

QUANTUM KINETIC EQUATION IN THE PRESENCE OF MUTUAL ENTRAINMENT OF ELECTRONS AND PHONONS

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A theory is developed for the thermoelectric coefficients in a quantized magnetic field in the case of mutual entrainment of phonons and electrons. A set of kinetic equations for the phonon distribution functions, and the electron density (nondiagonal) matrix f is obtained with the aid of the diagram technique developed in reference 5. It is shown that solution of the integral equations for g and the diagonal part of f should precede the expansion in powers of $(\omega\tau)^{-1} \ll 1$ (ω is the Larmor frequency and τ the electron relaxation time). An arbitrary electron and phonon spectrum is assumed.

THE important role of the deviation of the phonon distribution function from equilibrium in thermoelectric phenomena, i.e., the effect of entrainment of the electrons by phonons (or vice-versa), was reported some time ago.^{1,2} The starting point in these papers was the Boltzmann transport equation for the distribution functions of the phonons and electrons, with allowance for deviations of both systems from equilibrium. However, in the case when the energy is quantized and the distance between discrete levels is commensurate with or greater than $T = \beta^{-1}$ (T is the temperature in energy units), the problem is radically changed. Thus, for example, in a magnetic field the electron velocity component transverse to the field has no diagonal matrix elements, so that to calculate the corresponding current components it is necessary to know the nondiagonal elements of the density matrix, and the problem cannot even be formulated in terms of the customary classical theory.

The purpose of the present investigation was to obtain suitable quantum equations for the entrainment theory. Although we shall be interested in what follows in the thermoelectric tensor, we shall determine the Peltier tensor, which is related to the former by simple symmetry relations³ (the Herring Π -approach²). In investigations of thermoelectric phenomena we deal with entrainment of phonons by electrons acted upon by an electric field. In this case the total heat flow consists of two parts, the ordinary part produced by the electrons, and a part due to the entrainment of the phonons by the electrons and produced by the phonons.

1. SYSTEM OF KINETIC EQUATIONS FOR THE ELECTRONS AND PHONONS IN A QUANTIZING MAGNETIC FIELD

If a crystal with arbitrary electron spectrum $\epsilon(\hat{P})$ is placed in a magnetic field $\mathbf{H} = (0, 0, H)$, we can choose the energy operator in the form $\hat{\epsilon} = \hat{\epsilon}(P_x, (eH/c)(\hat{x}_0 - \hat{x}), \hat{P}_z)$, where $\hat{x}_0 = (c/eH)\hat{P}_y$. The corresponding wave functions are of the form

$$\psi = (L_y L_z)^{-1/2} \exp [(i\hbar)^{-1}(P_y y + P_z z)] \varphi_{nP_z}(x - x_0) \quad (1.1)$$

$L_{y,z}$ are the crystal dimensions in the y, z direction.

The functions φ satisfy the equation

$$\epsilon(\hat{P}_x, - (eH/c)x, P_z) \varphi_{nP_z}(x) = \epsilon_n(P_z) \varphi_{nP_z}(x),$$

where $\epsilon_n(P_z)$ are the eigenvalues of the energy $\hat{\epsilon}$.

If the electrons do not interact with one another, the complete Hamiltonian of the electron-phonon system is of the form

$$\begin{aligned} \hat{\mathcal{H}} &= \hat{\mathcal{H}}_0 + \hat{V}; & \hat{\mathcal{H}}_0 &= \sum_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha} \epsilon_{\alpha} + \sum_{\mathbf{q}} \hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}} \hbar \omega_{\mathbf{q}}, \\ \hat{V} &= \sum_{\mathbf{q}} \sum_{\alpha\alpha'} \sum_j V_{ed}(\mathbf{q}) J_{\alpha\alpha'}(\mathbf{q}) \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha'} \exp[-i\mathbf{q}\mathbf{r}_j/\hbar] \\ &+ \sum_{\mathbf{q}} \sum_{\alpha\alpha'} \{c_{\mathbf{q}} \hat{b}_{\mathbf{q}} J_{\alpha\alpha'}(\mathbf{q}) + c_{\mathbf{q}}^* \hat{b}_{\mathbf{q}}^{\dagger} J_{\alpha'\alpha}(\mathbf{q})\} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha'} + \hat{V}_{ff} + \hat{V}_{fd}. \end{aligned}$$

Here α is the aggregate of the quantum numbers of the electron ($nP_y P_z$), $\omega_{\mathbf{q}}$ is the cyclic frequency of a phonon with momentum \mathbf{q} ; $V_{ed}(\mathbf{q})$ is the Fourier component of the potential of the interaction between the electrons and the defects; \mathbf{r}_j is the coordinate of the j -th defect (the eventual averaging is over \mathbf{r}_j); $J_{\alpha\alpha'}(\mathbf{q})$ is the matrix element of the operator $\exp[i\mathbf{q} \cdot \mathbf{r}/\hbar]$; $c_{\mathbf{q}}$ characterizes the interaction between the electrons and the

phonons, and is proportional to $q^{1/2}$ for small q ; \hat{V}_{ff} and \hat{V}_{fd} are the operators of the phonon-phonon and phonon-defect interactions.

In the presence of a constant and homogeneous electric field \mathbf{E} , the deviation of the density matrix $\hat{\rho}_1$ of the system from the equilibrium matrix $\hat{\rho}_0$ is^{4,5}

$$\hat{\rho}_1 = \hat{\rho}_0 \int_{-\infty}^0 d\tau e^{s\tau} \int_0^\beta d\lambda \int d^3r e^{\mathbf{J}(\mathbf{r}, \tau - i\hbar\lambda) \mathbf{E}}$$

$$= \hat{\rho}_0 \int_{-\infty}^0 d\tau e^{s\tau} \int_0^\beta d\lambda e^{\hat{\mathbf{v}}(\tau - i\hbar\lambda) \mathbf{E}}, \quad s \rightarrow +0,$$

where $\hat{\mathbf{v}}$ and $\hat{\mathbf{J}}(\mathbf{r})$ are the electron-velocity and the particle-flux-density operators.

