PHYSICAL REVIEW B VOLUME 9, NUMBER 4 15 FEBRUARY 1974

Anisotropic piezoelectric polaron

James J. Licari and George Whitfield
Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802
(Received 4 September 1973)

A continuum theory is used to derive an anisotropic piezoelectric polaron Hamiltonian. The intermediate-coupling theory is applied to this Hamiltonian and it is shown that the polaron has a maximum velocity is each direction. This maximum velocity is less than the velocity of the phonons moving in the same direction. This effect was previously shown only for an isotropic Hamiltonian. The angular dependence of the coupling constant is derived from the anisotropic Hamiltonian and average values for the quasilongitudinal and quasitransverse modes are obtained. The increase in effective mass due to the polaron effect is also calculated for slow polarons.

I. INTRODUCTION

The piezoelectric polaron has been the subject of much discussion in recent years. The importance of the interaction between an electron and the acoustic phonons of a piezoelectric crystal such as CdS was pointed out by Hutson[1] and numerous experiments followed. The shift in the electron's effective mass due to this interaction was measured in these experiments and two sets of masses were found. Cyclotron-resonance experiments in CdS performed by Baer and Dexter[2] and Sawamoto[3] gave a slightly anisotropic mass tensor with components between $0.153m_0$ and $0.171m_0$, where m_0 is the free-electron mass. Other experiments involving analysis of impurity activation energies,[4] exciton spectra,[5] Faraday rotation,[6] electron mobility,[7] and free-carrier absorption[8] gave larger masses in the range of $0.19m_0$ to $0.22m_0$.

Mahan and Hopfield[9] tried to explain these differences by formulating a temperature-dependent semiclassical theory of the piezoelectric polaron. Their results indicated that the lower masses were polaron masses. This semiclassical theory, however, is not applicable to the experiments giving the lower masses, since these were performed in the quantum region of low temperature and high magnetic field. Larsen[10] then formulated a quantum theory at zero temperature, but this theory cannot be safely extrapolated to finite temperatures.

Other theories[11,12] and experiments[13] have appeared recently in the literature, but the problem of the correct polaron mass (and the interpretation of the experimental results given here) and the effect of the electron-phonon interaction in CdS has not been resolved.

In view of this situation, we feel that more might be gained by a critical study of the nature of the ground state of the piezoelectric polaron, than by directly trying to resolve the situation just described. This was initially done by using the approximation of an isotropic Hamiltonian.[14–18] It has been argued[15,17,18] that the lowest solution of this Hamiltonian has an anomalous energy-momentum relation, in that as momentum increases, the velocity approaches the speed of sound instead of being proportional to the momentum as is usual. These arguments are based on the intermediate-coupling theory.[19,20]

In the present paper we continue the study of the ground state of the piezoelectric polaron. Since the anomalous energy-momentum relation results from a singular integral obtained in the isotropic formulation of the problem, it was thought that perhaps the formulation of the problem in terms of a more realistic, anisotropic Hamiltonian might remove the singularity and the resulting anomaly. Following a method suggested by Henry,[21] we derive an anisotropic Hamiltonian and apply the intermediate-coupling theory, using the crystal parameters of CdS. The anomalous behavior is found to persist. The anisotropic coupling constant $\alpha(\theta)$ and the polaron effective mass are also calculated.

II. EQUATIONS OF STATE AND LATTICE DYNAMICS

When work is done on a piezoelectric crystal the internal energy per unit volume is increased by an amount dU given by[22]

$$dU = T_i\, dS_i + E_i\, dD_i/4\pi + \theta\, d\sigma ,$$

in cgs units (the Einstein summation convention is used throughout the paper). In the above, T_i is the stress, S_i the strain, E_i the electric field, D_i the electric displacement, θ the absolute temperature, and σ the entropy. A piezoelectric crystal is stiffened owing to the electric fields produced when a strain is applied. The second term in dU represents the work done against these forces in applying a given strain dS_i.

