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THE THEORY OF POLARONS

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THE THEORY OF POLARONS

S. I. Pekar

Summary:

This paper considers the polaron in an ionic crystal; the oscillations of the ions are treated quantum-mechanically. The effective mass of the polaron in its forward motion is calculated; obtained are the waves of the polaron states that (waves) possess a continuous energy spectrum. The author discusses the scattering of polaron waves by optical oscillations of ions and calculates the corresponding free flight and mobility (motility) of the polaron. The mobility as calculated (only as of its order of magnitude) coincides with the measured mobilities of current carriers in semiconductors.

Section 1. Setting up the problem; Approximate calculation of the energy.

Let us assume, even as in previous works [1], that the dimensions of of the polaron exceeds considerably the lattice constant and that only long waves essentially interact with the polaron in polarized (optical) oscillations of a crystal, for which (long waves) it is valid to pass to a dielectric continuum. Let us assume, further, that the electrons of the ions are polarized without inertia by the field of a conduction electron, as a result of which the latter (conduction electron) will be acted upon by a force possessing the periods of the crystal. Let us include this force in the total periodical potential of an electron in a crystal, which is successfully done in Schroedinger's equation by the introduction of the corresponding effective mass of an electron $m\mu$. [6]

The natural oscillations of ions in a crystal are composed, as is well known, of acoustic and polarized waves. Let us assume that acoustic waves are absent. The polarized waves (more accurately, the inertial part of specific polarization), we represent in the form of a trigonometric series:

$$\vec{P}(\vec{r},t)=\sum_k \vec{P}_k(t)\chi_k(\vec{r}) \quad \text{and} \quad \chi_k(r)=\sqrt{\frac{2}{L^3}}\begin{cases}\cos \vec{kr}, & k_x<0\\ \sin \vec{kr}, & k_x>0\end{cases} \qquad (1)$$

Here, as is well known, we introduced the conditions of cyclicness with

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large periods L; chi χ_k is normed in the volume of the "fundamental region" L^3. P_k oscillates (fluctuates) harmonically in time; limiting ourselves to crystals with a lattice of the rock-salt type, we can consider them as normal coordinates of the ions. The energy of a crystal, in the absence of the conductance electron, is written in the following form:

$$U = \sum_k \frac{2\pi}{c_k}\left(P_k^2 + \frac{\dot{P}_k^2}{\omega_k^2}\right) \qquad (2)$$

where omega ω_k are the frequencies of the natural optical oscillations of the ions and c_k are constants.

It is convenient for latter use, to introduce dimensionless canonical conjugate coordinates:

$$q_k = P_k\sqrt{\frac{4\pi}{\hbar\omega_k c_k}} \qquad (3)$$

and impulse:

$$p_k = \dot{P}_k\sqrt{\frac{4\pi}{\hbar\omega^3 c_k}} \qquad (4)$$

Thus we have:

$$U = \frac{1}{2}\sum_k \hbar\omega_k(q_k^2 + p_k^2) \qquad (5)$$

The classical equations of motion of the ions acquire the form of the canonical equations:

$$\hbar\dot{q}_k = \partial U/\partial p_k \text{ and } \hbar\dot{p}_k = -\partial U/\partial q_k \qquad (6)$$

If the conductance electron is present, the operator of the energy of the system is:

$$H = -\frac{\hbar^2}{2\mu}\Delta_r - e\int\frac{P(\vec{r}_1)\,(\vec{r}_1 - \vec{r})}{|\vec{r}_1 - \vec{r}|^3}d\tau_1 + U; \qquad (7)$$

r is the coordinates of the conductance electron; by $P(r_1)$ we understand the series (1); it is necessary to substitute in U the operator $-i\,\partial/\partial q_k$ for p_k. In (7) the first term represents the kinetic energy of the conductance electron, and the second is its energy of interaction with the ions. The energy of the system is assumed equal to zero when all the ions are at rest in the nodes of the lattice, but the electron is ~~in two conductance zones.~~ at the bottom of the conductance zone.