We introduce, following Konstantinov and Perel',⁴ the single-particle matrices

$$f_{\beta'\beta} = \text{Sp} \hat{\rho}_1 \hat{a}_{\beta'}^+ a_{\beta'} = e\mathbf{E} \sum_{\alpha\alpha'} (\mathbf{v})_{\alpha\alpha'} \int_{-\infty}^0 d\tau e^{s\tau} \int_0^\beta d\lambda$$

$$\times \text{Sp} \left\{ \hat{\rho}_0 T_C \left\{ \exp \left[(i\hbar)^{-1} \int_C \hat{V}(z) dz \right] (\hat{a}_{\beta'}^+ \hat{a}_{\beta'})_{-i\hbar\lambda} (\hat{a}_{\alpha'}^+ \hat{a}_{\alpha'})_{\tau} \right\} \right\},$$

$$g_{\mathbf{q}\mathbf{q}'} = \text{Sp} \hat{\rho}_1 \hat{b}_{\mathbf{q}}^+ \hat{b}_{\mathbf{q}'} = e\mathbf{E} \sum_{\alpha\alpha'} (\mathbf{v})_{\alpha\alpha'} \int_{-\infty}^0 d\tau e^{s\tau} \int_0^\beta d\lambda$$

$$\times \text{Sp} \left\{ \hat{\rho}_0 T_C \left\{ \exp \left[(i\hbar)^{-1} \int_C \hat{V}(z) dz \right] (\hat{b}_{\mathbf{q}}^+ \hat{b}_{\mathbf{q}'})_{-i\hbar\lambda} (\hat{a}_{\alpha'}^+ \hat{a}_{\alpha'})_{\tau} \right\} \right\}. \quad (1.2)$$

The integration contour C is shown in Fig. 1 (from τ via $\tau - i\hbar\lambda$ to $-i\hbar\lambda$, again to $\tau - i\hbar\lambda$, and finally to $\tau - i\hbar\beta$). The symbol T_C denotes the ordering of the Heisenberg operators along the contour C .

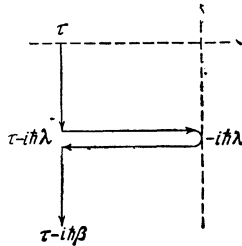


FIG. 1. The contour of integration C .

Konstantinov and Perel'⁴ have obtained an equation which the matrix f satisfies when the phonons are not entrained by electrons ($g = 0$). Using their method, we readily obtain a system of transport equations for the matrices f and g . The general form of this system is most conveniently formulated by using the diagram technique which they introduced, and which we must generalize somewhat because the eigenfunctions of the operator $\hat{\mathcal{K}}_0$ are not plane waves.

We shall represent the vertex corresponding to the electron-phonon interaction and containing

$\hat{a}_{\alpha'}^+ \hat{a}_{\alpha'} \hat{b}_{\mathbf{q}}$ (or $\hat{a}_{\alpha'}^+ \hat{a}_{\alpha'} \hat{b}_{\mathbf{q}}^+$) by means of a point, on the contour C , at which three lines meet: the incoming (α') and the outgoing (α) electron lines (solid) and one incoming ($\hat{b}_{\mathbf{q}}$) or outgoing ($\hat{b}_{\mathbf{q}}^+$) phonon line (dotted). The rules for calculating the diagrams are as follows:

1) To each "regular" electron line (i.e., moving from the earlier to the later point along the contour) there corresponds a factor $(1 - n_{\alpha})$, while to each "irregular" line (moving in the opposite direction) corresponds a factor n_{α} . To each "regular" phonon line corresponds a factor $1 + N_{\mathbf{q}}$, and to each "irregular" one — a factor $N_{\mathbf{q}}$ (n_{α} and $N_{\mathbf{q}}$ are the Fermi and Planck functions, respectively).

2) To each vertex corresponds a factor $c_{\mathbf{q}} J_{\alpha\alpha'}(\mathbf{q})$, if the incoming lines are α' and \mathbf{q} and the outgoing line is α , and a factor $c_{\mathbf{q}}^* J_{\alpha\alpha'}^*$ if the outgoing line is \mathbf{q} . In interactions with defects, incoming "defect" lines with no directions appear at the points. The corresponding factor is

$$V_{ed}(\mathbf{q}) J_{\alpha\alpha'}(\mathbf{q}) \exp[-i\mathbf{q}\mathbf{r}_j/\hbar].$$

3) To each point corresponds a factor $(i\hbar)^{-1}$ on the upper horizontal part of the contour C , a factor $(-i\hbar)^{-1}$ on the lower part, and a factor -1 on the vertical part.

4) Each diagram is multiplied by $(-1)^M$, where M is the number of intersections of the electron lines with each other. The electron lines approach the points only in a manner such that their direction coincides with the direction of motion along the contour near this point (see, for example, Figs. 8b, e, h, below).

5) To each interval between the points nearest in time on a horizontal part (upper or lower) corresponds a factor obtained in the following manner. The interval is cut by a vertical line and the factor $(s + i\omega_{MN})^{-1}$ is set up, where $\omega_{MN} = \hbar^{-1}(E_M - E_N)$, and E_M (or E_N) is the sum of the energies of the lines that cross the cutting line from left to right (or from right to left). If some cutting line crosses only two electron (or two phonon) lines, then the corresponding factor has a value s^{-1} when $\alpha = \alpha'$ (or $\mathbf{q} = \mathbf{q}'$) and diverges as $s \rightarrow 0$. This is the basis of the separation of the irreducible parts of the diagrams (see below).

6) A Laplace transform is taken in the variable $\beta = T^{-1}$ (T is the temperature in energy units):

$$f_{\alpha\alpha'}(\sigma) = \int_0^\infty d\beta e^{-\beta\sigma} f_{\alpha\alpha'}(\beta)$$

and analogously for $g_{\mathbf{q}\mathbf{q}'}$. The quantity β , which enters in $\hat{\rho}_0$, is not regarded as an integration variable. Then to each interval between two near-

est points on the vertical part corresponds a factor $(\sigma + \hbar\omega_{MN})^{-1}$, where E_M (or E_N) is the energy of the lines that cross the horizontal cutting line from top to bottom (or from bottom to top).

In setting up all the possible sections, account is taken also of intervals whose boundary points are τ , $\tau - i\hbar\lambda$, $-i\hbar\lambda$, and $\tau - i\hbar\beta$.