There are three pairs of variables used in the equations relating to piezoelectric crystals. These are stress and strain, electric field and displacement, and temperature and entropy. Any three of these (taking one from each pair) can be used as independent variables. Here we will use the strain, electric field, and entropy.

We consider the stress as a function of these variables and write

$$dT_i(S_j, E_j, \sigma) = \left(\frac{\partial T_i}{\partial S_j}\right)_{E,\sigma} dS_j + \left(\frac{\partial T_i}{\partial E_j}\right)_{S,\sigma} dE_j + \left(\frac{\partial T_i}{\partial \sigma}\right)_{E,S} d\sigma. \quad (1a)$$

We will confine the discussion to conditions under which linear relations exist between stress and strain, stress and electric field, and electric field and electric displacement. Thus the partial derivatives appearing in the above equation define a number of constants relating to the crystal. These are

$$\left(\frac{\partial T_i}{\partial S_j}\right)_{E,\sigma} = c_{ij}^{E,\sigma},$$

the elastic-stiffness constant measured at constant field and entropy; and

$$\left(\frac{\partial T_i}{\partial E_j}\right)_{S,\sigma} = -e_{ji}^{S,\sigma},$$

the piezoelectric constant which relates the stress to the electric field when the strain is held fixed (crystal clamped). Since we are interested in an acoustic wave propagating in the crystal, we will set $d\sigma$ equal to zero since such waves propagate adiabatically. Integrating Eq. (1a) we can write

$$T_i = c_{ij}^{E,\sigma} S_j - e_{ji}^{S,\sigma} E_j, \quad (1b)$$

where our initial state has zero stress, strain, and electric field.

In order to derive the equation of state for the electric displacement it is useful to consider the electric enthalpy H_{el}:

$$H_{el} = U - E_i D_i / 4\pi,$$

with differential dH_{el} given by

$$dH_{el} = T_i dS_i - D_i dE_i/4\pi + \theta d\sigma. \quad (2)$$

dH_{el} is an exact differential so the following result holds:

$$\left(\frac{\partial D_i}{\partial S_j}\right)_{E,\sigma} = -4\pi\left(\frac{\partial T_j}{\partial E_i}\right)_{S,\sigma} = 4\pi e_{ij}^{S,\sigma}.$$

Using the above and a procedure analogous to that used in deriving Eq. (1b), we get an expression for the electric displacement:

$$D_i = 4\pi e_{ij}^{S,\sigma} S_j + \epsilon_{ij}^{S,\sigma} E_j, \quad (3a)$$

where $(\partial D_i/\partial E_j)_{S,\sigma} = \epsilon_{ij}^{S,\sigma}$ is the dielectric constant at constant strain and entropy.

We will drop the σ superscripts on the constants, remembering that these must be measured adiabatically. Thus we can write the equations of state in full tensor notation:

$$T_{ij} = c_{ijlm}^{E} S_{lm} - e_{lij}^{S} E_l, \quad (1c)$$

$$D_i = \epsilon_{ij}^{S} E_j + 4\pi e_{ijk}^{S} S_{jk}. \quad (3b)$$

Equation (3b) illustrates the direct piezoelectric effect (mechanical strain producing a polarization and a resulting electric displacement), while Eq. (1c) describes the converse effect (electric field producing a mechanical stress). The above equations are analogous to the phenomenological equations of Born and Huang[23] describing an ionic crystal. We also note that the same piezoelectric constant appears in both Eq. (1c) and Eq. (3b).

