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On the Theory of Polaron Mobility

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The interaction of the translational motion of a polaron with the lattice vibrations and the associated energy loss of the polaron are investigated. Using a classical treatment, the energy transferred from one polaron to the vibrational degrees of greedom of the lattice is calculated. This type of excitation is possible for acoustic vibrations only if the polaron velocity exceeds the sound velocity in the crystal. It is thus analogous to the Cerenkov effect for an electron moving with a speed greater than that of light. The numerical results obtained for NaCl, KCl and KBr show that, although this mechmanim is not the main cause for slowing, nevertheless the interaction of the current carriers with the acoustical and transverse optical vibrations is by no means small for these crystals.

1. INTRODUCTION

THE theory of polaron mobility developed by Pekar on the basis of a macroscopic treatment of crystals[1,2] started from the picture of the scattering of polaron waves by the longitudinal optical vibrations of the lattice. The polarization of the crystal was split into two parts: a self-consistent part $\mathbf{P}_0(\mathbf{r}-\vec{\xi}) = (C/4\pi)\mathbf{D}(\mathbf{r}-\vec{\xi})$[where $\mathbf{D}(\mathbf{r})$ is the average induction of the polaron, $C = (1/n^2)-1/\epsilon$, ϵ and n are the dielectric constant and the index of refraction, $\vec{\xi}$ is the radius vector to the center of the polarization source] and a variable part $\mathbf{P}' = \sum_{\mathbf{K}} \mathbf{P}'_{\mathbf{K}} e^{i\,\mathbf{Kr}}$ describing the phonons. On the assumption that the radius of the polaron state is large compared to the lattice constant, one can neglect the interaction of the polaron with short wavelength longitudinal optical vibrations as well as with the acoustic and transverse optical vibrations, which in this approximation have no longitudinal component of the dipole moment. Actually, for many materials (e.g., all alkali-halide crystals), the radius of the polaron state is only slightly greater than the lattice constant. It is therefore of interest to evaluate the magnitude of the interaction of a moving polaron with the acoustical and transverse vibrations of the crystal.

We shall limit our treatment to polarons whose radius is large enough for the results of Pekar's theory to be applicable as a zeroth approximation, and shall calculate the next approximation in which the energy of interaction of the electron with the transverse optical and acoustical vibrations can still be treated as a small quantity.

As in Pekar's first papers[3,4], we shall treat the electron motion quantum-mechanically and the oscillations of the ions classically. The constants characterizing the electron interaction with the crystal vibrations are taken from the data of one of the authors[5,6].

2. FORCED VIBRATIONS OF A CRYSTAL UNDER THE ACTION OF THE FIELD OF A MOVING POLARON

According to Pekar, the wave function of a moving polaron is

$$\psi(r,\ t) = \psi_0(|\mathbf{r} - \mathbf{v}t|),$$

where $\mathbf{v}$ is the translational velocity of the polaron, and $\psi_0(r)$ is the wave function for the polaron at rest. The wave function can be chosen to be Gaussian,

$$\psi_0 = (2/\pi)^{3/4}\alpha^{3/2} e^{-\alpha^3/2}, \qquad (1)$$

with an error of less than 1% compared to the function used by Pekar[1]. We denote the average electrical induction produced by the charge density $\rho = e\,|\psi_0|^2$ by

$$\mathbf{D}(\mathbf{r}) = -\nabla\varphi = -\nabla \int \frac{e\,|\psi_0(\mathbf{r}')|^2\,d\tau'}{|\mathbf{r}-\mathbf{r}'|}, \qquad (2)$$

and the "instantaneous" induction produced by an electron at the point $\mathbf{r}'$ by

$$\mathbf{D}(\mathbf{r},\ \mathbf{r}') = e(\mathbf{r}-\mathbf{r}')/\,|\mathbf{r}-\mathbf{r}'|^3. \qquad (2')$$