The system of transport equations for f and g can be presented graphically by means of this technique as follows:

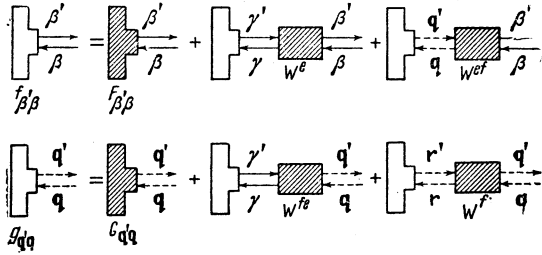


FIG. 2

The unshaded figures with two solid (or dotted) lines $\beta\beta'$ (or $q'q$) on the right represent the matrices $f_{\beta'\beta}$ (or $g_{q'q}$), which are equal to the sum of all the diagrams with all possible numbers and placements of the points on the horizontal and vertical sections, and with two "free" electron ($\beta'\beta$) (or phonon, $q'q$) lines on the right. The shaded figures $F_{\beta'\beta}$ (or $G_{q'q}$) on the right represent the sum of all the diagrams terminated by two electron lines $\beta\beta'$ (or phonon lines $q'q$) and are irreducible in the sense that any vertical cut on the horizontal part of the contour crosses more than two lines. The shaded figures W represent the sum of the diagrams which are irreducible in this sense and which have points only on the horizontal part of the contour. The quantities $F_{\beta'\beta}$ and $G_{q'q}$ do not include the factors $(s + i\omega_{\beta'\beta})^{-1}$ and $(s + i\omega_{q'q})^{-1}$, corresponding to the cutting of two right lines. The W 's do not include the factors corresponding to the cutting of two pairs of lines joined to W from the left and from the right (pair 5), nor the factors corresponding to the pair on the left (pair 1).

The system shown graphically in Fig. 2 has the form

$$\begin{aligned}
 f_{\beta'\beta} &= F_{\beta'\beta} (s + i\omega_{\beta'\beta})^{-1} + \sum_{\gamma\gamma'} W^e_{(\beta'\beta)(\gamma\gamma')} f_{\gamma'\gamma} (s + i\omega_{\beta'\beta})^{-1} \\
 &+ \sum_{q'q} W^{ef}_{(\beta'\beta)(q'q)} g_{q'q} (s + i\omega_{\beta'\beta})^{-1}, \\
 g_{q'q} &= G_{q'q} (s + i\omega_{q'q})^{-1} + \sum_{\beta\beta'} W^{fe}_{(q'q)(\beta\beta')} f_{\beta'\beta} (s + i\omega_{q'q})^{-1} \\
 &+ \sum_{r'r} W^f_{(q'q)(r'r)} g_{r'r} (s + i\omega_{q'q})^{-1}.
 \end{aligned}
 \tag{1.3}$$

The W 's represent the kernels of the "collision integrals" and have the meaning of transition probabilities. Our problem reduces thus to the calculation of F , G , and W . We require an accuracy to V^2 , so that the corresponding diagrams will have two vertices.

Figures 3–6 show typical diagrams for W . The diagrams W^{fe} are constructed similar to W^{ef} , and therefore only one is shown. In the diagonal components of W ($W^e_{(\beta\beta)(\gamma\gamma)}$, $W^{ef}_{(\beta\beta)(q'q)}$ etc.) the principal values of the integrals involved cancel out and only the delta functions remain. As regards the nondiagonal elements of W , we shall see later on that in the approximation of interest to us (the lowest approximation that does not vanish in V) we can neglect the principal values in these elements.

The diagrams contained in F and G , which have vertices only on the vertical parts of the contour, do not contain irreversibilities (the parameter s) and correspond to renormalization of the spectrum of the system as a result of the interaction V . Further, in analogy with the statements made concerning W , we shall discard in F and G the principal values of the integrals and retain only the delta functions, since F and G represent

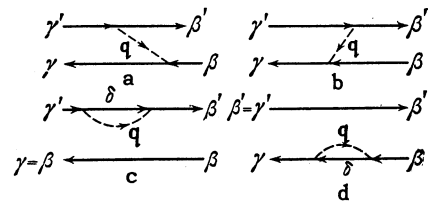


FIG. 3. Diagrams for W^e .

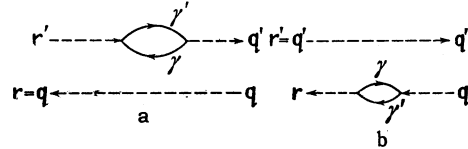


FIG. 4. Diagrams for W^f .

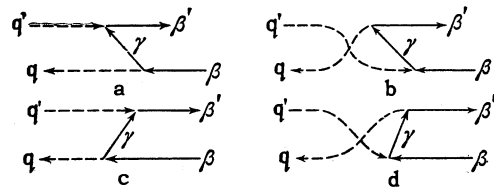


FIG. 5. Diagrams for W^{ef} .

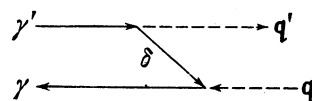


FIG. 6. Diagram for W^{fe} .

an inhomogeneity in the system of transport equations, and the discarded terms would yield only small additive corrections which are of no interest to us. Since diagrams in F and G with both vertices on the horizontal part of the contour are reducible, the only remaining diagrams are those indicated in Figs. 7 – 9, in which one point is on the vertical and one on the horizontal part of the contour. Figure 7 shows the free term F in the absence of interaction. The sum of the diagrams for F and G must be multiplied by $e(\mathbf{E} \cdot \mathbf{v})_{\alpha\alpha'}$ and summed over all α and α' .

We have included in the figures only the diagrams necessary to understand the method. To all the diagrams indicated for W, F, and G we must add those obtained by transferring the points from the upper horizontal section to the lower one (or vice versa). With this, it is necessary to take into account, in accordance with the rules indicated above, the change in the sign, the change in the number of intersections, and the change in the "regularity" of the incoming (or outgoing) lines to the right of the point. The "regularity" of the lines to the left does not change in such a transfer. As a result, the diagrams in which all the lines arrive at a point on the horizontal part from the

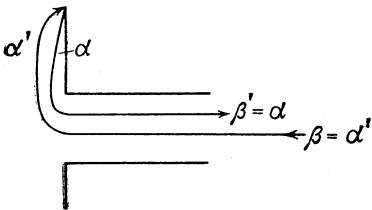


FIG. 7. Diagram for F without interaction.

