Mobility of piezopolaron in the case of strong coupling

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We consider the problem of strong interaction of particles with a quantum field (with phonons). An equation is derived for the amplitude of phonon scattering by a dressed particle. The equation is solved for the case of electron-phonon interaction in piezoelectric crystals. The mobility of the piezopolaron at low temperatures is calculated.

A piezopolaron is an electron interacting with acoustic modes in a piezoelectric crystal. A survey of research on the piezopolaron, for both strong and weak coupling between the piezopolaron and the acoustic phonons, can be found in.[1]

In this paper we determine the piezopolaron mobility, which is limited by scattering from thermal acoustic phonons. The problem of scattering under conditions of strong coupling is of interest in itself. It is attracting attention especially in connection with the problem of the polaron mobility in strong coupling. We therefore consider the general case of interaction of a particle with the field of phonons of arbitrary dispersion.

The scattering of phonons by a particle will be considered within the framework of the adiabatic perturbation theory proposed by Bogolyubov[2] and Tyabilikov.[3] This method makes it possible to expand consistently the Hamiltonian of the system in terms of the reciprocal coupling constant. By carrying out the Bogolyubov and Yyablikov transformation in conjunction with the transformation of Lee, Low, and Pines[4] we obtain the Hamiltonian of the system in the form of the sum of Hamiltonians of a dressed particle, free phonons, and interaction between the dressed particle and the phonons. Owing to the large mass of the dressed particle, the problem reduces to phonon scattering by a recoilless center. As a result, we obtain the Bethe-Salpeter equation, which expresses the total amplitude of the scattering in terms of the Born amplitude obtained from the transformed interaction Hamiltonian. In the case of the piezopolaron this equation can be easily solved in the limit of large wavelengths of the thermal acoustic phonons, so that its mobility at low temperatures can be calculated.

In the last section of this paper we consider also a logarithmic singularity in the piezopolaron energy.

1. TRANSFORMATION OF HAMILTONIAN

In the case of strong coupling, the Hamiltonian of a particle interacting with phonons is conveniently expressed in the dimensionless units $\hbar = m = \tilde{e} = 1$, where m is the bare mass of the particle, and $\tilde{e}$ is the effective charge:

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\sum_k V_k q_k e^{ikx}+\frac{1}{2}\sum_k [E^2(k)q_k^+q_k+\varepsilon^4 p_k^+ p_k]. \quad (1.1)$$

Here x is the coordinate of the particle; $q_k^+ = q_{-k}$ and $p_k^+ = p_{-k}$ are the canonically-conjugated coordinate and momentum operators of the k-th oscillator. The phonon spectrum is $\omega(k) = \epsilon^2 E(k)$ (ϵ is a small parameter, and V_k characterizes the interaction of the particle with the phonons). Our notation differs somewhat from that of Tyablikov.[3] In the case of the piezopolaron we have

$$V_k=\left(\frac{4\pi}{\Omega}\right)^{1/2},\quad E(k)=k,\quad \varepsilon^2=\frac{\hbar s}{\tilde{e}^2}=\frac{1}{2\alpha}, \quad (1.2)$$

where Ω is the volume of the system, s is the speed of sound, and $\alpha \gg 1$ is a dimensionless coupling constant (see[1]). In the case of a polaron

$$V_k=\left(\frac{4\pi}{\Omega}\right)^{1/2}\frac{1}{k},\quad E(k)=1,\quad \varepsilon^2=\frac{\hbar^3\omega_0}{m\tilde{e}^4}=\frac{1}{2\alpha^2}, \quad (1.3)$$

where ω_0 is the frequency of the optical phonons.

The system momentum operator takes the form

$$\hat{P}_a=-i\frac{\partial}{\partial x^a}-i\sum_k k_a q_k p_k. \quad (1.4)$$

We introduce new variables **r**, **R**, and Q_k by means of the formulas

$$x^a=r^a+R^a,\quad q_k=\xi_k e^{-ikR}+\varepsilon Q_k, \quad (1.5)$$

and impose on Q_k the three additional constraints:

$$\sum_k k\xi_k^* e^{ikR} Q_k=0, \quad (1.6)$$

in order to make the number of variables the same as before.

The coordinate **r** has the meaning of the coordinate of the internal motion of the particle in the phonon well made up by the displacements ξ_k, while **R** is the coordinate of the particle together with the well (or, in other words, of the dressed particle). Formulas (1.5)–(1.6) constitute the Bogolyubov and Tyablikov transformation[2,3] in conjunction with the inverse transformation of Lee, Low, and Pines[4]: $Q_k \exp(ik\cdot R)$. The transformation (1.5)–(1.6) enables us to obtain the Hamiltonian of the interaction of the dressed particle with the phonons, and by the same token enables us to formulate the scattering problem.

The derivatives $\partial/\partial x^a$ and $\partial/\partial q_k$ are transformed in accordance with the following law:

$$\partial/\partial x^a=\partial/\partial r^a,$$

$$\frac{\partial}{\partial q_k}=\frac{1}{\varepsilon}\frac{\partial}{\partial Q_k}-\frac{1}{2M}\xi_k^* k_a\left[e^{ikR}F^{ab}\left(K_b+\frac{\lambda_b}{\varepsilon}\right)+\left(K_b+\frac{\lambda_b}{\varepsilon}\right)F^{ab}e^{ikR}\right], \quad (1.7)$$

where

$$M=\frac{1}{3}\sum_k k^2|\xi_k|^2,\quad F=(1+\varepsilon A)^{-1},\quad A_{ab}=\frac{1}{M}\sum_k k_a k_b \xi_k^* e^{ikR},$$
$$K_a=-i\frac{\partial}{\partial R^a}+i\frac{\partial}{\partial r^a},\quad \lambda_a=\sum_k k_a\xi_k e^{-ikR}\frac{\partial}{\partial Q_k}, \quad (1.8)$$

and summation over the repeated indices a and b is implied.