To each vector k corresponds one longitudinal and two transverse polarized waves. For the transverse waves we have:

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$$\operatorname{div} \vec{P}_{\perp} = 0 \quad \text{and} \quad \int \frac{\vec{P}_{\perp}(\vec{r}_1)(\vec{r}_1 - \vec{r})}{|\vec{r} - \vec{r}|^3} d\tau \tag{8}$$

Consequently, in the case of a continuum in an energy operator, the normal coordinates of the transverse waves enter only the individual terms in U and are completely determined as independent closed subspace. Therefore, in the future we can ignore the transverse waves, and in expansion (1) we can include only the longitudinal waves. Similarly, only the variables of the longitudinal waves figure in the formulas (7) to (8).

For the approximate calculation of the energy of the ground state of the system, we shall employ the variational method of quantum mechanics. In the minimization of the energy functional we shall approximate the state of the system by the ~~of~~ functions of the form:

$$\Psi(\vec{r}, \cdots q_k \cdots) = \psi(\vec{r})\, \Phi(\cdots q_k \cdots) \tag{9}$$

By limiting the approximating function to the multiplicative form (9), we obtain a somewhat heightened value of the energy.

It is convenient to introduce the designations:

$$\overline{P}_k = \int P_k |\Phi|^2 dq \quad \text{and} \quad dq = \prod_k dq_k . \tag{10}$$

$$U = \int \Phi^* U \Phi \, dq \tag{11}$$

$$\vec{D}[\psi, \vec{r}_1] = e \int \frac{|\psi(\vec{r})|^2 (\vec{r}_1 - \vec{r})}{|\vec{r}_1 - \vec{r}|^3} d\tau \tag{12}$$

$$\vec{D}_k[\psi] = \int \vec{D}[\psi, \vec{r}_1]\, \chi_k(\vec{r}_1)\, d\tau_1 \tag{13}$$

Since $\vec{D}$ is a vortex-less vector, then $\vec{D}_k$ is always parallel to $\vec{P}_k$:

$$\overline{H} = \int \Psi^* H \Psi \, d\tau\, dq = \frac{\hbar^2}{2\mu} \int |\nabla \psi|^2 d\tau - \sum_k \overline{P}_k D_k[\psi] + \overline{U}. \tag{14}$$

It is necessary to minimize the functional $\overline{H}$, by varying independently psi ψ and phi Φ, but preserving their normalness. The variation of phi Φ leads to the Euler-Lagrange equation, which, as a result of separation of variables, breaks up into independent equations of the form:

$$H_k \Phi_{n_k}(q_k + q_{k_0}) = E_k \Phi_{n_k}(q_k - q_{k_0}) \tag{15}$$

$$H_k = \frac{1}{2}\hbar\omega_k \left[(q_k - q_{k_0})^2 - \frac{\partial^2}{\partial q^2} \right] - \frac{c_k}{8\pi} D_k^2$$

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$$q_{k_0} = D_k \sqrt{\frac{c_k}{4\pi\hbar\omega_k}} \qquad (16)$$

$$\Phi = \prod_k \Phi_{n_k} \qquad (17)$$

Equation (15) can be considered as the wave equation of a harmonic oscillator with the position of equilibrium displaced under the influence of an additional constant force. Its solution:

$$\Phi_{n_k}(q_k - q_{k_0}) = A_{n_k} e^{-\frac{1}{2}(q_k - q_{k_0})^2} H(q_k - q_{k_0}) \qquad (18)$$

$$E_k = \hbar\omega_k\left(n + \frac{1}{2}\right) - \frac{c_k}{8\pi} D_k^2 .$$

H_n are the Chebyshev-Hermite polynomials; the minimum is obtained by setting $n_k = 0$.