From the equations of state we can now derive the characteristic equation giving the sound speeds of a piezoelectric crystal. Writing the strain in terms of the displacements μ_l of an element of mass of the crystal, i.e.,

$$S_{lm} = \tfrac{1}{2}\left(\frac{\partial \mu_l}{\partial x_m} + \frac{\partial \mu_m}{\partial x_l}\right) = \tfrac{1}{2}(\nabla_m \mu_l + \nabla_l \mu_m), \quad (4)$$

we can write the equation of motion of this element of mass ρdV as

$$\nabla_j T_{ij} = \rho \ddot{\mu}_i = (\nabla_j c_{jilm}^{E} \nabla_m)\mu_l + (\nabla_l e_{lij}^{S} \nabla_j)\phi, \quad (5)$$

where ϕ is the electric potential. The elastic and piezoelectric tensors possess symmetry in their indices of the following forms[24]:

$$c_{ijlm} = c_{lmij} = c_{jilm} = c_{ijml} = c_{jiml} = c_{mlij} = c_{mlji} = c_{lmji},$$

and

$$e_{ijk} = e_{ikj}.$$

Maxwell's equation $\vec{\nabla}\cdot\vec{D} = 4\pi\rho_0$ is here written as

$$\nabla_i D_i = 4\pi\rho_0 = 4\pi(\nabla_i e_{ijk}^{S} \nabla_k)\mu_j - (\nabla_i \epsilon_{ij}^{S} \nabla_j)\phi. \quad (6)$$

We define the Fourier transform of $\mu_i(\vec{x})$ as

$$\mu_i(\vec{x}) = \sum_{\vec{k}} \mu_i(\vec{k}) \frac{e^{i\vec{k}\cdot\vec{x}}}{V^{1/2}}, \quad (7)$$

ignoring the $\vec{k} = 0$ mode of uniform translation. In order for $\mu_i(\vec{x})$ to be real we must have $\mu_i(-\vec{k}) = \mu_i(\vec{k})^*$. Similarly transforming $\phi(\vec{x})$ and $\rho_0(\vec{x})$, we can write Eqs. (5) and (6) (thus eliminating the spatial derivatives) as

$$\rho \ddot{\mu}_i(\vec{k})/k^2 = -(\bar{c}_{il}\mu_l(\vec{k}) + \bar{e}_i \phi(\vec{k})) \quad (8)$$

and

$$4\pi\rho_0(\vec{k})/k^2 = \bar{\epsilon}\phi(\vec{k}) - 4\pi\bar{e}_j \mu_j(\vec{k}). \quad (9)$$

In the above equations $\bar{c}_{il}$, $\bar{e}_i$, and $\bar{\epsilon}$ are defined as

$$\bar{c}_{il} \equiv \alpha_j c_{jilm}^{E} \alpha_m, \qquad \bar{e}_i \equiv \alpha_j e_{jik}^{S} \alpha_k, \quad (10)$$

$$\bar{\epsilon} \equiv \alpha_i \epsilon^S_{ij} \alpha_j ,$$

where the α_i are direction cosines for the vector $\vec{k}$. Equations (10) depend only on the direction of $\vec{k}$.

Solving Eq. (9) for $\phi(\vec{k})$ and substituting in Eq. (8) gives

$$\rho \ddot{\mu}_i(\vec{k})/k^2 = -\bar{d}_{il}\mu_l(\vec{k}) - [4\pi\rho_0(\vec{k})/k^2\bar{\epsilon}]\bar{e}_i , \qquad (11)$$

where

$$\bar{d}_{il} = \bar{c}_{il} + 4\pi\bar{e}_i\bar{e}_l/\bar{\epsilon} . \qquad (12)$$

The first term on the right of Eq. (11) is the restoring force due to the lattice (elastic force and piezoelectric stiffening), and the second term is the force exerted by the free charges through their electric field, coupled to the lattice by the $\bar{e}_i$.

To get an expression for the lattice frequencies and sound speeds let us take $\rho_0(\vec{k}) = 0$, i.e., no free charges present. The equation of motion, Eq. (11), now becomes