For a lattice made up of deformable ions, the ion displacements $\mathbf{u}_s^l$ and the associated dipole moments $\mathbf{p}_s^l = e_s\mathbf{u}_s^l$ (s numbers the ions and l the cells of the lattice) are determined by the average field $\mathbf{D}(r)$; according to the adiabatic approximation, the dipole moments $\mathbf{P}^l_s$ of the electronic shells are determined[2] both by the momentary position of the electron [and consequently, by the field $\mathbf{D}(\mathbf{r}, \mathbf{r}')$] and the field resulting from the displacements $\mathbf{u}^l_s$. The equations describing the displacements and deformation of the ions can be written in the form[7]

$$m_s\ddot{p}^l_{sx} = -e_s^2\left(\partial U^0/\partial p^l_{sx}\right) + e_s^2 D_x(\mathbf{r}^l_s, \mathbf{r}'), \quad (3a)$$

$$0 = -\left(\partial U^0/\partial P^l_{sx}\right) + D_x(\mathbf{r}^l_s, \mathbf{r}'), \quad (3b)$$

where U^0 is the potential energy of the crystal expressed as a function of $\mathbf{p}^l_s$ and $\mathbf{P}^l_s$. This function was given in Ref. 7 (with some differences in notation) as

$$U^0 = \frac{1}{2a^3}\sum\left(a^{l-l'}_{ss'xy}p^l_{sx}p^{l'}_{s'y}\right. \quad (4)$$

$$\left. + 2b^{l-l'}_{ss'xy}p^l_{s'x}P^{l'}_{s'y} + c^{l-l'}_{ss'xy}P^l_{sx}P^{l'}_{s'y}\right),$$

where the coefficients a, b, c depend only on the coordinate differences $\mathbf{r}^l_s - \mathbf{r}^{l'}_s$, and are dimensionless constants; the summation extends over all indices.

Since we are interested only in the vibrations of the ions, and not in the part $\check{\mathbf{P}}^l_s$ of the polarization which follows the electron motion without any lag, we can choose as the zero of energy of interaction of the electron with the crystal the state where $p^l_s = 0$ and the electron is at the bottom of the conduction band. In such a motion the inertialess part of the polarization, $\check{\mathbf{P}}^l_s$, remains the same as the case we are considering, where $\mathbf{p}^l_s \neq 0$. Then Eq. (3b) becomes

$$0 = -\left[\partial U^0(0, \check{\mathbf{P}}^l_s)/\partial P^l_{sx}\right] + D_x(\mathbf{r}^l_s, \mathbf{r}'). \quad (5)$$

To eliminate the quantities $\check{\mathbf{P}}^l_s$, we subtract Eq. (5) from Eq. (3b) and get

$$0 = -\partial U^0\left(\mathbf{p}^l_s, \mathbf{P}^l_s - \check{\mathbf{P}}^l_s\right)/\partial P^l_{sx}. \quad (6)$$

Thus the quantities $\tilde{\mathbf{P}}^l_s = \mathbf{P}^l_s - \check{\mathbf{P}}^l_s$ are determined only by the ion displacements $\mathbf{u}^l_s$ and do not depend on the instantaneous position of the electron. Consequently, they are equal to their quantum-mechanical average values, calculated with $|\psi(\mathbf{r}')|^2$. Averaging Eqs. (3) over $\mathbf{r}'$, we get

$$(m_s/e_s^2)\,\ddot{p}^l_{sx} = \quad (7a)$$

$$-\left(\partial U^0(\mathbf{p}^l_s, \overline{\mathbf{P}}^l_s)\right)/\partial p^l_{sx} + D_x(\mathbf{r}^l_s);$$

$$0 = -\left(\partial U^0(\mathbf{p}^l_s, \overline{\mathbf{P}}^l_s)/\partial P^l_{sx}\right) + D_x(\mathbf{r}^l_s), \quad (7b)$$

where $\overline{\mathbf{P}}^l_s = \tilde{\mathbf{P}}^l_s + \overline{\check{\mathbf{P}}}^l_s$.

The potential energy of the electron interaction with the polarized crystals (measured from the bottom of the conduction band) will obviously be

$$U^l(r') = -\sum_{sl}\mathbf{D}(\mathbf{r}^l_s, \mathbf{r}')\cdot(\mathbf{p}^l_s + \tilde{\mathbf{P}}^l_s), \quad (8)$$

and since $\mathbf{p}^l_s + \tilde{\mathbf{P}}^l_s$ does not depend on the instantaneous position of the electron, the quantum-mechanical average of U^0 is

$$\overline{U^l} = -\sum_{sl}\mathbf{D}(\mathbf{r}^l_s, \mathbf{r}')\cdot(\mathbf{p}^l_s + \tilde{\mathbf{P}}^l_s) = \quad (9)$$

$$-\sum_{s,l}\mathbf{D}(\mathbf{r}^l_s)\cdot(\mathbf{p}^l_s + \overline{\mathbf{P}^l_s} - \overline{\check{\mathbf{P}}^l_s}).$$