Substituting the found Φ in equation (14) we obtain the following expression:

$$\overline{H}[\psi] = \frac{\hbar^2}{2\mu}\int |\nabla\psi|^2 d\tau - \frac{1}{8\pi}\sum c_k D_k^2[\psi] + \sum_k \frac{1}{2}\hbar\omega \qquad (19)$$

Minimization of this functional determines psi ψ. Having determined psi ψ we can clearly calculate $\vec{D}$, $\vec{D}_k$, q_{k_0} and the energy of the system's ground state. It is necessary, however, to be free, before hand, of the infinite summation ~~[illegible]~~ in the second term of (19). From a determination of c_k /see formula (2)/ it is obvious that $c_{-k} = c_k$. Therefore in the expansion:

$$c_k = c(k_x, k_y, k_z) = \sum_{m_1 m_2 m_3} c_{m_1 m_2 m_3} k_x^{m_1} k_y^{m_2} k_z^{m_3} \qquad (20)$$

only the terms enter whose summed power $(m_1 + m_2 + m_3)$ ~~are odd~~ is even. Substituting into the expansion (20) in k_x, k_y, k_z, respectively, the following partials: $i\partial/\partial x$, $i\partial/\partial y$, $i\partial/\partial z$, we obtain the operator which is essentially expressed thus:

$$c' = c\left(i\frac{\partial}{\partial x}, i\frac{\partial}{\partial y}, i\frac{\partial}{\partial z}\right) \qquad (21)$$

It is easy to show that

$$c'\chi_k(\vec{r}) = c_k \chi_k(\vec{r}) \qquad (22)$$

Resolving $\vec{D}$ into a series in chi χ_k and relying on equation (22), we can be satisfied that the following holds:

$$\sum_k c_k \vec{D}_k^2 = \int \vec{D}[\psi, \vec{r}]\, c'\, \vec{D}[\psi, \vec{r}]\, d\tau . \qquad (23)$$

Thus we have:

$$\overline{H}[\psi] = \frac{\hbar^2}{2\mu}\int |\nabla\psi|^2 d\tau \cdot \frac{1}{8\pi}\int \vec{D} c' \vec{D}\, d\tau + \sum_k \frac{1}{2}\hbar\omega_k \qquad (24)$$

For short polarized waves whose length is comparable with the lattice

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constant, the dependence of c_k upon k does exist and differs for various crystals. However, in the sum (23), the terms pr dominate in which k corresponds to wavelengths of the order of the polaron's diameter; that is, considerably exceeding the lattice constant. In this case, c_k can be approximately replaced by the corresponding suitable coefficient of the specific (infinite) wave and can be expressed in terms of macroscopic constants (see [17):

$$c_k \rightarrow c = \frac{1}{n^2} - \frac{1}{\varepsilon} \qquad (25)$$

where n is the index of refraction of light characterizing the inertialess polarization of electrons that belong to the ions, and epsilon ε is a dielectric constant. Thus, the first two terms in (24) are transformed into the functional $J[\psi]$, which was discussed in detail and minimized in previous works [1, 2]. On the basis of the results of these works, we obtain:

$$\overline{H}_{min} = J[\psi_0] + \sum_k \frac{1}{2}\hbar\omega_k \text{ and } J[\psi_0] = -0.0544\frac{\mu e^4}{\hbar^2}c^2 \qquad (26)$$

$$\psi_0 = 0.1229\,\alpha_4^{3/2}(1+\alpha_4 r + 0.4516\alpha_4^2 r^2)\cdot e^{-\alpha_4 r} \qquad (27)$$

$$\alpha_4 = 0.6585\,\mu e^2 c/\hbar^2.$$

If the electron were at the bottom of the conductance zone ~~in two conductance zones~~ in a nonpolarized crystal, then the energy of the system would simply equal the energy of the zero oscillations of the ions; that is, equal to only the ~~one~~ second term in formula (26). Consequently, the energy of dissociation of an electron equals $-J[\psi_0]$; that is, equals the same as in previous polycrystallic calculations [1,2]. The stability, indicated here, of a polaron cannot be disputed in an exact solution of the problem, since one can, taking into account the multiplicative limitation of approximation (9), affirm that the exact value of the energy of the polaron state lies somewhat lower.