To ensure unitarity of the transformation (1.5), the following transformation of the wave function was carried out:

$$\Psi=U\Psi',\quad U=\exp\{-{}^1\!/_2 \mathrm{Sp}\ln(1+\varepsilon A)\}. \quad (1.9)$$

Using (1.7), we obtain for the momentum and energy operators the expressions

$$\hat{P}_a=-i\frac{\partial}{\partial R^a}-i\sum_k k_a Q_k P_k, \quad (1.10)$$

$$H=H_0(\mathbf{r})+\varepsilon\sum_{\mathbf{k}}Q_{\mathbf{k}}e^{i\mathbf{k}\mathbf{R}}(V_{\mathbf{k}}e^{i\mathbf{k}\mathbf{r}}+E^2(\mathbf{k})\xi_{\mathbf{k}}^*)$$
$$+\frac{1}{2}\varepsilon^2\sum_{\mathbf{k}}[E^2(\mathbf{k})Q_{\mathbf{k}}Q_{-\mathbf{k}}+P_{\mathbf{k}}'(\mathbf{R})P_{-\mathbf{k}}'(\mathbf{R})] \quad (1.11)$$
$$+\frac{\varepsilon^4}{8M}\sum_c[(K_a-A_{ab}\lambda^b)F^{ac}+F^{ac}(K_a-\lambda^bA_{ab})]^2-\frac{\varepsilon^4}{8M^2}\sum_{\mathbf{k}}|\xi_{\mathbf{k}}|^2(k_aF^{ab}k_b)^2,$$

where

$$P_{\mathbf{k}}=-i\frac{\partial}{\partial Q_{\mathbf{k}}},\quad P_{\mathbf{k}}'(\mathbf{R})=P_{\mathbf{k}}-\frac{e^{i\mathbf{k}\mathbf{R}}}{\sqrt{M}}k^a\xi_{\mathbf{k}}^*\sum_{\mathbf{k}'}\frac{e^{-i\mathbf{k}'\mathbf{R}}}{\sqrt{M}}k_a'\xi_{\mathbf{k}'}P_{\mathbf{k}'}, \quad (1.12)$$

$$H_0(\mathbf{r})=-\frac{1}{2}\frac{\partial^2}{\partial\mathbf{r}^2}+\sum_{\mathbf{k}}V_{\mathbf{k}}\xi_{\mathbf{k}}e^{i\mathbf{k}\mathbf{r}}+\frac{1}{2}\sum_{\mathbf{k}}E^2(\mathbf{k})|\xi_{\mathbf{k}}|^2. \quad (1.13)$$

We denote by φ_n the eigenfunctions of the operator H_0:

$$H_0\varphi_n=E_n\varphi_n \quad (1.14)$$

and change over into a matrix representation in terms of these functions

$$\langle m|H|n\rangle=\int d^3r\,\varphi_m^*(\mathbf{r})H\varphi_n(\mathbf{r}). \quad (1.15)$$

To eliminate from (1.15) the off-diagonal terms that are linear in ϵ, it is necessary to carry out the unitarity transformation

$$H'=e^{-S}He^{S}, \quad (1.16)$$

where

$$S_{mn}=\begin{cases}0, & E_n=E_m,\\ \dfrac{\varepsilon}{E_m-E_n}\sum_{\mathbf{k}}Q_{\mathbf{k}}e^{i\mathbf{k}\mathbf{R}}V_{\mathbf{k}}\int d^3r\varphi_n^*e^{i\mathbf{k}\mathbf{r}}\varphi_m(r), & E_n\neq E_m.\end{cases}$$

The transitions between states with different E_n will now make a contribution $\sim\epsilon^4$ to the energy. We can therefore assume, with the same degree of accuracy, that the particle in the phonon well is in the ground state at all times, and the Hamiltonian of the system is $\langle 0|H'|0\rangle$. The term linear in ϵ in the Hamiltonian $\langle 0|H'|0\rangle$ is illuminated by the following choice of ξ_k:

$$\xi_{\mathbf{k}}^*=-\frac{V_{\mathbf{k}}}{E^2(\mathbf{k})}\int d^3r|\varphi_0(\mathbf{r})|^2e^{i\mathbf{k}\mathbf{r}}. \quad (1.17)$$

Equations (1.17) and (1.14) with n = 0 can also be obtained by varying the functional

$$J=\int d^3r\varphi^*(\mathbf{r})H_0(\mathbf{r})\varphi(\mathbf{r}) \quad (1.18)$$

with respect to φ and ξ_k. The energy E_0 is the absolute minimum of this function which is realized on the function $\varphi_0(\mathbf{r})$. The functional describes the motion of the particle in a classical field. It was first derived for the case of the polaron by Pekar.[5] 1)

Let us write out $\langle 0|H'|0\rangle$, retaining the terms $\sim\epsilon^2$ and the principal terms containing $\partial/\partial R^a$:

$$\langle 0|H'|0\rangle-E_0=\frac{\varepsilon^2}{2}\sum_{\mathbf{k}}[E^2(\mathbf{k})Q_{\mathbf{k}}^+Q_{\mathbf{k}}+P_{\mathbf{k}}^+P_{\mathbf{k}}]-\frac{\varepsilon^4}{2M}\frac{\partial^2}{\partial R^2}$$
$$-\varepsilon^2\sum_{\mathbf{k}\mathbf{k}'}D_{-\mathbf{k},\mathbf{k}'}e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}}Q_{\mathbf{k}}^+Q_{\mathbf{k}'}-\frac{\varepsilon^2}{2M}\sum_{\mathbf{k}\mathbf{k}'}(k^ak_a')\xi_{\mathbf{k}}\xi_{\mathbf{k}'}^*e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}}P_{\mathbf{k}}P_{\mathbf{k}'}^+ \quad (1.19)$$
$$-\frac{\varepsilon^4}{2M}\sum_{\mathbf{k}\mathbf{k}'}(k^bk_b')\xi_{\mathbf{k}}^*\xi_{\mathbf{k}'}Q_{\mathbf{k}}P_{\mathbf{k}'}\left[e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}}k_a\frac{\partial}{\partial R^a}+k_a\frac{\partial}{\partial R^a}e^{i(\mathbf{k}-\mathbf{k}')\mathbf{R}}\right],$$