The quantities $\overline{\check{\mathbf{P}}}^l_s$ are found by averaging Eq. (5):

$$0 = -\left[\partial U^0(0, \overline{\check{\mathbf{P}}}^l_s)/\partial P^l_{sx}\right] + D_x(\mathbf{r}^l_s). \quad (10)$$

We transform Eqs. (7) to normal coordinates by the substitutions

$$p^l_{sx} = \sum_{\mathbf{K},\alpha} p^\alpha_{sx}(\mathbf{K})\exp\{i\mathbf{K}\mathbf{r}^l_s\}\, q_{\alpha\mathbf{K}}(t); \quad (11)$$

$$P^l_{sx} = \sum_{\mathbf{K}}\left[\sum_\alpha P^\alpha_{sx}(\mathbf{K})\, q_{\alpha\mathbf{K}}(t) + R_{sx}(\mathbf{K}, t)\right]e^{i\mathbf{K}\mathbf{r}^l_s},$$

where p^α_{sx}, P^α_{sx} are the normalized amplitudes of the free oscillations of the lattice, and satisfy the equations:

$$\mu_s p^\alpha_{sx}\Omega^2_{\alpha\mathbf{K}} = \sum_{s'y}\left(A_{ss'xy}p^\alpha_{s'y} + B_{ss'xy}P^\alpha_{s'y}\right); \quad (12)$$

$$0 = \sum_{s'y}\left(B^*_{ss'yx}p^\alpha_{s'y} + C_{ss'xy}P^\alpha_{s'y}\right), \quad (13)$$

where

$$A_{ss'xy} = \sum_{l'} a^{l-l'}_{ss'xy}\exp\{-i\mathbf{K}(\mathbf{r}^l_s - \mathbf{r}^{l'}_{s'})\}$$

etc. (cf. Ref. 7),

$$\mu_s = m_s/\mu; \qquad \mu = m_1 m_2/(m_1 + m_2);$$

$$\Omega^2_{\alpha\mathbf{K}} = (\mu a^3/e^2)\,\omega^2_{\alpha\mathbf{K}};$$

the $\omega_{\alpha\mathbf{K}}$ are the eigenfrequencies. Then (3) becomes

$$\frac{\mu a^3}{e^2}\ddot{q}_{\alpha\mathbf{K}} + \Omega^2_{\alpha\mathbf{K}} q_{\alpha\mathbf{K}} = a^3 \sum_{sx} p^{\alpha *}_{sx}\left\{\frac{1}{N}\sum_{l} D_x(\mathbf{r}^l_s) \times \exp\{-i\mathbf{K}\cdot\mathbf{r}^l_s\} - \sum_{s'y} B_{ss'xy} R_{s'y}\right\}; \tag{14}$$

$$\sum_{s'y} C_{ss'xy} R_{s'y} = \frac{a^3}{N}\sum_{l} D_x(\mathbf{r}^l_s)\, e^{-i\mathbf{K}\mathbf{r}^l_s}, \tag{15}$$

where N is the number of cells in the fundamental domain of the crystal.

It is easy to see from a comparison of Eqs. (15) and (10) that the quantities $R_{s'y}$ are precisely the Fourier components of $\check{\bar{\mathrm{P}}}^l_s$. Solving Eq. (15) for the $R_{s'y}$ and substituting in (14), we get

$$\ddot{q}_{\alpha\mathbf{K}} + \omega^2_{\alpha\mathbf{K}} q_{\alpha\mathbf{K}} = Q_\alpha(\mathbf{K}, t) \tag{16}$$

$$= \frac{e^2}{N\mu}\sum_{s,x} p^{\alpha *}_{sx} \exp\{-i\mathbf{K}\cdot\mathbf{r}^l_s\} \times [D_x(\mathbf{r}^l_s) - \sum_{s's''yz} B_{ss'xy} C^{-1}_{s's''yz} D_z(\mathbf{r}^l_{s''}) \exp\{i\mathbf{K}\cdot(\mathbf{r}_s - \mathbf{r}_{s''})\}].$$