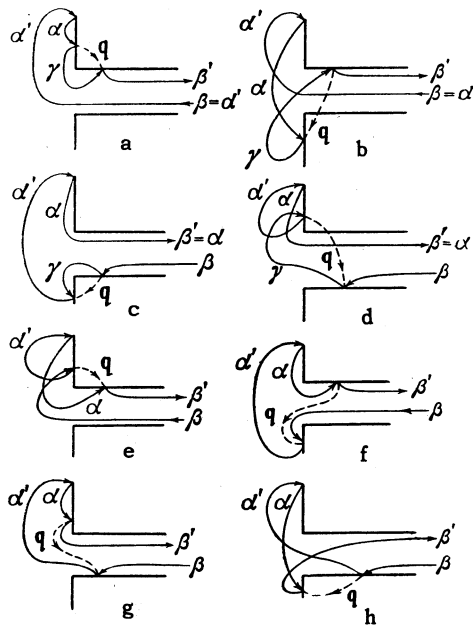


FIG. 8. Diagrams for F in the V^2 approximation.

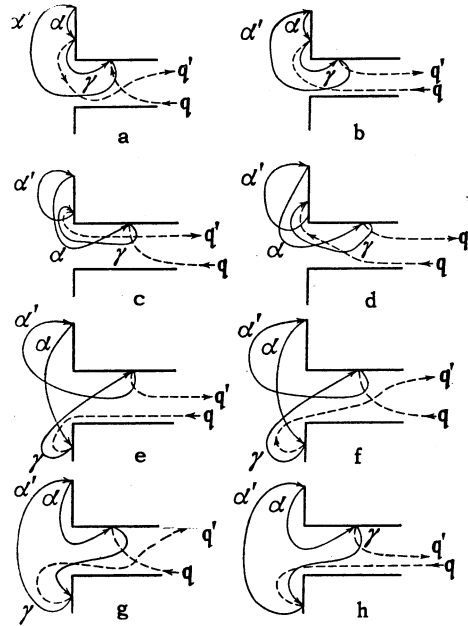


FIG. 9. Diagrams for G in the V^2 approximation.

left can be disregarded. Further, it is necessary to sum over the two possible directions of the phonon lines with dummy indices. It goes without saying that it is necessary to sum over the dummy indices in all diagrams.

Using the general form of the wave functions (1.1), and also the fact that $v_{\alpha\alpha'}$ is diagonal over \mathbf{P} [$\mathbf{P} = (P_y, P_z)$], it is easy to conclude that F is diagonal over \mathbf{P} and is independent of P_y while G is diagonal over \mathbf{q} . Further, it is easy to show that

$$W_{(PP)(P'P')}^e \sim \delta_{P'P}, \quad W_{(P'P)(qq)}^{ef} \sim \delta_{P'P},$$

$$\int dP_y W_{(q'q)(PP)}^{fe} \sim \delta_{q'q}, \quad W_{(qq)(r'r)}^f \sim \delta_{r'r}.$$

In addition, all the W are independent of P_y .

It follows from the properties of W that the matrix elements f, diagonal over \mathbf{P} , and the diagonal matrix elements g, are not "coupled" in the equations with matrix elements f and g which are not diagonal over \mathbf{P} (or \mathbf{q}). But then it follows from the aforementioned properties of F and G that $f_{(n\mathbf{P})(n'\mathbf{P}')} \sim \delta_{\mathbf{P}\mathbf{P}'}$ and $g_{\mathbf{q}'\mathbf{q}} \sim \delta_{\mathbf{q}'\mathbf{q}}$. Since neither F nor W depend on P_y , f is also independent of P_y , and we can introduce $f_{(n\mathbf{P})(n'\mathbf{P}')} = f_{nn'}(P_z)$. The foregoing properties are obviously the consequence of the spatial homogeneity of the problem, and take place only in the absence of spatial dispersion.

Calculating W with allowance for the approximations listed above, we obtain

$$\begin{aligned}
W_{(\beta'\beta)(\alpha'\alpha)}^e &= \pi\hbar^{-2} \sum_{\mathbf{q}} |c_{\mathbf{q}}|^2 J_{\alpha'\beta'}^* J_{\alpha\beta} \{ \delta(\omega_{\beta'\alpha} + \omega_{\mathbf{q}}) \\
&\times [(1 - n_{\beta'}) (N_{\mathbf{q}} + 1) + n_{\beta'} N_{\mathbf{q}}] + \delta(\omega_{\beta'\alpha} - \omega_{\mathbf{q}}) [(1 - n_{\beta'}) N_{\mathbf{q}} \\
&+ n_{\beta'} (N_{\mathbf{q}} + 1)] + \delta(\omega_{\beta\alpha'} + \omega_{\mathbf{q}}) [(1 - n_{\beta}) (N_{\mathbf{q}} + 1) + n_{\beta} N_{\mathbf{q}}] \\
&+ \delta(\omega_{\beta\alpha'} - \omega_{\mathbf{q}}) [(1 - n_{\beta}) N_{\mathbf{q}} + n_{\beta} (N_{\mathbf{q}} + 1)] \} \\
&- \pi\hbar^{-2} \delta_{\beta\alpha} \sum_{\mathbf{q}} \sum_{\gamma} |c_{\mathbf{q}}|^2 J_{\alpha'\gamma}^* J_{\beta\gamma} \{ \delta(\omega_{\beta\gamma} - \omega_{\mathbf{q}}) \\
&\times [(1 - n_{\gamma}) (N_{\mathbf{q}} + 1) + n_{\gamma} N_{\mathbf{q}}] \\
&+ \delta(\omega_{\beta\gamma} + \omega_{\mathbf{q}}) [(1 - n_{\gamma}) N_{\mathbf{q}} + n_{\gamma} (N_{\mathbf{q}} + 1)] \} \\
&- \pi\hbar^{-2} \delta_{\beta'\alpha'} \sum_{\mathbf{q}} \sum_{\gamma} |c_{\mathbf{q}}|^2 J_{\alpha\gamma} J_{\beta'\gamma}^* \{ \delta(\omega_{\beta'\gamma} - \omega_{\mathbf{q}}) \\
&\times [(1 - n_{\gamma}) (N_{\mathbf{q}} + 1) + n_{\gamma} N_{\mathbf{q}}] \\
&+ \delta(\omega_{\beta'\gamma} + \omega_{\mathbf{q}}) [(1 - n_{\gamma}) N_{\mathbf{q}} + n_{\gamma} (N_{\mathbf{q}} + 1)] \}, \quad (1.4a)
\end{aligned}$$