Section 2. The Energy of the System in Adiabatic Approximation.

More accurate results can be obtained with the aid of adiabatic approximation. The ions' frequency of oscillations are assumed to be so small that the state of the conductance electron can adiabatically follow the motion of

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the ions. The advantage of adiabatic approximation consists in this--it permits one in a discussion of the electron state to take into consideration the actual instantaneous value of the field of oscillating ions, when, as in Section 1 here, only the average value of the ions' field was considered, thanks to the multiplicative limitation (9).

Let us assume that the configuration of ions in the crystal is determined by the normal coordinates P_k or q_k. The electron's state, corresponding adiabatically to this configuration of ions, is determined from the following equation:

$$\left[-\frac{\hbar^2}{2\mu}\Delta + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}) \tag{28}$$

$$V(\vec{r}) = -e\int \frac{\vec{P}(\vec{r}_1)(\vec{r}_1-\vec{r})}{|\vec{r}_1-\vec{r}|^3}\,d\tau \tag{29}$$

If we replace this equation by the equivalent variational method and make use of the designations in (12), then we have:

$$E(\ldots P_k\ldots) = \min\left\{\frac{\hbar^2}{2\mu}\int|\nabla\psi|^2 d\tau - \int \vec{P}(\vec{r}_1)\vec{D}[\psi,\vec{r}]\,d\tau_1\right\} \tag{30}$$

This functional can be minimized by varyin psi ψ for fixed polarization $\vec{P}(\vec{r})$; that is, for fixed P_k. The total energy of the conductance electron and of the longitudinal polarized waves in adiabatic approximation is equal to:

$$H = E(\ldots P_k\ldots) + U. \tag{31}$$

As already mentioned, the polaron interacts mainly with the long polarized waves, for which one consider c_k and ω_k as independent of $\vec{k}$. Therefore, in a discussion of the problems of interest to us we take c_k and ω_k in expression (2) from behind the summation sign and represent it in the form:

$$U = \frac{2\pi}{c}\int\left[P^2(\vec{r}) + \frac{1}{\omega^2}\dot{P}^2(\vec{r})\right]d\tau. \tag{32}$$

The energy (31) is a Hamiltonian function describing the longitudinal polarized oscillations of ions in the presence of a conductance electron.

It is impossible to solve exactly the problem with such a Hamiltonian, because the exact explicit expression for $E(\ldots P_k\ldots)$ is unknown, besides

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other difficulties; to determine $L(\ldots P_k \ldots)$ for arbitrary P_k's would require finding the solution of equation (28) for arbitrary polarized potential hole $V(\vec{r})$, which is practically impossible. One can, however, solve the problem approximately if one considers that ions oscillate, for not too high temperatures, mainly close to the configurations for which the following equation for the potential energy of ions is a minimum:

$$\min_{\psi}\left\{\frac{\hbar^2}{2\mu}\int|\nabla\psi|^2 d\tau - \int \vec{P}(\vec{r}_1)\vec{D}[\psi,\vec{r}_1]d\tau\right\} + \frac{2\pi}{c}\int P^2 d\tau. \quad (33)$$

In order to determine these configurations, it is necessary to find the absolute minimum of the functional (33) both in psi ψ and in $\vec{P}(\vec{r})$. This was successfully done in previous works [1,2], in which the polaron at rest was considered. The result obtained was:

$$\vec{P}_0(\vec{r}) = \frac{c}{4\pi}\vec{D}[\psi_0, r] \quad (34)$$

where psi ψ_0 is the minimum of the above-mentioned functional $J[\psi]$; its approximate expression is given in formula (27).