3.TRANSFER OF ENERGY FROM A MOVING POLARON TO THE CRYSTAL

In order to determine the time dependence of the generalized force $Q_\alpha(\mathbf{K}, t)$, we calculate the Fourier components of $\rho = e/\psi(\mathbf{r}-\mathbf{v}t)|^2$ for an arbitrary point $\mathbf{r}$:

$$\rho = \sum_{\mathbf{K}} \rho_{\mathbf{K}}(t)\, e^{i\mathbf{K}\mathbf{r}}, \tag{17}$$

$$\rho_{\mathbf{K}}(t) = \frac{e}{V}\int |\psi(\mathbf{r} - \mathbf{v}t)|^2 e^{-i\mathbf{K}\mathbf{r}} d\tau = \frac{e}{V}\exp\left\{-\frac{\mathbf{K}^2}{8\alpha^2} - i\mathbf{K}\cdot\mathbf{v}t\right\},$$

where V is the volume of the fundamental domain.

The Fourier transforms of the Poisson equation $\Delta\varphi = -4\pi\rho$ and the relation $\mathrm{D} = -\nabla\varphi$ are

$$\mathbf{D}(\mathbf{r}, t) = \sum \mathbf{D}(\mathbf{K}, t)\, e^{i\mathbf{K}\mathbf{r}}, \tag{18}$$

$$\mathbf{D}(\mathbf{K}, t) = -\frac{4\pi i e\mathbf{K}}{K^2}\exp\left\{-\frac{\mathbf{K}^2}{8\alpha^2} - i\,\mathbf{K}\cdot\mathbf{v}\,t\right\}.$$

Substituting (17) in (15) and noting that $\sum_l e^{i(\mathbf{K}-\mathbf{K}')\mathbf{r}^l_s} \neq 0$ only if $\mathbf{K} - \mathbf{K}' = 2\pi\mathbf{q}^m$ (where $\mathbf{q}^m$ is an arbitrary vector of the reciprocal lattice), we obtain a complicated expression for Q_α, consisting of a sum of terms with different frequencies $\mathbf{v}\cdot(\mathbf{K}+2\pi\mathbf{q}^m)$. However, in the macroscopic approximation where we consider polarons of large radius, only terms with wave vectors small compared to the vectors of the reciprocal lattice appear in the expansion of $\mathrm{D}(\mathbf{r})$. Therefore, since we are neglecting the components $\mathbf{D}(2\pi\mathbf{q}^m) \sim \exp\{-(2\pi q^m)^2/8\alpha^2\}$, it would be inconsistent to keep them in the expression for the external force. Thus, in the sum over m in the expression for Q_α, we should keep only the leading term with $m = 0$. Using (13) and (15), we can transform $Q_\alpha(\mathbf{K}, t)$ to the simpler form

$$Q_\alpha(\mathbf{K}, t) = e^{-i\mathbf{v}\cdot\mathbf{K}t}; \tag{19}$$

$$Q_\alpha(\mathbf{K}) = \frac{e^2}{\mu}\mathbf{D}(\mathbf{K}, t)\sum_s (\mathbf{p}^{\alpha *}_s\, t\, \mathbf{P}^{\alpha *}_s).$$

The solution of Eq. (16) can be put in the form

$$q_{\alpha\mathbf{K}} = \frac{Q_\alpha(\mathbf{K})}{\omega^2_{\alpha\mathbf{K}} - (\mathbf{K}\cdot\mathbf{v})^2}\{\cos\mathbf{K}\cdot\mathbf{v}\,t - \cos\omega_{\alpha\mathbf{K}} t - i\sin\mathbf{v}\cdot\mathbf{K}\,t + b_{\alpha\mathbf{K}}\sin(\omega_{\alpha\mathbf{K}} t + \beta_{\alpha\mathbf{K}})\}, \tag{20}$$

where $b_{\alpha\mathbf{K}}$ and $\beta_{\alpha\mathbf{k}}$ are arbitrary integration constants. If the crystal was not deformed at $t=0$, then all the $\beta_{\alpha\mathbf{K}} = 0$.