where

$$D_{\mathbf{k}\mathbf{k}'}=V_{\mathbf{k}}V_{\mathbf{k}'}\sum_{n\neq 0}\frac{I_{\mathbf{k}}^{0n}I_{\mathbf{k}'}^{n0}}{E_n-E_0},\quad I_{\mathbf{k}}^{mn}=\int d^3r\varphi_m^*(\mathbf{r})e^{i\mathbf{k}\mathbf{r}}\varphi_n(\mathbf{r}). \quad (1.20)$$

The second term in (1.19) is the kinetic energy of a dressed particle with mass

$$M^*=\varepsilon^{-4}M. \quad (1.21)$$

The three last two terms describe the two-phonon interactions of the particle with the field. As will be shown later on, the condition (1.6) makes an additional contribution to the two-phonon interaction, which has the same order of magnitude as the last term in (1.19).

The single-phonon interaction is described by terms of higher order in ϵ. Confining ourselves to the principal terms containing $\partial/\partial\mathbf{R}$, we obtain for them the following expression:

$$H_1=\frac{\varepsilon^5}{4M^2}\sum_{\mathbf{k}}k_ak_b\xi_{\mathbf{k}}^*Q_{\mathbf{k}}\left[e^{i\mathbf{k}\mathbf{R}}\frac{\partial^2}{\partial R_a\partial R_b}+2\frac{\partial}{\partial R_a}e^{i\mathbf{k}\mathbf{R}}\frac{\partial}{\partial R_b}+\frac{\partial^2}{\partial R_a\partial R_b}e^{i\mathbf{k}\mathbf{R}}\right]. \quad (1.22)$$

In an electric field $\mathbf{E}$, it is necessary to add to the Hamiltonian (1.11) the term

$$H_e=-e\mathbf{E}\mathbf{r}-e\mathbf{E}\mathbf{R}. \quad (1.23)$$

Since we are interested in the linear response of the system, we can regard each term of (1.23) separately. The first term commutes with the momentum operator of the system (1.10) and leads only to a small shift of the electron levels in the polarization well, and also to nonlinear effects connected with the quasistationary character of these levels in the electric field. These effects become significant in sufficiently strong fields, when the probability of the transition to the continuous spectrum increases. Thus, in weak fields, the dissipation of the energy is determined by the second term of (1.23), and, in accordance with the general formulas of statistical mechanics, it is given by

$$\dot{E}=e\mathbf{E}\langle\dot{\mathbf{R}}\rangle,$$

where the angle brackets denote averaging over the Gibbs distribution. On the other hand, from the fact that the energy dissipation should be equal to the work performed by the electric field on the electron moving with average velocity $\langle \mathbf{v}\rangle$, we conclude that $\langle \mathbf{v}\rangle = \langle\dot{\mathbf{R}}\rangle$.

It follows therefore that in a weak field the mobility of the electron coincides with the mobility of a particle having a spectrum $E_0p^2/2M^*$ and interacting with the phonons in accordance with the Hamiltonian (1.19) and (1.22).

Since this interaction is weak in the sense that it does not change significantly the energy and the mass of the particle, we can use the Boltzmann equation in the calculation of the mobility. To satisfy the condition $\hbar/\tau \ll T$, we assume that the number of thermal phonons is small, i.e., $T \ll \epsilon^2$.

Let us ascertain which processes make the main contribution to the collision integral. We consider first the emission and absorption processes. The amplitude for the emission of a phonon with momentum $\mathbf{k}$ is determined with the aid of formula (1.22):

$$W_{\mathbf{p},\mathbf{p}-\mathbf{k}}=\frac{1}{\Omega^{\cdot}}\int d^3Re^{-i(\mathbf{p}-\mathbf{k})\mathbf{R}}\langle\mathbf{k}|H_1|0\rangle e^{i\mathbf{p}\mathbf{R}}$$
$$=\frac{\varepsilon}{\sqrt{2E(\mathbf{k})}}V_{\mathbf{k}}\int d^3re^{i\mathbf{k}\mathbf{r}}|\varphi_0(r)|^2.$$

We have used formula (1.17) for ξ_k and the conservation of the energy in phonon emission. A similar formula is obtained for the absorption. At particle momenta $p^2/2M^* \sim T \ll \xi^2$, the momentum of the emitted and absorbed phonons is $k \sim \epsilon^{-1}$ for optical phonons and $k \sim \epsilon^{-2}$ for acoustic phonons, and therefore the amplitude $W_{p,p-k}$ is exponentially small (the function $\varphi_0(r)$ has no singularities on the real axis).

We consider now the scattering processes.