$$\begin{aligned}
W_{(\beta'\beta)(\mathbf{q}\mathbf{q})}^{ef} &= \pi\hbar^{-2} |c_{\mathbf{q}}|^2 \sum_{\gamma} \{ (n_{\gamma} - n_{\beta}) [\delta(\omega_{\gamma\beta} + \omega_{\mathbf{q}}) J_{\beta'\gamma} J_{\beta\gamma}^* \\
&+ \delta(\omega_{\gamma\beta} - \omega_{\mathbf{q}}) J_{\gamma\beta} J_{\beta'\gamma}^*] + (n_{\gamma} - n_{\beta'}) [\delta(\omega_{\gamma\beta'} + \omega_{\mathbf{q}}) J_{\beta'\gamma} J_{\beta\gamma}^* \\
&+ \delta(\omega_{\gamma\beta'} - \omega_{\mathbf{q}}) J_{\gamma\beta'} J_{\beta'\gamma}^*] \}, \quad (1.4b)
\end{aligned}$$

$$\begin{aligned}
W_{(\mathbf{q}\mathbf{q})(\beta'\beta)}^{fe} &= \pi\hbar^{-2} |c_{\mathbf{q}}|^2 \sum_{\gamma} \{ J_{\beta\gamma} J_{\beta'\gamma}^* [(1 + N_{\mathbf{q}}) (1 - n_{\gamma}) \\
&+ N_{\mathbf{q}} n_{\gamma}] \delta(\omega_{\beta\gamma} - \omega_{\mathbf{q}}) \\
&- J_{\gamma\beta} J_{\gamma\beta}^* [(1 - n_{\gamma}) N_{\mathbf{q}} + n_{\gamma} (N_{\mathbf{q}} + 1)] \delta(\omega_{\beta'\gamma} + \omega_{\mathbf{q}}) \\
&+ J_{\beta\gamma} J_{\beta'\gamma}^* [(1 + N_{\mathbf{q}}) (1 - n_{\gamma}) + N_{\mathbf{q}} n_{\gamma}] \delta(\omega_{\beta\gamma} - \omega_{\mathbf{q}}) \\
&- J_{\gamma\beta} J_{\gamma\beta}^* [(1 - n_{\gamma}) N_{\mathbf{q}} + n_{\gamma} (N_{\mathbf{q}} + 1)] \delta(\omega_{\beta\gamma} + \omega_{\mathbf{q}}) \}. \quad (1.4c)
\end{aligned}$$

We do not write out W^f , since this operator is obtained by linearizing the usual integrals for collisions between phonons and equilibrium electrons, for collisions between phonons, or collisions with defects. As regards the operator of collisions between the electrons and the defects, this operator is obtained in the Born approximation from the one written out above by discarding the factors $N_{\mathbf{q}}$ or $N_{\mathbf{q}} + 1$ and the addend $\omega_{\mathbf{q}}$ from the arguments of the delta function, and replacing $|c_{\mathbf{q}}|^2$ by $|V_{ed}(\mathbf{q})|^2 N_d$ (N_d is the number of defects).

In the longitudinal case, when $\mathbf{E} = E_z$ and $(\mathbf{E} \cdot \mathbf{v})_{\alpha\alpha'} \sim \delta_{\alpha\alpha'}$ so that $F_{\beta'\beta}$ which is diagonal in the zeroth approximation (sufficient for this case) of the interaction, we obtain, after taking the inverse Laplace transform in the variable σ , a system of transport equations of the ordinary form for diagonal matrices (occupation numbers) f and g .*

In the transverse case (for example $\mathbf{E} = E_x$), if the motion of the electron along the x axis is finite (i.e., we do not consider open trajectories⁶), then $(\mathbf{E} \cdot \mathbf{v})_{\alpha\alpha'} = 0$.

*Subject to the condition $\omega\tau \gg 1$ (in the notation of Sec. 2).

It is convenient to present F in the form

$$F_{\beta'\beta} = F_{\beta'\beta}^0 - \sum_{\gamma\gamma'} W_{(\beta'\beta)(\gamma'\gamma)}^e F_{\gamma'\gamma}^0 (i\omega_{\gamma'\gamma})^{-1} + \Delta F_{\beta'\beta}; \quad (1.5)$$

$$F_{\beta'\beta}^0 = eE v_{\beta'\beta}^{(x)} (\hbar\omega_{\beta'\beta})^{-1} (n_{\beta} - n_{\beta'}), \quad (1.6a)$$

$$\begin{aligned}
\Delta F_{\beta'\beta} &= -\pi eE (i\hbar^2 T)^{-1} \sum_{\gamma'\gamma\mathbf{q}} |c_{\mathbf{q}}|^2 N_{\mathbf{q}} \{ v_{\gamma'\beta}^{(x)} \omega_{\gamma'\beta}^{-1} \\
&\times [J_{\gamma'\gamma}^* J_{\beta\gamma} \delta(\omega_{\gamma\beta} + \omega_{\mathbf{q}}) n_{\gamma} (1 - n_{\beta}) \\
&+ J_{\gamma'\beta}^* J_{\gamma\gamma'} \delta(\omega_{\gamma\beta} - \omega_{\mathbf{q}}) n_{\beta} (1 - n_{\gamma})] \\
&+ v_{\beta'\gamma}^{(x)} \omega_{\beta'\gamma}^{-1} [J_{\beta'\gamma}^* J_{\gamma\gamma'} \delta(\omega_{\gamma'\beta'} + \omega_{\mathbf{q}}) n_{\gamma'} (1 - n_{\beta'}) \\
&+ J_{\gamma'\gamma}^* J_{\gamma'\beta} \delta(\omega_{\gamma'\beta'} - \omega_{\mathbf{q}}) n_{\beta'} (1 - n_{\gamma'})] \\
&- v_{\gamma'\gamma}^{(x)} \omega_{\gamma'\gamma}^{-1} [J_{\beta\gamma}^* J_{\beta'\gamma'} \delta(\omega_{\gamma\beta} + \omega_{\mathbf{q}}) n_{\gamma} (1 - n_{\beta}) \\
&+ J_{\gamma'\beta}^* J_{\gamma\beta} \delta(\omega_{\gamma\beta} - \omega_{\mathbf{q}}) n_{\beta} (1 - n_{\gamma'}) \\
&+ J_{\beta\gamma}^* J_{\beta'\gamma'} \delta(\omega_{\gamma\beta'} + \omega_{\mathbf{q}}) n_{\gamma} (1 - n_{\beta'}) \\
&+ J_{\gamma'\beta}^* J_{\gamma\beta} \delta(\omega_{\gamma\beta'} - \omega_{\mathbf{q}}) n_{\beta'} (1 - n_{\gamma}) \}. \quad (1.6b)
\end{aligned}$$