It is necessary to emphasize that the polaron at rest can be localized with unique success at any point of the crystal, and in all cases the potential energy of the ions will have one and the same minimum value. If $\vec{P}_0(\vec{r})$, $V_0(\vec{r})$, $\vec{D}_0(\vec{r})$ are understood to be quantities corresponding to minimum potential energy of the ions and relating to a polaron whose center is at the origin, then for a polaron with center a point xi $\vec{\xi}$ these quantities are written in the form $\vec{P}_0(\vec{r}-\vec{\xi})$, $V_0(\vec{r}-\vec{\xi})$,.... These functions represent a simple translation of the preceding functions by the amount of the vector xi $\vec{\xi}$. If the ions oscillate close to the configuration for which the potential energy is a minimum, then this means that polarization always approximates to $\vec{P}_0(\vec{r}-\vec{\xi})$, if only each time the vector $\vec{\xi}$ is chosen in a suitable way. Consequently, polarization can be represented in the following way:

$$\vec{P}(\vec{r}) = \vec{P}_0(\vec{r}-\vec{\xi}) + \vec{P}'(\vec{r}) \quad (35)$$

where $\vec{P}'(\vec{r})$ can be considered as a small perturbation. In the zero approximation

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the term $\vec{P}'(\vec{r})$ can be omitted and then the solution of equations (26), (29) will be $(\psi_0(\vec{r}-\vec{\xi}))$. Thereupon one can introduce the term $\vec{P}'(\vec{r})$ as a small perturbation. The energy of an electron in the first approximation equals:

$$E(\cdots P_k \cdots) = \frac{\hbar^2}{2\mu}\int |\nabla\psi_0|^2 d\tau - \int \vec{P}(\vec{r})\vec{D}_0(\vec{r}-\vec{\xi})d\tau. \qquad (36)$$

If we insert expressions (36), (32), (33), (34) into formula (31), then we obtain:

$$H = J[\psi_0] + \frac{2\pi}{c}\int \dot{P}'^2(\vec{r})d\tau + \frac{2\pi}{c\omega_0}\int \dot{P}^2(\vec{r})d\tau. \qquad (37)$$

In order to describe the motion of ions we shall select such a system of generalized coordinates that among them are the components of the vector $\vec{\xi}$. These three generalized coordinates must not enter the potential energy of the ions and will describe the free forward motion of the polaron. Let us represent the second term of equation (37) in the form of a trigonometric series:

$$\vec{P}'(\vec{r}) = \sum_k{}' P_k' \chi_k(\vec{r}) \qquad (38)$$

Here all chi's χ_k are the same as in formula (1), after exclusion of the six terms in which $\vec{k}$ has the following components: $\pm 2\pi/L, 0, 0$; $0, \pm 2\pi/L, 0$; $0, 0, \pm 2\pi/L$. In place of these six terms in formula (38) are three terms with the functions:

$$\chi_{k_i}(\vec{r}) = \sqrt{\frac{2}{L^3}} \cdot \sin \vec{k}_i(\vec{r}-\vec{\xi}) \qquad (i=1,2,3) \qquad (39)$$

$$\vec{k}_1\left(\frac{2\pi}{L},0,0\right), \quad \vec{k}_2\left(0,\frac{2\pi}{L},0\right), \quad \vec{k}_3\left(0,0,\frac{2\pi}{L}\right).$$

These three functions contain arbitrary and independent initial phases $k_1 \cdot \xi_x$, $k_2 \cdot \xi_y$, $k_3 \cdot \xi_z$, but therefore one can replace the above-mentioned six terms without disruption of the completeness of the system. In formula (38), the dash-mark on the summation sign indicates the absence of the three terms with the indexes $\vec{-k}_1$, $\vec{-k}_2$, $\vec{-k}_3$.

One is easily satisfied that an arbitrary function $\vec{P}(\vec{r})$ can be represented in the form:

$$\vec{P}(\vec{r}) = \vec{P}_0(\vec{r}-\vec{\xi}) + \sum_k{}' \vec{P}_k' \chi_k(\vec{r}); \qquad (40)$$

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here it is assumed that one and the same vector xi $\vec{\xi}$ enters into the term $\vec{P}_0$ and in the function chi χ k1 of (39). Thus the closedness of coefficients of $\vec{P}_k$ together with the vector xi $\vec{\xi}$ forms a complete system of independent generalized coordinates that define polarization in a crystal.