2. EQUATION FOR THE AMPLITUDE OF PHONON SCATTERING BY A DRESSED PARTICLE

To calculate the scattering amplitude we could use the Hamiltonian (1.19) with conditions (1.6). The problem becomes simpler if we take into consideration the fact that the mass of the dressed particle is large: $M^* \sim \epsilon^{-4}$. This means that it is possible to neglect the recoil energy and, changing over to the c.m.s., consider the scattering phonons by an immobile center. The transition to the c.m.s. is carried out by means of the transformation of Lee, Low, and Pines[4], which is realized by the unitary matrix

$$U=\exp\left\{-R^a\sum_{\mathbf{k}}k_aQ_{\mathbf{k}}P_{\mathbf{k}}\right\}. \tag{2.1}$$

Recognizing that

$$U^+Q_{\mathbf{k}}U=Q_{\mathbf{k}}e^{-i\mathbf{k}\mathbf{R}}, \tag{2.2}$$

$$U^+\left(-i\frac{\partial}{\partial R^a}\right)U=-i\frac{\partial}{\partial R^a}+i\sum_{\mathbf{k}}k_aQ_{\mathbf{k}}P_{\mathbf{k}},\quad U^+\hat{P}_aU=-i\frac{\partial}{\partial R^a}, \tag{2.3}$$

we obtain the Hamiltonian in the same form as obtained by Bogolyubov and Tyablikov[2,3]

$$\begin{aligned}U^+\langle 0|H'|0\rangle U=E_0+\frac{P^2}{2M^*}+\frac{\varepsilon^2}{2}\sum_{\mathbf{k}\mathbf{k}'}[E^2(\mathbf{k})\delta_{\mathbf{k}\mathbf{k}'}-2D_{-\mathbf{k}\mathbf{k}'}]Q_{\mathbf{k}}^+Q_{\mathbf{k}'}\\+\frac{\varepsilon^2}{2}\sum_{\mathbf{k}}P_{\mathbf{k}}'^+P_{\mathbf{k}}'+i\frac{P^a}{M^*}\sum_{\mathbf{k}}k_aQ_{\mathbf{k}}P_{\mathbf{k}}',\quad P_{\mathbf{k}}'=P_{\mathbf{k}}'(0).\end{aligned} \tag{2.4}$$

In (2.4) we have neglected the term $(\Sigma \mathbf{k}Q_{\mathbf{k}}P_{\mathbf{k}})^2/2M^*$, which represents the recoil energy and which is small in terms of the parameter ϵ, and have replaced the momentum operator by a c-number, namely $i\partial/\partial R^0 = P^a$.

The constraints (1.6) take the form

$$\sum_{\mathbf{k}}k_a\xi_{\mathbf{k}}^*Q_{\mathbf{k}}=0. \tag{2.5}$$

We can get rid of these conditions in the following manner. We place $Q_{\mathbf{k}}$ formally in (2.4) by the expression

$$Q_{\mathbf{k}}'=Q_{\mathbf{k}}-\frac{1}{\sqrt{M}}k^a\xi_{\mathbf{k}}\sum_{\mathbf{k}'}\frac{1}{\sqrt{M}}k_a'\xi_{\mathbf{k}'}^*Q_{\mathbf{k}'}. \tag{2.6}$$

We denote the obtained Hamiltonian H'':

$$\begin{aligned}H''=E_0+\frac{P^2}{2M^*}+\frac{\varepsilon^2}{2}\sum_{\mathbf{k}}[E^2(\mathbf{k})\delta_{\mathbf{k}\mathbf{k}'}-2D_{-\mathbf{k},\mathbf{k}'}]Q_{\mathbf{k}}^{+\prime}Q_{\mathbf{k}'}'\\+\frac{\varepsilon^2}{2}\sum_{\mathbf{k}}P_{\mathbf{k}}^{+\prime}P_{\mathbf{k}}'+i\frac{P^a}{M^*}\sum_{\mathbf{k}}k_aQ_{\mathbf{k}}'P_{\mathbf{k}}'.\end{aligned} \tag{2.7}$$

We note that the operator $P_{\mathbf{k}}'$ commutes with the operator $\Sigma k^a\xi_{\mathbf{k}}^*Q_{\mathbf{k}}$. Therefore the Hamiltonian H'' with the conditions (2.5) is equivalent to the Hamiltonian (2.4) with the same conditions.

We shall show now that for the Hamiltonian H'' the conditions (2.5) are unnecessary and can be omitted. To this end we consider the $N \times N$ matrix

$$M_{\mathbf{k}\mathbf{k}'}=E^2(\mathbf{k})\delta_{\mathbf{k}\mathbf{k}'}-2D_{-\mathbf{k},\mathbf{k}'}, \tag{2.8}$$

where N is the number of oscillators in the volume Ω. This matrix is Hermitian and has three eigenvectors:

$$U_{\mathbf{k}}^a=i\frac{1}{\sqrt{M}}k^a\xi_{\mathbf{k}}, \tag{2.9}$$

corresponding to a zero eigenvalue (see[7,8]), i.e.,

$$\sum_{\mathbf{k}'}M_{\mathbf{k}\mathbf{k}'}U_{\mathbf{k}'}^a=0. \tag{2.10}$$

The remaining eigenvalues of the matrix $M_{\mathbf{k}\mathbf{k}'}$ are positive; this follows from the fact that the matrix $M_{\mathbf{k}\mathbf{k}'}$ is the second variation of the functional J (1.18) at $\varphi = \varphi_0$. The presence of three zero eigenvalues corresponds to the fact that the functional J is invariant with respect to translations. We denote the remaining N−3 orthonormal eigenvectors of the matrix $M_{\mathbf{k}\mathbf{k}'}$ by $U_{\mathbf{k}}^\sigma$, and the eigenvalues by M^σ. The following orthogonality relations hold:

$$\sum_{\mathbf{k}}U_{\mathbf{k}}^{*\sigma}U_{\mathbf{k}}^{\sigma'}=\delta_{\sigma\sigma'},\quad \sum_{\mathbf{k}}U_{\mathbf{k}}^{*\sigma}U_{\mathbf{k}}^a=0,\quad \sum_{\mathbf{k}}U_{\mathbf{k}}^{*a}U_{\mathbf{k}}^b=\delta_{ab}. \tag{2.11}$$

We effect with the aid of these vectors a unitary transformation of the variables $Q_{\mathbf{k}}$ to new variables z_σ and z_a:

$$Q_{\mathbf{k}}=\sum_{\sigma=1}^{N-3}U_{\mathbf{k}}^\sigma z_\sigma+\sum_{a=1}^{3}U_{\mathbf{k}}^az_a. \tag{2.12}$$