Noting that

$$(i\omega_{\gamma'\beta})^{-1} v_{\gamma'\beta}^{(x)} = x_{\gamma'\beta} \quad (\gamma' \neq \beta),$$

$$\begin{aligned}
\sum_{\gamma' \neq \beta} x_{\gamma'\beta} J_{\gamma'\gamma}^* (\mathbf{q}) &= \sum_{\gamma' \neq \beta} x_{\gamma'\beta} J_{\gamma'\gamma} (-\mathbf{q}) \\
&= \sum_{\gamma'} J_{\gamma'\gamma} (-\mathbf{q}) x_{\gamma'\beta} - x_{\beta\beta} J_{\beta\beta} (-\mathbf{q}) \\
&= (e^{-iq\tau/\hbar} x)_{\gamma\beta} - x_{\beta\beta} J_{\beta\beta}^* (\mathbf{q}),
\end{aligned}$$

and carrying out analogous transformations in the remaining terms of (1.6), we obtain, recognizing that the operators $\exp(i\mathbf{q} \cdot \mathbf{r})$ and \mathbf{x} commute, and also that $J_{\gamma\gamma'}(-\mathbf{q}) = J_{\gamma'\gamma}^*(\mathbf{q})$ and $\omega(\mathbf{q}) = \omega(-\mathbf{q})$,

$$\begin{aligned}
\Delta F_{\beta'\beta} &= \pi eE (\hbar^2 T)^{-1} \sum_{\gamma\mathbf{q}} |c_{\mathbf{q}}|^2 N_{\mathbf{q}} J_{\beta\gamma}^* J_{\beta'\gamma} \\
&\times \{ X_{\beta\gamma} [\delta(\omega_{\gamma\beta} + \omega_{\mathbf{q}}) n_{\gamma} (1 - n_{\beta}) \\
&+ \delta(\omega_{\gamma\beta} - \omega_{\mathbf{q}}) n_{\beta} (1 - n_{\gamma})] \\
&+ X_{\beta'\gamma} [\delta(\omega_{\gamma\beta'} + \omega_{\mathbf{q}}) n_{\gamma} (1 - n_{\beta'}) \\
&+ \delta(\omega_{\gamma\beta'} - \omega_{\mathbf{q}}) n_{\beta'} (1 - n_{\gamma'}) \}. \quad (1.7)
\end{aligned}$$

Here $X_{\alpha\beta} = x_{\alpha\alpha} - x_{\beta\beta}$.

Analogously we obtain

$$\begin{aligned}
G_{\mathbf{q}} &= -\sum_{\beta\beta'} W_{(\mathbf{q}\mathbf{q})(\beta'\beta)}^{fe} F_{\beta'\beta}^0 (i\omega_{\beta'\beta})^{-1} \\
&+ |c_{\mathbf{q}}|^2 2\pi eE (\hbar^2 T)^{-1} \sum_{\beta\beta'} N_{\mathbf{q}} n_{\beta} (1 - n_{\beta'}) \\
&\times \delta(\omega_{\beta'\beta} - \omega_{\mathbf{q}}) |J_{\beta'\beta}|^2 X_{\beta\beta'}. \quad (1.8)
\end{aligned}$$

We note that the matrices f and g are Hermitian, because

$$\begin{aligned}
W_{(\beta'\beta)(\gamma'\gamma)}^e &= W_{(\beta\beta')(\gamma\gamma')}^{e*}, & W_{(\beta'\beta)(\mathbf{q}\mathbf{q})}^{ef} &= W_{(\beta\beta')(\mathbf{q}\mathbf{q})}^{ef*}, \\
W_{(\mathbf{q}\mathbf{q})(\beta'\beta)}^{fe} &= W_{(\mathbf{q}\mathbf{q})(\beta\beta')}^{fe*}, & W_{(\mathbf{q}\mathbf{q})(\mathbf{r}\mathbf{r})}^f &= W_{(\mathbf{q}\mathbf{q})(\mathbf{r}\mathbf{r})}^{f*}, \\
F_{\beta'\beta} &= F_{\beta\beta'}^*, & G_{\mathbf{q}} &= G_{\mathbf{q}}^*.
\end{aligned}$$

2. CASE OF STRONG ($\omega\tau \gg 1$) TRANSVERSE MAGNETIC FIELD. DERIVATION OF A SYSTEM OF EQUATIONS FOR THE DIAGONAL PARTS OF THE MATRICES f AND g

In the case of a strong magnetic field transverse to the electric field, we can expand the non-diagonal part of the matrix f in powers of $(\omega\tau)^{-1} \ll 1$, where ω is the Larmor frequency of the electrons and τ is their relaxation time. This corresponds to assuming W and ΔF in (1.5) to be small. In this case it is sufficient to calculate the values of $W \sim \tau^{-1}$ in the lower approximation in V (in the case of scattering by impurities — in the lower approximation in the concentration).

Diagrams of higher order contain parameters of the type $\hbar(\tau T)^{-1}$ or $\hbar(\tau\xi)^{-1}$ (ξ is the chemical potential of the electrons), which are small in most cases, and can be disregarded here. As regards F (or G), the addition of points on the horizontal parts of the corresponding diagrams obviously yields corrections of the same type as due to the addition of points in the diagrams of W . The addition of points on the vertical parts corresponds, on the other hand, to thermodynamic perturbation theory (i.e., to the expansion of the operator $\hat{\rho}_0 = Z^{-1} \exp[-\beta(\hat{\mathcal{H}}_0 + \hat{V} - \xi N)]$ in powers of \hat{V}), and therefore cannot lead to either appearance or disappearance of currents, but can only give rise to corrections to these quantities, which are of no interest to us. Therefore, at least for the calculation of F (or G), it is sufficient to consider only diagrams with a single point on the vertical part, and in our case also with a single point on the horizontal portion, as we have done in Sec. 1.