From Eqs. (7a) and (7b), the work done on the crystal by the moving polaron during the time from 0 to t is

$$A = \int_0^t \frac{d}{dt}\left[\sum_{slx}\frac{1}{2}\frac{m_s}{e^2_s}\dot{p}^{l2}_{sx} + U^0(p^l_s, \overline{P}^l_s)\right]dt = \int_0^t \sum_{slx}\mathbf{D}_x(\mathbf{r}^l_s)(\dot{p}^l_{sx} + \dot{\bar{P}}^l_{sx})\,dt. \tag{21}$$

Taking Fourier transforms and using the relation

$$C^{-1}_{ss'xy} = C^{-1*}_{s'syx}, \tag{22}$$

we get, after simple transformations

$$A = \int_0^t \Big\{ \sum_{\mathbf{K}\alpha} Q_{\alpha\mathbf{K}}(t)\, \dot{q}_{\alpha\mathbf{K}}(-\mathbf{K}) \tag{23}$$

$$+ \sum_{ss'xy\mathbf{K}} D_x(-\mathbf{K})\, C^{-1}_{ss'xy}\, \dot{D}_y(\mathbf{K}) \Big\}\, N\mu/e^2\, dt.$$

The second term in the integral is identically zero, since the expression to be summed over K is an odd function of **K**. Integrating the first term in (23) with respect to t and dropping terms which go to zero or cancel one another when we sum over K, we find for sufficiently long times t

$$A = \frac{2\mu N}{e^2} \sum_{\alpha,\mathbf{K}} \frac{|Q_\alpha(\mathbf{K})|^2\, \omega_{\alpha\mathbf{K}}}{\omega_{\alpha\mathbf{K}} + \mathbf{K}\cdot\mathbf{v}}\; \frac{\sin^2 {}^1\!/_2\, (\omega_{\alpha\mathbf{K}} - \mathbf{K}\cdot\mathbf{v})\, t}{(\omega_{\alpha\mathbf{K}} - \mathbf{K}\cdot\mathbf{v})^2}. \tag{24}$$

As $t \to \infty$, A becomes proportional to t, and thus the special choice of solution with $q_{\alpha\mathbf{K}}(t = 0) = 0$, where A also includes the energy of formation of the polaron, has no significance.

4. COMPUTATION OF ENERGY LOSS OF A POLARON FOR SPECIFIC CRYSTALS

Further calculations in general form are not possible, so we shall limit ourselves to considering the simplest case of the motion of a polaron of relatively large radius in a cubic crystal. Numerical results will be obtained for crystals of NaCl, KCl and KBr.

We may assume that, for a polaron of large radius, $Q_\alpha(\mathbf{K})$ is significantly different from zero only for K's which are so small that the $\omega_{\alpha\mathbf{K}}$ can be assumed to be equal to their limiting frequency in the case of optical waves, and proportional to $|\mathbf{K}|$ in the case of acoustic waves.

For the optical branches $\omega_{1\mathbf{K}} \approx \omega_\parallel$ (longitudinal waves), and $\omega_{2\mathbf{K}} = \omega_{3\mathbf{K}} = \omega_\perp$ (transverse waves), where $\omega_\parallel/\omega_\perp = \sqrt{\epsilon}/n$. Taking the z-axis along the direction of the velocity v and changing to polar coordinates, we can carry out the summation over the angle ϑ. Replacing the sum over K by an integral, we have

$$A_{\alpha}^{:} = t\, \frac{VN}{16\pi^2}\, \frac{\mu}{e^2 |\mathbf{v}|} \iint |Q(\mathbf{K}, \vartheta_\alpha, \varphi)|^2\, K dK d\varphi, \tag{25}$$

where $\cos \vartheta_\alpha = \omega_\alpha/Kv$, 1,2, 3.

For the acoustic branches, we can set $\omega_{\alpha\mathbf{K}} = KC_\alpha(\vartheta, \varphi)$. Then the integration over the angle ϑ gives the same formula (25), where $\vartheta_\alpha^{:}$ is the "resonance" value of the angle ϑ, for which

$$C_i(\vartheta_\alpha^{:}, \varphi) = v \cos \vartheta_\alpha^{:}. \tag{26}$$

In a paper of one of the authors, solutions of the equations for the normal modes (12) were obtained including terms of order $k^2 = (aK)^2$, (where a is the separation of neighboring ions); numerical values of the amplitudes were found for the four crystals: LiF, NaCl, KCl and KBr[5].