Inasmuch as in accordance with (2.6) and (2.4) we have

$$Q_{\mathbf{k}}'=\sum_{\sigma=1}^{N-3}U_{\mathbf{k}}^\sigma z_\sigma,\quad P_{\mathbf{k}}'=-i\sum_{\sigma=1}^{N-3}U_{\mathbf{k}}^{*\sigma}\frac{\partial}{\partial z^\sigma},$$

the Hamiltonian H'' depends neither on z^a nor on $\partial/\partial z^a$:

$$\begin{aligned}H''=E_0+\frac{P^2}{2M^*}+\frac{\varepsilon^2}{2}\sum_{\sigma=1}^{N-3}\left(M^\sigma z_\sigma^2-\frac{\partial^2}{\partial z_\sigma^2}\right)\\+\frac{P^a}{M^*}\sum_{\sigma\sigma'}z^\sigma\frac{\partial}{\partial z^{\sigma'}}\sum_{\mathbf{k}}U_{\mathbf{k}}^{*\sigma'}k_aU_{\mathbf{k}}^\sigma.\end{aligned} \tag{2.13}$$

The conditions (2.5) now take the form $z^a = 0$. These conditions have no bearing whatever on the Hamiltonian (2.13) and can therefore be omitted. Obviously, the system described by the Hamiltonian (2.13) does not change physically when a term $0\cdot(z_a^2-\partial^2/\partial z_a^2)$ is added to it. Then, changing over to the variables $Q_{\mathbf{k}}$ in accordance with formula (2.12), we obtain the Hamiltonian (2.7), which can be used in the calculation of the scattering amplitude even without taking the conditions (2.5) into account.

This procuedure of eliminating the conditions (2.5) is valid in all orders in ϵ, since the Hamiltonian $U^+\langle 0|H'|0\rangle U$ depends on $P_{\mathbf{k}}$, in all orders in ϵ, only via $P_{\mathbf{k}}'$(see[2]). On the other hand, if the recoil energy cannot be neglected, then after substituting $Q_{\mathbf{k}}'$ in place of $Q_{\mathbf{k}}$ in the Hamiltonian $U^+\langle 0|H'|0\rangle U$, it is necessary to rewrite again in the form (1.19). This naturally gives rise to the appearance of additional terms in the interaction.

We now express the Hamiltonian (2.7) in terms of the Bose phonon creation and annihilation operators:

$$H''=E_0+\frac{P^2}{2M^*}+H_{ph}+H_{int}, \tag{2.14}$$

where

$$H_{ph}=\sum_{\mathbf{k}}\left[\varepsilon^2E(\mathbf{k})-\frac{k_aP^a}{M^*}\right]\left(a_{\mathbf{k}}^+a_{\mathbf{k}}+\frac{1}{2}\right),$$

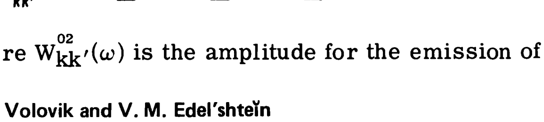
$$\begin{aligned}H_{int}=-\frac{\varepsilon^2}{2}\sum_{\mathbf{k}\mathbf{k}'}B_{-\mathbf{k},\mathbf{k}'}(a_{\mathbf{k}'}+a_{-\mathbf{k}'}^+)(a_{\mathbf{k}}^++a_{-\mathbf{k}})\\-\frac{\varepsilon^2}{2}\sum_{\mathbf{k}\mathbf{k}'}C_{\mathbf{k}'\mathbf{k}}(a_{-\mathbf{k}'}-a_{\mathbf{k}'}^+)(a_{-\mathbf{k}}^+-a_{\mathbf{k}})\end{aligned} \tag{2.15}$$

$$-\frac{P^a}{M^*}\sum_{\mathbf{k}\mathbf{k}'}(k_a+k_a')C_{\mathbf{k}'\mathbf{k}}\frac{(a_{\mathbf{k}}+a_{-\mathbf{k}}^+)(a_{-\mathbf{k}'}-a_{\mathbf{k}'}^+)}{E(\mathbf{k})}, \tag{2.16}$$

$$\begin{aligned}B_{\mathbf{k}\mathbf{k}'}=D_{\mathbf{k}\mathbf{k}'}/[E(\mathbf{k})E(\mathbf{k}')]^{1/2},\\C_{\mathbf{k}\mathbf{k}'}=\xi_{\mathbf{k}}\xi_{\mathbf{k}'}^*[E(\mathbf{k})E(\mathbf{k}')]^{1/2}k^ak_a'/2M;\end{aligned} \tag{2.17}$$

H_{int} describes the interaction of the phonons with the center located at the point R = 0.

The amplitude $W_{\mathbf{k}\mathbf{k}'}^{int}(\omega)$ for the scattering of a phonon by the center satisfies the following graphic equation



(2.18)

where $W_{\mathbf{k}\mathbf{k}'}^{02}(\omega)$ is the amplitude for the emission of two phonons. The internal lines are the nonrenormalized Green's function of the phonon:

$$\left[\omega-\varepsilon^2E(\mathbf{k})+\frac{k^aP_a}{M^*}+i\delta\right]^{-1}, \qquad (2.19)$$

and the unshaded squares represent the nonrenormalized scattering amplitude, and also the amplitudes for the emission and omission of two phonons. Their analytic expressions are respectively

$$\langle a_{\mathbf{k}}H_{\rm int}a_{\mathbf{k}'}{}^+\rangle,\ \langle H_{\rm int}a_{-\mathbf{k}}{}^+a_{\mathbf{k}'}{}^+\rangle,\ \langle a_{\mathbf{k}}a_{-\mathbf{k}'}H_{\rm int}\rangle. \qquad (2.20)$$

3. PIEZOPOLARON MOBILITY AT LOW TEMPERATURES

According to (1.2), the spectrum of the acoustic phonons is of the form $\omega(k) = \epsilon_k^2$. We are interested in the case of low temperatures $T \ll \epsilon^2$, when the characteristic momentum of the thermal phonon is $k \sim T\epsilon^{-2} \ll 1$, and the characteristic momentum of the piezopolarn is $p \sim \sqrt{M^*T} \sim \sqrt{T}\epsilon^{-2}$. It follows therefore that $k \ll p \ll \epsilon^{-1}$. The condition $p \ll \epsilon^{-1}$ denotes that the particle velocity is $v = p/M^* \sim P/M^* \ll \epsilon^3$, so that the terms containing P/M^* can be neglected.