$$\rho\ddot{\mu}_i(\vec{k})/k^2 = -\bar{d}_{il}\,\mu_l(\vec{k}) . \qquad (13)$$

Since $\bar{d}_{il}$ is a symmetric tensor, the matrix formed from its elements possesses three orthogonal eigenvectors $\hat{g}_1$, $\hat{g}_2$, and $\hat{g}_3$, with corresponding eigenvalues d_{g_1}, d_{g_2}, and d_{g_3}. These are obtained by solving $d\cdot\hat{g}_i = d_{g_i}\hat{g}_i (i=1, 2, 3)$. The directions of the $\hat{g}$'s depend on that of $\vec{k}$ and we choose them to be unit in length. If we write the vectors $\vec{\mu}(\vec{k})$ and $\ddot{\vec{\mu}}(\vec{k})$ using the $\hat{g}$'s as a basis, i.e., $\vec{\mu}(\vec{k}) = \sum_{\hat{g}} \mu_g(\vec{k})\hat{g}$, we can write

$$\rho\ddot{\mu}(\vec{k})/k^2 = -d\cdot\vec{\mu}(\vec{k})$$

and

$$\ddot{\mu}_{g_1}(\vec{k}) + (d_{g_1}k^2/\rho)\,\mu_{g_1}(\vec{k}) = 0 \qquad (14)$$

for one of the $\hat{g}$'s (with similar equations for $i=2$, 3). The general solution for $\mu_{g_i}(\vec{k})$ is

$$\mu_{g_i}(\vec{k}) = A(\vec{k})e^{i\omega_{g_i}t} + B(\vec{k})e^{-i\omega_{g_i}t},$$

where

$$\omega_{g_i} = (d_{g_i}/\rho)^{1/2}k = v_{g_i}k .$$

The sound speeds v_{g_i} can be determined for any direction in the crystal by finding the eigenvalues of d.

We will do this for wurtzite-structured CdS, taking the $\hat{z}$ coordinate axis to be the hexagonal $\hat{c}$ axis. The values for the elastic, piezoelectric, and dielectric constants are given in Table I. Specifying the direction of $\vec{k}$ by θ, the angle between the $\hat{z}$ axis and the $\vec{k}$ vector, and ϕ, the azimuthal angle, let us rotate the coordinate system about the $\hat{z}$ axis through ϕ (see Fig. 1). Since $\vec{k}$ now lies in the $\hat{x}$-$\hat{z}$ plane the d matrix becomes

$$\begin{pmatrix} d'_{11} & 0 & d'_{13} \\ 0 & d'_{22} & 0 \\ d'_{13} & 0 & d'_{33} \end{pmatrix} \qquad (15)$$

where

$$\begin{aligned} d'_{11} &= d_{11}\cos^2\phi + d_{22}\sin^2\phi + 2d_{12}\sin\phi\cos\phi , \\ d'_{22} &= d_{11}\sin^2\phi + d_{22}\cos^2\phi - 2d_{12}\sin\phi\cos\phi , \\ d'_{33} &= d_{33}, \\ d'_{13} &= d_{13}\cos\phi + d_{23}\sin\phi. \end{aligned} \qquad (16)$$

The eigenvectors, while mutually orthogonal, are not necessarily longitudinal and transverse to $\vec{k}$. However, one eigenvector is transverse and lies in the $\hat{y}$ direction as shown in Fig. 1. This is seen by writing

$$\begin{pmatrix} d'_{11} & 0 & d'_{13} \\ 0 & d'_{22} & 0 \\ d'_{13} & 0 & d'_{33} \end{pmatrix} \begin{pmatrix} 0 \\ g_2 \\ 0 \end{pmatrix} = d'_{22} \begin{pmatrix} 0 \\ g_2 \\ 0 \end{pmatrix} ,$$

where the speed of this transverse mode is given by

$$v_T = \left(\frac{d'_{22}}{\rho}\right)^{1/2} = \left[\frac{\frac{1}{2}(c_{11}-c_{12})\sin^2\theta + c_{44}\cos^2\theta}{\rho}\right]^{1/2} . \qquad (17)$$

This mode is not piezoelectrically stiffened.

The other eigenvectors, therefore, have no $\hat{y}$ component and the eigenvalue problem for them is a two-dimensional one. Solving for the two remaining modes gives v_{QT} and v_{QL}, the velocities of the quasitransverse and quasilongitudinal modes, respectively. These are given in the Appendix. The angular dependence of these velocities is shown in Fig. 2, where we note that they are independent of the azimuthal angle ϕ.