For the longitudinal optical vibrations, the effect is already different from zero in the zeroth approximation with respect to k where, according to Ref. 5,

$$p_{sx} = k_x/k\mu_s; \qquad P_{sx} = (k_x/k)(c_s/a_0), \tag{27}$$

where the quantities μ_s and c_s/a_0 are numerical constants whose values for the crystals mentioned are given in Table I. Substituting (27) and (18) in (19) and (19) in (25) and integrating over φ we get

$$A_1 = t\, \frac{\pi e^4}{2\mu a^3 v} \left(1 + \frac{c_1 + c_2}{a_0}\right)^2 \int_{(\omega_\parallel/2\alpha v)^2}^{\infty} \frac{e^{-x}}{x}\, dx. \tag{28}$$

For low velocities v, when $\omega_\parallel/2\alpha v \gg 1$ and the asymptotic expansion of the exponential integral is applicable, we get for the approximate dependence of A_1/t on v

$$\frac{A_1}{t} = Bv \exp\{-(\omega_\parallel/2\alpha v)^2\} \tag{29}$$

$$\times \left[1 - \left(\frac{2\alpha v}{\omega_\parallel}\right)^2 + 2!\left(\frac{2\alpha v}{\omega_\parallel}\right)^4 - \cdots\right],$$

$$B = \frac{\pi e^4\, 2\alpha^2}{\mu a^3 \omega_\parallel^2} \left(1 + \frac{c_1 + c_2}{a_0}\right)^2. \tag{30}$$

Thus the energy loss is greater, the greater α, i.e., the smaller the radius of the polaron state, and increases exponentially with increasing velocity.

For the crystals NaCl, KCl and KBr, for which the parameter α in the polaron wave function is known, the result of computation with the exact formula (26) is given in Fig. 1.

For transverse optical vibrations the sum of $\mathbf{P}_s + \mathbf{p}_s$, which is parallel to the vector k, is given by the formula

TABLE I. Amplitudes of Dipole Moments of Optical Vibrations

Crystal	$1/\mu_1$	$1/\mu_2$	c_1/a_0	c_2/a_0	b
NaCl	0.6066	0.3934	—0.01485	—0.51755	0.084295
KCl	0,4756	0.5244	—0.05516	—0.43228	—0.042374
KBr	0.6715	0,3285	—0.04367	—0.48942	0.107363

$$\sum_{s=1}^{2} (\mathbf{P}_s + \mathbf{p}_s)_k = b\,\mathbf{k}/k\tau_{\pm}(k). \tag{31}$$

The value of the constant b depends on the properties of the crystal (values calculated from Ref. 5 are given in the last column of Table I), while $1/\tau_{\pm}(k)$ is a universal function and depends only on the direction of the vector k. Its expansion in spherical harmonics was found in Ref. 5. Approximately,

$$1/\tau_{\pm}(k) = \tau_{\pm}^{0} + \tau_{\pm}^{(4)} Y_4(\theta, \varphi) \tag{32}$$

$$+ \tau_{\pm}^{(6)} Y_6(\theta, \varphi) + \tau_{\pm}^{(8)} Y_8(\theta, \varphi) + \tau_{\pm}^{(10)} Y_{10}(\theta, \varphi);$$

where τ_q^0, $\tau_{\pm}^4$etc. are numerical factors and the + and – refer to the two branches of the transverse optical vibrations. Because of the complicated dependence of $\tau_{\pm}$ on ϑ and φ, the energy loss of the polaron will be strongly dependent on the direction of the velocity v with respect to the crystal axes (ϑ and φ in formula (32) are the angles describing the vector k in a polar coordinate system fixed in the crystal). However, for a rough estimate of the energy loss, we can limit ourselves to the first term in (32). We then get

$$\frac{1}{t} A_{2,3} = \frac{8\pi b^2 a\alpha^4 e^4}{\mu} (\tau_{\pm}^{0})^2 \frac{1}{v} \tag{33}$$

$$\times \exp\{-(\omega_{\perp}/2\alpha v)^2\}\left[1 + \left(\frac{\omega_1}{2\alpha v}\right)^2\right],$$

where $\tau_{+}^{0} = 0.1481$; $\tau_{-}^{0} = 0.0408$. Comparing (33) and (29), we see that for low velocities, where $\omega_{\perp}/2\alpha v \gg 1$, $A_{2,3}$ differs from A_1 by the factor

$$(\alpha a)^4 \left(\frac{2\omega_{\parallel}}{\alpha v}\right)^2 \exp\left\{\frac{\omega_{\parallel}^2 - \omega_{\perp}^2}{(2\alpha v)^2}\right\}$$

which comes from the quantity $(b\tau_{\pm}^{0})^2$.