The condition $p \gg k$ denotes smallness of the momentum transfer in the collision, and indicates by the same token that the Fokker-Planck equation can be used for the piezopolaron momentum distribution function. The piezopolaron mobility μ is then expressed in terms of the mean-squared momentum loss per unit time in scattering by thermal phonons:

$$\mu^{-1}=\frac{1}{6eT}\sum_{\mathbf{k},\mathbf{k}'}|W_{\mathbf{k}\mathbf{k}'}^{11}(\omega(\mathbf{k}))|^2n(\mathbf{k})[1+n(\mathbf{k}')](\mathbf{k}-\mathbf{k}')^22\pi\delta[\omega(\mathbf{k})-\omega(\mathbf{k}')]. \qquad (3.1)$$

Here ie is the electron charge and $n_k = [\exp(\omega(k)/T)-1]^{-1}$.

We now obtain $W_{kk'}{}^{11}(\omega)$ at $k, k' \ll 1$, $\omega = \epsilon^2 k = \epsilon^2 k'$. To this end we eliminate W^{02} from (2.18). After a number of simple transformations (see the Appendix) we obtain for $W_{kk'}^{11}$ the equation

$$\widetilde{W}_{\mathbf{k}\mathbf{k}'}^{11}(\tilde\omega)+2\sum_{\mathbf{q}}B_{-\mathbf{k},\mathbf{q}}E(\mathbf{q})\frac{1}{\tilde\omega^2-E^2(\mathbf{q})+i\delta}\widetilde{W}_{\mathbf{q}\mathbf{k}'}^{11}(\tilde\omega)=-B_{-\mathbf{k},\mathbf{k}'}, \qquad (3.2)$$

where

$$\widetilde{W}_{\mathbf{k}\mathbf{k}'}^{11}(\tilde\omega)=\varepsilon^{-2}W_{\mathbf{k}\mathbf{k}'}^{11}(\omega),\ \tilde\omega=\varepsilon^{-2}\omega,\ \tilde\omega\ll1. \qquad (3.3)$$

The quation for $\widetilde{W}^{11}$ does not contain the parameter ϵ. We note that the characteristic q in the sum (3.2) are of the order of unity, so that the kernel in the sum can be expanded in the small $\tilde\omega^2$. After expansion up to first order inclusive, we obtain

$$\widetilde{W}_{\mathbf{k}\mathbf{k}'}^{11}(\tilde\omega)-2\sum_{\mathbf{q}}B_{-\mathbf{k},\mathbf{q}}E^{-1}(\mathbf{q})\widetilde{W}_{\mathbf{q}\mathbf{k}'}^{11}(\tilde\omega)-2\tilde\omega^2\sum_{\mathbf{q}}B_{-\mathbf{k},\mathbf{q}}E^{-3}(\mathbf{q})\widetilde{W}_{\mathbf{q}\mathbf{k}'}^{1}(\tilde\omega)=-B_{-\mathbf{k},\mathbf{k}'}. \qquad (3.4)$$

As seen from (2.10), the homogeneous equation (3.4) (without the right-hand side) has at $\tilde\omega = 0$ solutions of the type

$$f(\mathbf{k}')E^{1/2}(\mathbf{k})U_{\mathbf{k}}{}^a,$$

where f(k) is an arbitrary function of k. Therefore the solution of the inhomogeneous equation (3.4) as $\tilde\omega \to 0$ is represented in the form

$$\widetilde{W}_{\mathbf{k}\mathbf{k}'}^{11}(\tilde\omega)=\mathrm{const}[E(\mathbf{k})E(\mathbf{k}')]^{1/2}\tilde\omega^{-2}U_{\mathbf{k}}{}^aU_{\mathbf{k}'a}^*+\widetilde{\widetilde{W}}{}_{\mathbf{k}\mathbf{k}'}^{11}+O(\tilde\omega^2), \qquad (3.5)$$

where the constant is determined from the solvability condition for $\widetilde{\widetilde{W}}$, and turns out to equal 1/2.

Retaining in (3.5) the first term and substituting it into (3.3), we obtain for the amplitude of phonon scattering by a center the following expression at $k, k' \ll 1$, $\omega = \omega(k) = \omega(k')$:

$$W_{\mathbf{k}\mathbf{k}'}^{11}(\omega)\approx V_{\mathbf{k}}V_{\mathbf{k}'}\frac{\varepsilon^2}{\sqrt{kk'}}\frac{k^ak_a'}{2M^*\omega(\mathbf{k})\omega(\mathbf{k}')}. \qquad (3.6)$$

A similar result is obtained in second order of perturbation theory with Hamiltonian (1.1), in which the bare mass m is replaced by the piezopolaron mass M*.