We shall now show that before we expand in powers of W and ΔF [i.e., in $(\omega\tau)^{-1}$], we must solve the system of integral equations for the matrix g and the diagonal part of the matrix f . We introduce the symbol f^d and f^n for the diagonal and non-diagonal parts of f , and analogously for other matrices. Then the system (1.3) can be represented in the form

$$\begin{aligned} i\omega_{\beta'\beta} f_{\beta'\beta}^{(n)} &= F_{\beta'\beta}^{(n)} - \left(\sum_{\gamma'\gamma} W_{(\beta'\beta)(\gamma'\gamma)}^e F_{\gamma'\gamma}^{(n)} (i\omega_{\gamma'\gamma})^{-1} \right)^{(n)} + \Delta F_{\beta'\beta}^{(n)} \\ &+ \left(\sum_{\gamma'\gamma} W_{(\beta'\beta)(\gamma'\gamma)}^e f_{\gamma'\gamma}^{(n)} \right)^{(n)} + \left(\sum_{\gamma} W_{(\beta'\beta)(\gamma\gamma)}^e f_{\gamma\gamma}^d \right)^{(n)} \\ &+ \left(\sum_q W_{(\beta'\beta)(qq)}^{ef} g_q \right)^{(n)}, \end{aligned} \quad (2.1a)$$

$$\begin{aligned} - \sum_{\gamma'\gamma} W_{(\beta\beta)(\gamma'\gamma)}^e F_{\gamma'\gamma}^{(n)} (i\omega_{\gamma'\gamma})^{-1} + \Delta F_{\beta\beta} + \sum_{\gamma'\gamma} W_{(\beta\beta)(\gamma'\gamma)}^e f_{\gamma'\gamma}^{(n)} \\ + \sum_{\gamma} W_{(\beta\beta)(\gamma\gamma)}^e f_{\gamma\gamma}^d + \sum_q W_{(\beta\beta)(qq)}^{ef} g_q = 0, \end{aligned} \quad (2.1b)$$

$$\begin{aligned} - \sum_{\gamma'\gamma} W_{(qq)(\gamma'\gamma)}^e F_{\gamma'\gamma}^{(n)} (i\omega_{\gamma'\gamma})^{-1} + \Delta G_q + \sum_{\beta'\beta} W_{(qq)(\beta'\beta)}^e f_{\beta'\beta}^{(n)} \\ + \sum_{\beta} W_{(qq)(\beta\beta)}^e f_{\beta\beta}^d + \sum_r W_{(qq)(rr)}^e g_r = 0. \end{aligned} \quad (2.1c)$$

In the zeroth approximation $f_{\beta'\beta}^{(0(n))} = F_{\beta'\beta}^{(0(n))} (i\omega_{\beta'\beta})^{-1}$, and f^{0d} , and g^0 remain indeterminate. To determine these we must substitute in (2.1b) and (2.1c) the values of $f^{(0(n))}$. We then obtain a system of integral equations for f^{0d} and g^0 , which is more convenient to write down by introducing the quantities φ_α and γ_q , related to f^d and g by the equations

$$f_{\alpha\alpha}^d = -(\partial n_\alpha / \partial \varepsilon_\alpha) \varphi_\alpha, \quad g_q = -[\partial N_q / \partial (\hbar\omega_q)] \gamma_q. \quad (2.2)$$

φ_α^0 and γ_q^0 satisfy the system of equations

$$\begin{aligned} 2\pi (\hbar^2 T)^{-1} \sum_{\alpha q} |c_q|^2 |J_{\beta\alpha}|^2 [\delta(\omega_{\alpha\beta} + \omega_q) n_\alpha (1 - n_\beta) \\ + \delta(\omega_{\alpha\beta} - \omega_q) n_\beta (1 - n_\alpha)] \\ \times [eEX_{\beta\alpha} - (\varphi_\beta^0 - \varphi_\alpha^0) + \gamma_q^0] N_q + 2\pi (\hbar^2 T)^{-1} \\ \times \sum_{\alpha q} |V_{ed}(\mathbf{q})|^2 |J_{\beta\alpha}|^2 \delta(\omega_{\alpha\beta}) n_\beta (1 - n_\beta) \\ \times [eEX_{\beta\alpha} - (\varphi_\beta^0 - \varphi_\alpha^0)] N_d = 0; \\ 2\pi (\hbar^2 T)^{-1} \sum_{\alpha\beta} |c_q|^2 n_\alpha (1 - n_\beta) N_q \delta(\omega_{\beta\alpha} - \omega_q) |J_{\beta\alpha}|^2 \\ \times [eEX_{\alpha\beta} - (\varphi_\alpha^0 - \varphi_\beta^0) - \gamma_q^0] + \hat{W}_{ff}(\gamma_q) + \hat{W}_{fd}(\gamma_q) = 0. \end{aligned} \quad (2.3)$$

Here W_{ff} and W_{fd} are the operators of the phonon-phonon and phonon-defect collisions, respectively.

Substituting the solution of these equations into (2.1a) in the first approximation, we obtain for $f^{1(n)}$

$$\begin{aligned} f_{\beta'\beta}^{1(n)} &= \pi (i\omega_{\beta'\beta} \hbar^2 T)^{-1} \sum_{\alpha q} J_{\beta\alpha}^* J_{\beta'\alpha} \{ |c_q|^2 N_q \{ [\delta(\omega_{\alpha\beta} + \omega_q) n_\alpha \\ \times (1 - n_\beta) + \delta(\omega_{\alpha\beta} - \omega_q) n_\beta (1 - n_\alpha)] [eEX_{\beta\alpha} - (\varphi_\beta^0 - \varphi_\alpha^0) \\ + \gamma_q^0] + [\delta(\omega_{\alpha\beta'} + \omega_q) n_\alpha (1 - n_\beta) \\ + \delta(\omega_{\alpha\beta'} - \omega_q) n_{\beta'} (1 - n_\alpha)] [eEX_{\beta'\alpha} - (\varphi_{\beta'}^0 - \varphi_\alpha^0) \\ + \gamma_q^0] \} + |V_{ed}(\mathbf{q})|^2 N_d \{ \delta(\omega_{\alpha\beta}) n_\beta (1 - n_\beta) \\ \times [eEX_{\beta\alpha} - (\varphi_\beta^0 - \varphi_\alpha^0)] + \delta(\omega_{\alpha\beta'}) n_{\beta'} (1 - n_{\beta'}) \\ \times [eEX_{\beta'\alpha} - (\varphi_{\beta'}^0 - \varphi_\alpha^0)] \} \}. \end{aligned} \quad (2.4)$$

The resultant values $f^{1(n)}$ are again inserted in (2.1b) and (2.1c), after which we obtain f^d and g in the next approximation. This process of successive approximation corresponds to expansion in powers of the parameter $(\omega\tau)^{-1}$.

