(2)}=\frac{J^4}{2\pi^3\hbar^4}\int_0^{q_{max}}dq\cdot q^4\frac{|\gamma_{\mathbf{q}}|^4\bar{a}_{\mathbf{q}}^2\omega_{\mathbf{q}}^4}{\operatorname{sh}^2(\hbar\omega_{\mathbf{q}}\beta/2)}\frac{1}{d\omega_{\mathbf{q}}/dq}$$

$$\times\Omega^2\Big/\left(\frac{1}{N}\sum_{\mathbf{q}}|\gamma_{\mathbf{q}}|^2 a_{\mathbf{q}}\omega_{\mathbf{q}}\right)^6\approx\left(\frac{J}{E_a}\right)^4\frac{\bar{\omega}}{\operatorname{sh}^2(\hbar\bar{\omega}\beta/2)}, \qquad \text{(AIII.6)}$$

where Ω is the volume of the elementary cell, $q_{max} \approx 1/a$, and a is the lattice constant.

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