Substituting (3.6) in formula (3.1) for the mobility, we obtain

$$\mu^{-1}=\frac{8\pi^3}{135eM^{*2}}\left(\frac{T}{\varepsilon^2}\right)^4,$$

or, in dimensional units,

$$\mu=\frac{135}{32\pi^3\alpha^2}\frac{(M^*s^2)^2}{T^4}es^2. \qquad (3.7)$$

In the case of the polaron, the equation with the amplitude for scattering by optical phonons was obtained in.[9] In our notation it takes the form

$$W_{\mathbf{k}\mathbf{k}'}^{11}=-\varepsilon^2B_{-\mathbf{k},\mathbf{k}'}+\varepsilon^2\sum_{\mathbf{q}}B_{-\mathbf{k},\mathbf{q}}\frac{1}{q_av^a-k_a'v^a+i\delta}W_{\mathbf{q}\mathbf{k}'}^{11}, \qquad (3.8)$$

where

$$W_{\mathbf{k}\mathbf{k}'}^{11}=W_{\mathbf{k},\mathbf{k}'}^{11}(\omega=\varepsilon^2-k_av^a=\varepsilon^2-k_a'v^a);$$

v_a is the polaron velocity, and the inequality $\epsilon^{11/3} \ll v \ll \epsilon^2$ is assumed satisfied.

It is easily seen that Eq. (3.8) can be obtained from (2.18) by eliminating W^{02} and neglecting the small terms $v\epsilon^{-2} \ll 1$. (It follows from the condition $v \gg \epsilon^{11/3}$ that the polaron momentum is $p \gg k$, where k is the characteristic momentum of the scattered optical phonon. Therefore the quantity P_a/M^* in (2.14) is the polaron velocity: $P_a/M^* = (p_a + k_a)/M^* \approx p_a/M^* = v^a$.)

The translational coordinate R was introduced in[9] in the following manner: the phonon coordinates in the Lagrangian of the system were subjected to the transformation $q_k \to q_k^0 e^{-ikR(t)} + q_k'$, where R(t) is an arbitrary function of the time, after which the Lagrangian became formally dependent on R(t) and $\dot{R}(t)$. The function R(t) was then regarded as a dynamic variable, the translational coordinate of the polaron. Although this procedure is not quite correct, the errors incurred thereby are small in terms of the parameter ϵ and do not effect the value of the scattering amplitude.

4. LOGARITHMIC SINGULARITY IN THE PIEZOPOLARON ENERGY

Corrections of the order of ϵ^2 to the energy of the ground state of the piezopolaron at P = 0 are the result of a change in the energy of the zero-point oscillations of the crystal in the presence of an electron (see (2.13)):

$$\delta E^{(2)}=\frac{\varepsilon^2}{2}\sum_{\sigma=1}^{N-3}\sqrt{M_\sigma}-\frac{\varepsilon^2}{2}\sum_{\mathbf{k}}E(\mathbf{k}). \qquad (4.1)$$

Adding three zero eigenvalues $M^a = 0$ to the sum over σ, we obtain

$$\sum_{\sigma=1}^{N-3}\sqrt{M_\sigma}=\sum_{\sigma=1}^{N-3}\sqrt{M_\sigma}+\sum_{a=1}^{3}\sqrt{M_a}=\mathrm{Sp}\sqrt{M}=\mathrm{Sp}\sqrt{E^2-2D}, \qquad (4.2)$$

where E denotes the matrix $E(k)\,\delta_{kk'}$ and D denotes the matrix $D_{-k,k'}$ (see (1.20)).

Substituting (4.2) in (4.1) we obtain the perturbation-theory series

$$\delta E^{(2)}=-\frac{\varepsilon^2}{2}\sum_{\mathbf{k}}B_{-\mathbf{k},\mathbf{k}}-\frac{\varepsilon^2}{2}\sum_{\mathbf{k}\mathbf{k}'}B_{-\mathbf{k}\mathbf{k}'}[E(\mathbf{k})+E(\mathbf{k}')]^{-1}B_{-\mathbf{k}',\mathbf{k}}+\dots \qquad (4.3)$$

We shall show that the linear term in (4.3) diverges logarithmically. Let us examine this term:

$$\mathrm{Sp}\,B=\frac{4\pi}{\Omega}\sum_{\mathbf{k}}\frac{1}{k}\sum_{n\neq0}\frac{1}{E_n-E_0}\left|\int d^3r\varphi_n^*(\mathbf{r})e^{i\mathbf{kr}}\varphi_0(\mathbf{r})\right|^2 \quad (4.4)$$

The main contribution to (4.4) is made by large k and by large n. At large n we arrive at the continuous spectrum of the Hamiltonian $H_0(r)$ (see (1.13)):

$$E_n\to E_{\mathbf{p}}=\frac{\mathbf{p}^2}{2},\quad \varphi_n\to\varphi_{\mathbf{p}}=\frac{1}{\sqrt{\Omega}}e^{i\mathbf{pr}},$$

and then

$$\mathrm{Sp}\,B\approx\frac{4\pi}{\Omega^2}\sum_{\substack{k\gg1\\ p\gg1}}\frac{1}{k}\frac{2}{p^2}|(\varphi_0)_{\mathbf{p}-\mathbf{k}}|^2=\frac{8\pi}{\Omega^2}\sum_{\substack{\mathbf{p}\\ k\gg1}}\frac{1}{k}\frac{|(\varphi_0)_{\mathbf{p}}|^2}{|\mathbf{k}+\mathbf{p}|^2}, \quad (4.5)$$

where $(\varphi_0)_p$ is the Fourier component of the function $\varphi_0(r)$. Since the momentum p in the sum over p is of the order of unity, it can be negelcted in the denominator of (4.5) in comparison with $k \gg 1$. Then, taking into account the equality

$$\frac{1}{\Omega}\sum_{\mathbf{p}}|(\varphi_0)_{\mathbf{p}}|^2=1,$$

which follows from the normalization of φ_0 to unity, we obtain

$$\mathrm{Sp}\,B\approx\frac{8\pi}{\Omega}\sum_{k\gg1}\frac{1}{k^3}\approx\frac{4}{\pi}\ln q_m, \quad (4.6)$$

where q_m is the limiting momentum, equal in order of magnitude to the crystal reciprocal-lattice vector. It is easy to verify that the remaining terms in (4.3) have no divergence at large k. We therefore have, with logarithmic accuracy,

$$\delta E^{(2)}=-\frac{2\varepsilon^2}{\pi}\ln q_m,$$

or, in dimensional units,

$$\delta E^{(2)}=-\frac{4\alpha}{\pi}ms^2\ln\frac{q_m}{\alpha ms}. \quad (4.7)$$

The value of $\delta E^{(2)}$ differs from the piezopolaron energy in the case of weak coupling ($\alpha \ll 1$) only that in the case of weak coupling the argument of the logarithm does not depend on α.