Thus as the velocity decreases, the importance of the transverse vibrations in the slowing down increases. Figure 2 shows the behavior of $A_{2,3}/t$ for the same three crystals.

We find the quantities $Q_{\alpha}(\mathrm{K}, t)$, $\alpha = 4, 5, 6$ for the acoustic vibrations from forumla (9), using the results of Ref. 5. In the zeroth approximation for k, $\mathbf{p}_1^{\alpha} = -\mathbf{p}_2^{\alpha}$, $\mathbf{P}_1^{\alpha} = \mathbf{P}_2^{\alpha} = 0$ for the acoustic vibrations. In second order in **k**, using formula (67′) of Ref. 5, the sum $\sum_{s=1}^{2} (\mathbf{p}_s^{\alpha} + \mathbf{P}_s^{\alpha})\cdot\mathbf{k}/k$ gives

$$[n^0 + n^{(4)} Y_4(\theta, \varphi) + n^{(6)} Y_6(\theta, \varphi) \tag{34}$$

$$+ n^{(8)} Y_8(\theta, \varphi) + n^{(10)} Y_{10}(\theta, \varphi)]\,k^2;$$

the values of $n^{(0)}$, $n^{(4)}$, etc., are given in Table V of Ref. 5. Then

$$Q_{\alpha}(\mathrm{K}, t) = -\frac{4\pi i e^3 a^3 k}{\mu V} e^{-k^2/8(\alpha a)^2} \tag{35}$$

$$\times\{n^0 + n^{(4)} Y_4 + \ldots\}.$$

When substituting Q_{α} in formula (25) we must set the angle between k and v equal to the resonance value $\vartheta^{\cdot}_{\alpha}$ given by (26).

From Eq. (6) of Ref. 5, the sound velocity in the crystal is

$$C = \frac{\omega}{|K|} = \sqrt{\frac{e^2}{a\mu}}\, v^0 \{1 + v^{(4)} Y_4(\theta, \varphi) \tag{36}$$

$$+ v^{(6)} Y_6(\theta, \varphi) + \ldots\}.$$

The solution of Eq. (26) for $\vartheta^{\cdot}_{\alpha}$ is generally impossible for such a complicated dependence of C on the direction of k, so we shall replace the curly bracket by unity. From Table IV of Ref. 5 we see that all the $v^{(i)}$ ($i = 4, 6, \ldots, 10$) are small

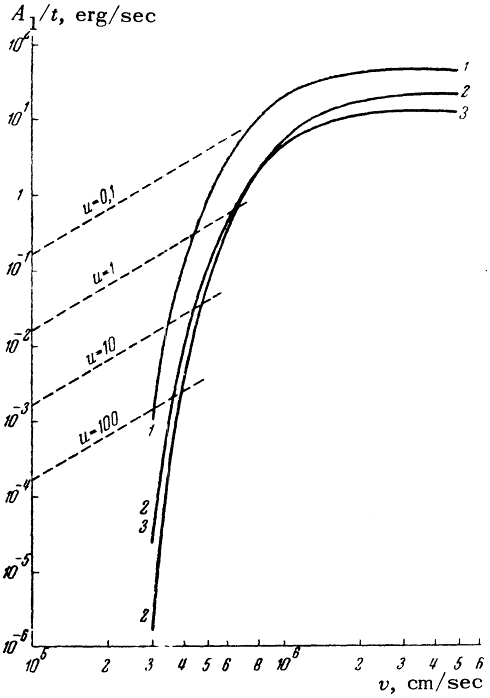

FIG. 1. Energy transferred from a polaron to the longitudinal optical vibrations of the lattice as a function of its velocity v: *1*-NaCl, *2*-KCl, *3*-KBr. The dotted lines shown the energy transferred to the lattice per second for various values of the mobility u, expressed in cm^2/volt sec and calculated according to the formula $W = eEv = ev^2/u$.

compared to one, so the resultant error is small.