Differentiating (40) with respect to time, we have:

$$\dot{\vec{P}}(\vec{r}) = -(\dot{\vec{\xi}}\nabla)\vec{P}_0(\vec{r}-\vec{\xi}) + \sum_k \dot{\vec{P}}_k \chi_k(\vec{r}) - \sum_i \vec{P}'_{k_i}(\dot{\vec{\xi}}\nabla\chi_{k_i}). \tag{41}$$

As the dimensions of the region of cyclicity (periodicity) L tends toward infinity, $\vec{k}_1$ and $\nabla\chi$ tend toward zero as 1/L. In this situation each term in the third term of formula (41) becomes vanishingly small in comparison with the corresponding terms of the second term of (41). Therefore, the third term in formula (41) can be neglected.

Inserting expressions (36) and (41) into formula (37) we obtain:

$$H = J[\psi_0] + \frac{2\pi}{c}\sum{}' \left[P_k'^2 + \frac{\dot{P}_k^2}{\omega^2}\right] + \frac{1}{2}M\dot{\xi}^2 + H_1 \tag{42}$$

where $M = \frac{c}{4\pi\omega^2}\int\left(\frac{\partial\vec{D}_0}{\partial x}\right)^2 d\tau = 9.08\cdot 10^3\left(\frac{\mu}{m}\right)^3\frac{c^4}{\omega^2}$ grams, (43)

$$H_1 = -\frac{4\pi}{c\omega^2}\sum_k{}' \dot{\vec{P}}'_k \int \chi_k(\vec{r})(\dot{\vec{\xi}}\nabla)\vec{P}_0(\vec{r}-\vec{\xi})d\tau. \tag{44}$$

Here m is the mass of the free electron, mu μ is the effective mass of an electron in the conductivity zone. As is evident from formula (42), M represents the effective mass of an electron in its forward motion. The quantity M coincides with the one obtained in one of our previous works [5], where the polaron's forward motion was considered in the absence of thermal oscillations of ions (in comparing results one must take into account that the coefficient c_2, figuring in a previous work, for rock-salt type crystals equals c/ω^2).

Now let us proceed to a quantum-mechanical discussion of motion which is described by the Hamiltonian (42). We shall consider the term H_1 as a small perturbation and shall omit it in the zero approximation. In the same way as was done in Section 1 here, let us pass to dimensionless canonical conjugate coordinates and impulses:

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$$q_k' = p'\sqrt{\frac{4\pi}{\hbar\omega c}} \quad \text{and} \quad \xi_k' = \dot{p}'\sqrt{\frac{4\pi}{\hbar\omega^3 c}} \,. \tag{45}$$

Impulses g_k' must be replaced by the operators $-i\,\partial/\partial q_k$; $M\dot{\xi}$ must be replaced by the operator $-i\hbar\nabla_\xi$. As a result the energy operator acquires the following form:

$$H = J[\psi_0] + \frac{1}{2}\hbar\omega\sum_k{}'\left(q_k'^2 - \frac{\partial^2}{\partial q_k'^2}\right) - \frac{\hbar^2}{2M}\nabla_\xi \,. \tag{46}$$

The wave equation with such an energy operator is solved exactly. The solution has the form:

$$\Psi_{f\ldots n_k\ldots} = L^{-\frac{3}{2}} e^{i\vec{f}\vec{\xi}} \cdot \prod{}' \Phi_{n_k}(q_k') \,. \tag{47}$$

The functions phi's Φ_{n_k} are given by formula (18). The eigenvalues of the system's energy equal:

$$H_{f\ldots n_k\ldots} = J[\psi_0] + \hbar\omega\sum{}'\left(n_k + \frac{1}{2}\right) + \hbar^2\vec{f}/2M \,. \tag{48}$$

The states (47) we shall conditionally call the polaron waves. Formula (48) gives the dependence of the energy of such a wave upon the wave vector $\vec{f}$. The movement of a polaron wave in a crystal is accompanied by an electrical current. The "integral" current (current density integrated over the volume of the fundamental region L^3) equals the electron charge e multiplied by the group velocity of the wave:

$$v = \frac{1}{\hbar}\cdot\frac{d}{df}H_{f\ldots n_k\ldots} = \hbar f/M \,. \tag{49}$$