It is easy to see that the equations for f^d and g in the different approximations differ only in the form of the inhomogeneity. We note that the non-

diagonal elements of W (i.e., $W_{(\beta'\beta)(\gamma'\gamma)}^e$, in which the equations $\beta' = \beta$ and $\gamma' = \gamma$ are not satisfied simultaneously, and analogously for W^{ef} and W^{fe}) enter into the integral equations only as inhomogeneities, and we can therefore discard in these quantities the principal values of the integrals, as in the case of F (or G). The same pertains also to the terms with W in (2.4).

The integral equations (2.3) have the form of ordinary transport equations, and the singularities of the problem are due only to the inhomogeneity. Since the wave functions (1.1) depend on the argument $(c/eH)p_y$, where $p_y = P_y - (eH/c)x$, the matrix elements are $x_{\alpha\alpha} = (c/eH)[(P_y)_{\alpha\alpha} - (p_y)_{\alpha\alpha}]$. The quantity $(p_y)_{\alpha\alpha}$ obviously has the meaning of the average value of the momentum p_y on the quasi-classical orbit $\epsilon(\mathbf{p}) = \text{const}$, $p_z = \text{const}$.

If the crystal has mirror symmetry with respect to the xz plane, then the first equation in (2.3) is satisfied by $\varphi_\alpha = u_e(p_y)_{\alpha\alpha}$, where $u_e = -cE/H$ is the electron drift (Hall) velocity, for in this case $(P_y)_{\beta\beta} - (P_y)_{\alpha\alpha} = q_y$, $\gamma(q_y) = -\gamma(-q_y)$. Then in the second equation in (2.3) the term corresponding to the phonon-electron interaction has the form $[u_e q_y - \gamma(\mathbf{q})] \tau_{fe}^{-1}$, corresponding precisely to the phenomenological theory if $\gamma(\mathbf{q}) = u_f q_y$, where u_f has the meaning of the phonon drift velocity. (Here τ_{fe} is the ordinary relaxation time of phonons on equilibrium electrons).

In the case of an isotropic spectrum $(p_y)_{\alpha\alpha} = 0$ and therefore $\varphi_\alpha = 0$. In the particular case of an isotropic quadratic spectrum, neglecting the entrainment of electrons by the phonons, we obtain the results of Adams and Holstein⁷ for $f_{\alpha\alpha'}^{in}$, and our matrix $n_\alpha \delta_{\alpha\alpha'} + f_{\alpha\alpha'}^{on}$ is identical with the matrix $\rho(0)$ of this paper, written in the \mathcal{H}_0 representation.

In the absence of defects (and also in the absence of Umklapp processes) the system (2.3) is satisfied by the values $\varphi_\alpha = u_e(p_y)_{\alpha\alpha}$ and $\gamma(\mathbf{q}) = u_e q_y$, corresponding to an over-all drift of the electron-phonon system with a velocity u_e [the term $W^{ff}(\gamma_q)$ also vanishes in this case]. We now get in (2.4) $f^{1(n)} = 0$, which is understandable, for in the absence of scattering by the defects the total momentum of the system is conserved, corresponding formally to $\tau = \infty$.

We also note the following. Let the phonons be in equilibrium. Then the equation for φ_α has the form $\hat{L}\chi = 0$, where $\chi_\alpha = eEx_{\alpha\alpha} - \varphi_\alpha$. Obviously the solution $\chi_\alpha \equiv 0$ (from which follows $f_{\beta'\beta}^{1(n)} \equiv 0$) corresponds merely to a Boltzmann charge distribution in a potential electric field, not accompanied

by an irreversible current. The nontrivial solution for χ is determined, in view of the homogeneity of the equation, accurate to a constant factor, which can be defined in such a manner as to make $\varphi_\alpha = eEx_{\alpha\alpha} - \chi_\alpha$ independent of P_y (which is possible, as was already noted in Sec. 1). With this, since $f_{\alpha\alpha'}$ is diagonal over P_z and is independent of P_y , and the wave functions have the form (1.1), the charge density

$$e \sum_{\alpha\alpha'} \hat{f}_{\alpha\alpha'} \Psi_{\alpha'}^*(x) \Psi_\alpha(x) = \sum_{nn'P_z} \hat{f}_{nn'}(P_z) \sum_{P_y} \Psi_{n'P_z}^*(x - x_0) \Psi_{nP_z}(x - x_0)$$

is independent of x .

Knowing the functions φ and γ in the zeroth approximation, we can determine $f^{1(n)}$ and consequently, the component of the current density along the electric field

$$j^{(x)} = \frac{2e}{V} \sum_{\beta'\beta} v_{\beta'\beta}^{(x)} f_{\beta'\beta}^{1(n)}$$

(V is the volume of the sample and the factor 2 corresponds to the two spin orientations). After transformations analogous to those used to transform (1.6) into (1.7), we obtain

$$j^{(x)} = \frac{1}{V} \frac{4\pi e}{\hbar^2 T} \sum_{\alpha\beta q} |J_{\beta\alpha}|^2 \{ |c_q|^2 N_q n_\alpha (1 - n_\beta) \delta(\omega_{\alpha\beta} + \omega_q) \times X_{\beta\alpha} [eEX_{\beta\alpha} - (\varphi_\beta^0 - \varphi_\alpha^0) + \gamma^0(\mathbf{q})] + |V_{ed}(\mathbf{q})|^2 N_d n_\beta (1 - n_\beta) \delta(\omega_{\alpha\beta}) \times X_{\beta\alpha} [eEX_{\beta\alpha} - (\varphi_\beta^0 - \varphi_\alpha^0)] \}. \quad (2.5)$$

The formula obtained by Adams and Holstein⁷ is a particular case of this formula.

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