Formula (4.7) was obtained in not quite a consistent manner in[1], where it was assumed that perturbation theory rather than the adiabatic approach is applicable to short-wave phonons with energies larger than the piezopolaron energy.

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APPENDIX

In terms of the notation (3.3), Eqs. (2.18) at P = 0 have the following analytic form:

$$\tilde W^{11}_{\mathbf{kk}'}(\tilde\omega)=-B_{-\mathbf{k},\mathbf{k}'}-C_{\mathbf{kk}'}-\sum_{\mathbf{q}}(B_{-\mathbf{k},\mathbf{q}}+C_{\mathbf{kq}})\frac{\tilde W^{11}_{\mathbf{q},\mathbf{k}'}(\tilde\omega)}{\tilde\omega-E(\mathbf{q})+i\delta}+\sum_{\mathbf{q}}(B_{-\mathbf{k},\mathbf{q}}-C_{\mathbf{kq}})\frac{\tilde W^{02}_{\mathbf{qk}'}(\tilde\omega)}{\tilde\omega+E(\mathbf{q})-i\delta}, \quad (A.1)$$

$$\tilde W^{02}_{\mathbf{kk}'}(\tilde\omega)=-B_{-\mathbf{k},\mathbf{k}'}+C_{\mathbf{kk}'}-\sum_{\mathbf{q}}(B_{-\mathbf{k},\mathbf{q}}-C_{\mathbf{kq}})\frac{\tilde W^{11}_{\mathbf{qk}'}(\tilde\omega)}{\tilde\omega-E(\mathbf{q})+i\delta}+\sum_{\mathbf{q}}(B_{-\mathbf{k},\mathbf{q}}+C_{\mathbf{kq}})\frac{\tilde W^{02}_{\mathbf{qk}'}(\tilde\omega)}{\tilde\omega+E(\mathbf{q})-i\delta} \quad (A.2)$$

We introduce in place of $\tilde W^{11}$ and $\tilde W^{02}$ new functions, X and Y, in accordance with the formulas

$$\tilde W^{11}_{\mathbf{kk}'}=[\tilde\omega-E(\mathbf{k})][X_{\mathbf{kk}'}+Y_{\mathbf{kk}'}].$$
$$\tilde W^{02}_{\mathbf{kk}'}=[\tilde\omega+E(\mathbf{k})][X_{\mathbf{kk}'}-Y_{\mathbf{kk}'}]. \quad (A.3)$$

Using the matrix equations

$$2\sum_{\mathbf{q}}B_{-\mathbf{k},\mathbf{q}}C_{\mathbf{qk}'}=E(\mathbf{k})C_{\mathbf{kk}'},\quad 2\sum_{\mathbf{q}}C_{\mathbf{kq}}B_{-\mathbf{q},\mathbf{k}'}=C_{\mathbf{kk}'}E(\mathbf{k}'), \quad (A.4)$$

which follow from (2.10), we obtain for X and Y the equations

$$(\tilde\omega^2-E^2)X+2BEX=-\tilde\omega B,\quad (\tilde\omega^2-E^2)Y+2EBY=-EB, \quad (A.5)$$

where E stands for the matrix $E(k)\,\delta_{kk'}$.

Making the new substitution

$$\tilde X=(\tilde\omega^2-E^2)XE^{-1},\quad \tilde Y=E^{-1}(\tilde\omega^2-E^2)Y, \quad (A.6)$$

we obtain the equations

$$\tilde X+2B\frac{E}{\tilde\omega^2-E^2}\tilde X=-B\frac{\tilde\omega}{E},\quad \tilde Y+2B\frac{E}{\tilde\omega^2-E^2}\tilde Y=-B. \quad (A.7)$$

From (A.3) and (A.6) we see that X and Y coincide with $\tilde W^{11}$ for a real process, i.e., at $\tilde\omega = E(k) = E(k')$. Therefore, to find $W^{11}_{kk'}(\tilde\omega)$ at $\tilde\omega = E(k) = E(k')$ we can use any of the equations in (A.7), which are equivalent in this sense. When expanded, the second equation of (A.7) takes form (3.2).

[1)]Pekar's method was applied to the piezopolaron problem by Pokatilov [6].

[1]G. Whitfield and P. M. Platzman, Phys. Rev. B6, 3987, (1972).
[2]N. N. Bogolyubov, Ukr. matem. zhur. 2, 3 (1950).
[3]S. V. Tyablikov, Zh. Eksp. Teor. Fiz. 21, 377 (1951).
[4]T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. 90, 297 (1953).
[5]S. I. Pekar, Issledovaniya po elektronnoĭ teoriĭ kristallov (Research on Electron Theory of Crystals), Gostekhizdat (1961).
[6]E. P. Pokatilov, Fiz. Tverd. Tela 6, 2809 (1964) [Sov. Phys.-Solid State 6, 2233 (1965)].
[7]S. V. Tyablikov and V. A. Moskalenko, Uchenye zapiski (Scientific Notes) Kishinev University 55, 113 (1960).
[8]G. R. Allcock, Polarons and Excitons, edited by C. G. Kuper and G. D. Whitfield (Edinburgh and London, 1962), p. 45.
[9]V. I. Mel'nikov and G. E. Volovik, Zh. Eksp. Teor. Fiz. 65, 1637 (1973) [Sov. Phys.-JETP 38, 000 (1974)].

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