Setting $\vec{f} = 0$ and $n_k = 0$ in formula (48), we obtain the energy of the system's ground state:

$$H_0 = J[\psi_0] + \sum_k{}'\frac{1}{2}\hbar\omega \tag{50}$$

This energy is $(3/2)\hbar\omega$ less than the approximate increased value of the energy in (26), which (increased value) was obtained by a direct variational method. When an electron is found in two conductance zones and the crystal is depolarized, the energy of the system equals simply the energy of the zero oscillations of the ions, $\sum\frac{1}{2}\hbar\omega$.

Taking this into consideration (5), we obtain the polaron's energy of dissociation (for the case T = 0):

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Then $f' \approx f$ and therefore:

$$4\alpha^2 x = |\vec{f}' - \vec{f}|^2 \approx 2f^2(1-\cos\theta) \quad (\theta < \vec{f}, \vec{f}') \tag{62'}$$

$$d\Omega = 2\pi \cdot \sin\theta \cdot d\theta = \frac{4\pi\alpha^2}{f^2} \cdot dx;$$

so that

$$W_{ff'}\, d\Omega = \frac{M\omega c e^2}{2f\hbar^2}\left\{\frac{\bar{n}+1}{\bar{n}}\right\}\frac{(1+\frac{1}{7}x)^2}{(1+x)^8}\, dx. \tag{63}$$

Section 4. The Mobility of Polarons.

It is easy to show that in the case of thermal equilibrium there takes place a Maxwell distribution of group velocities of the polarons. If a small homogeneous electrical field is set up in a crystal, then the average value of the velocity of polaron in the direction of the field—and also the density of the electrical field—turns out to be proportional to the field. Let us calculate the mobility (motility) of the polarons (the ratio of the average velocity of a polaron to the field tension) on the assumption that the mobility is determined by the above-mentioned scattering of polarons by optical oscillation of ions.

1. The case of low temperatures ($kT \ll \hbar\omega$):

In this case, inequality (59) is fulfilled for most polarons and formula (60) is correct. The probability of scattering is not dependent either upon the angle of scatter or upon the polaron energy. This very convenient situation permits one to calculate exactly by elementary means the mobility, without having recourse to the kinetic formula. The mobility turns out to equal:

$$u = e\tau/M \tag{64}$$

where

$$\tau = \frac{1}{4\pi W_{ff'}} \tag{65}$$

is the average time of "free flight" of the polaron. Inserting $W_{ff'}$ from formula (60) and setting $\bar{n} \approx e^{-\hbar\omega/kT}$, we obtain:

$$u = \frac{\hbar^{3/2}}{M^{3/2} c e \sqrt{2\omega}} \cdot \frac{(1+x)^8}{(1+\frac{1}{7}x)^2}\, e^{\hbar\omega/kT} \tag{66}$$

If here we insert the value of M from formula (43), we then obtain:

$$u = 5.8 \cdot 10^{-38} \frac{\omega^{5/2}(1+x)^8}{\left(\frac{\mu}{m}\right)^{9/2} c^7 (1+\frac{1}{7}x)^2}\, e^{\hbar\omega/kT} \text{ cgse}. \tag{67}$$

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A numerical example: if $\varepsilon = 5$, $n = 1.58$, $\mu = m$, $\omega = 5 \cdot 10^{13}$/sec, and $\hbar\omega/kT = 3$, then we have: $c = 1/5$, $x = 0.383$, and $u = 2 \cdot 10^4$ cgse.