With this simplification, Q_α no longer depends on the direction of **k**, and integration of (25) gives

$$A_i/t = (\pi e^4/\mu a^3 v)(\overset{0}{n}_{\dot{\alpha}})^2 (2\alpha a)^4, \qquad (37)$$

$$\dot{\alpha} = 4, 5, 6.$$

Formula (37) is of course applicable only if $v \geq C$, since otherwise, Eq. (26) cannot be satisfied. In Table II the values of the constants in Eq. (37) are given for the various crystals and the various branches of acoustical vibrations. From a comparison of formulas (37), (33) and (29) it is clear that for low velocities, so long as $v \geq C$, most of the energy loss occurs via excitation of acoustical vibrations (except fo NaCl). The numerical values of the energy transfer are small for $v \sim C$ but of the same order of magnitude for all six branches. Thus we may expect that a quantum-mechanical calculation of the scattering will show an important contribution from interaction with the acoustical and transverse optical vibrations.

To estimate the role of the mechanism of energy loss which we are considering, we compare the quantity A_i/t with the power W from the external force $e\mathbf{E}$ which maintains the translational motion of the polaron at the fixed velocity $\mathbf{v} = u\mathbf{E}$, where u is the mobility of the polaron and $W = e\mathbf{E}\cdot\mathbf{v} = ev^2/u$. For a mobility $u \sim 1$-10 cm^2/volt sec, which is typical of alkali halide crystals, the line ev^2/u is above the curves of A_α/t. Only for polaron velocities $v \gtrsim 5 \times 10^5$ cm/sec does the energy loss to excitation of longitudinal optical vibrations become greater than W. This means that for such velocities the mobility of the polaron must decrease.

In conclusion, we note that the transfer of energy from a moving polaron to a crystal was calculated by Buckingham[8] on the basis of band theory, where the interaction of the electron with the vibrations was taken to be

$$\int c\rho \operatorname{div} \mathbf{u} \, d\tau \qquad (38)$$

where **u** is the displacement vector, and the crystal was treated macroscopically and the electron was

TABLE II. Constants of Formula (37) which Gives the Energy Transfer from the Polaron to the Acoustical Vibrations of the Lattice

Crystal	Branch No. α	$C_\alpha = v^0\sqrt{e^2/\mu_\alpha}$ in 10^5 cm/sec	$-n_\alpha^0 \cdot 10^3$	$\frac{A_{\max}}{t} = \frac{A_\alpha v}{tC}$ in 10^{-2} erg/sec
NaCl	4	2.53	0,694	0,277
	5	2.79	2.177	2.67
	6	4.65	1.003	0,276
KCl	4	2.01	1.061	0.120
	5	2.5	3.031	0.839
	6	4.1	12.48	8.36
KBr	4	1.6	1.176	0.0791
	5	2.1	3.155	0.433
	6	3.3	6.002	0.996

treated as a point: $\rho = e\,\delta(\mathbf{r} - \mathbf{v}t)$, c is a constant which cannot be calculated from the band theory. Such a calculation cannot possibly be correct, since a point electron obviously interacts not only with the longitudinal acoustic waves as given by formula (36), but with all other vibrations. Then the magnitude of the interaction turns out to be of the same order for both long and short wave vibrations. But the expression (38) is obviously not suitable for short wave oscillations. In addition, for $v \to C$ Buckingham's result diverges like $1/(v - C)$ (because the electron is treated as a point). As we see, all these difficulties are absent from the polaron theory.

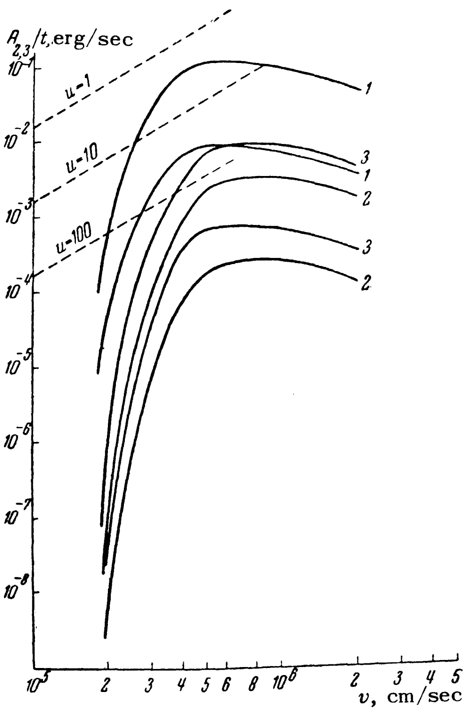

FIG. 2. Energy transferred from a polaron to the transverse optical vibrations of the lattice. The notation is the same as in Fig. 1. The upper curves show A_2/t, the lower curves A_3/t.

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