2. The case of high temperatures ($kT \gg \hbar\omega$):

In this case, inequality (62) is fulfilled for most polarons and formula (63) is correct. For high temperatures we have $\bar{n} \approx kT/\hbar\omega \gg 1$. Therefore, in accordance with formula (63), the probabilities of scattering through an angle theta θ with the emission of a quantum $\hbar\omega$ and with the absorption of a quantum $\hbar\omega$ are approximately similar. The total probability of scattering of a polaron with kinetic energy $\mathcal{E}$ through an angle θ equals:

$$W(\mathcal{E},\theta)\cdot 2\pi \sin\theta\, d\theta \approx \frac{Mce^2kT}{f\hbar^3}\cdot\frac{(1+\frac{1}{4}x)^2}{x(1+x)^8}\,dx \qquad (68)$$

The function of velocity distribution $F(\vec{v})$ of polarons is determined from the usual kinetic equation:

$$\frac{\partial F}{\partial t} + \frac{eE}{M}\frac{\partial F}{\partial v_x} + (a-b)F = 0\,. \qquad (69)$$

The term (a-b)F represents the variation per second of the distribution function in consequence of the scattering of polarons. If we set, as this is usually done,

$$F = F_0(\mathcal{E}) + F_1(\mathcal{E})\cos\beta \qquad (F_1 \ll F_0) \qquad (70)$$

(beta β is the angle between $\vec{v}$ and the x-axis), then we obtain:

$$(a-b)F = F_1(\mathcal{E})\cos\beta\cdot 2\pi\int_0^\pi W(\mathcal{E},\theta)(1-\cos\theta)\sin\theta\, d\theta. \qquad (71)$$

The usual expression for this term in free flight L has the form:

$$(a-b)F = \frac{v}{L}F_1(\mathcal{E})\cos\beta\,. \qquad (72)$$

Comparison of formulas (71) and (72) leads to the following determination of free flight:

$$\frac{v}{L(\mathcal{E})} = 2\pi\int_0^\pi W(\mathcal{E},\theta)(1-\cos\theta)\sin\theta\, d\theta. \qquad (73)$$

If expression (68) is used for $W(\mathcal{E},\theta)$, then there is obtained:

$$L(\mathcal{E}) = 13.34\,\mathcal{E}^2/ce^2\alpha^2kT\,. \qquad (74)$$

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In the stationary case of (72), we obtain:

$$F(\mathcal{E}) = -eEL \cdot \frac{\partial F_0}{\partial \mathcal{E}} . \qquad (75)$$

Inserting in place of $F_0(\mathcal{E})$ the Maxwell distribution function of velocities, we arrive by the usual way to the mobility:

$$u = \frac{42.7}{c e \alpha^2} \sqrt{\frac{kT}{M}} . \qquad (76)$$

If we insert here M from formula (43) and alpha α from formula (53), then we have:

$$u = 1.05 \cdot 10^{-7} \frac{\omega \sqrt{kT}}{\left(\frac{\mu}{m}\right)^{7/2} \cdot c^5} \quad cgse. \qquad (77)$$

As a numerical example, let us consider the same crystal as in the previous case ($c = 1/5$, $\mu = m$, $\omega = 5 \cdot 10^{13}$/sec), but for a temperature $T = 500^\circ$. With this data we obtain $u = 4300$ cgse.

From the numerical examples considered it is evident that in both the case of low and the case of high temperatures the calculated mobilities of polarons agree in the order of magnitude with experimentally-determined mobilities of current-carriers in semi-conductors. Detailed comparions of theory and experimental data for actual crystals will be given in a special article.

As is evident from formulas (67) and (77), with increase in temperature, the mobility initially decreases exponentially, and then, after passing through a minimum, begins to increase slowly.

For very cold crystals, the probability of the above-discussed scattering of polarons decreases with temperature more rapidly than the probability of their scattering by acoustical (sonic) oscillations of ions. Therefore, for sufficiently low temperatures, the mobility of polarons is determined by acoustical (sonic) oscillations, and also by "polaron stoppage", as discussed by the author in a previous work [4]. The latter work leads to a finite mobility of the polaron even for $T = 0^\circ$.

I take this opportunity to express my sincere thanks to Academician L. D. Landau for his very useful criticism and discussion.

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[No figures in the original.]

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