TABLE I. Elastic, dielectric, and piezoelectric constants of wurtzite structured CdS at 25 °C.

elastic[a] ($\times 10^{11}$ dynes/cm^2)					dielectric[b]		Piezoelectric[b] ($\times 10^5$ statcoulombs/cm^2)		
c_{11}	c_{33}	c_{44}	c_{12}	c_{13}	$\epsilon^S_{11}/\epsilon_0$	$\epsilon^S_{33}/\epsilon_0$	e_{31}	e_{33}	e_{15}
8.431	9.183	1.458	5.208	4.567	9.02	9.53	−0.73	1.32	−0.63

[a]E. Gerlich, J. Phys. Chem. Solids 28, 2575 (1967).

[b]D. Berlincourt, H. Jaffe, and L. R. Shiozawa, Phys. Rev. 129, 1009 (1963). The piezoelectric constants were multiplied by 3×10^5 for conversion to cgs units.

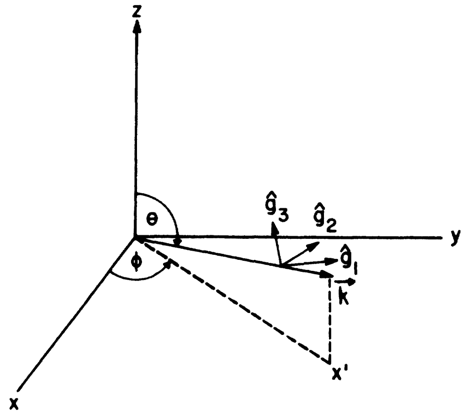

FIG. 1. $\hat{g}_2$ is the transverse, $\hat{g}_1$ the quasilongitudinal, and $\hat{g}_3$ the quasitransverse polarization vector.

III. POLARON HAMILTONIAN

We now put the free charges (by free charges we mean electrons in the bottom of the conduction band) back in the crystal and derive the polaron Hamiltonian. Our method is analogous to that used by Born and Huang[25] in deriving the optical-polaron Hamiltonian. We start with Maxwell's equations:

$$\vec{\nabla}\cdot\vec{D} = \vec{\nabla}\cdot(\vec{E}+4\pi\vec{P}) = 4\pi\rho_0(\vec{x}) \ ,$$
$$\vec{\nabla}\times\vec{H} = (1/c)(\dot{\vec{D}}+4\pi\vec{J}_0), \tag{18}$$
$$\vec{\nabla}\cdot\vec{H} = 0,$$

and

$$\vec{\nabla}\times\vec{E} = -(1/c)\dot{\vec{H}} \ ,$$

where

$$\vec{J}_0(\vec{x}) = -\sum_i e\dot{\vec{x}}_i\delta(\vec{x}-\vec{x}_i) \ .$$

$\vec{J}_0(\vec{x})$ is the current density due to the conduction electrons (e is the magnitude of the electron's charge). Forming the Poynting vector $(c/4\pi)\,\vec{E}\times\vec{H}$, and using the vector identity

$$\vec{\nabla}\cdot(\vec{E}\times\vec{H}) = \vec{H}\cdot(\vec{\nabla}\times\vec{E}) - \vec{E}\cdot(\vec{\nabla}\times\vec{H})$$

along with Maxwell's equations, we write

$$\int_V \frac{c}{4\pi}\vec{\nabla}\cdot(\vec{E}\times\vec{H})d\tau$$
$$= -\int_V \left[\frac{1}{4\pi}(\vec{H}\cdot\dot{\vec{H}}+\vec{E}\cdot\dot{\vec{E}})+\vec{E}\cdot\dot{\vec{P}}+\vec{E}\cdot\vec{J}_0\right]d\tau \ . \tag{19}$$

Equation (19) gives the total rate of flow of energy out of the arbitrary volume V. The last term in the integral can be cast into a more instructive form:

$$-\int_V \vec{E}\cdot\vec{J}_0 d\tau = \int_V \sum_i e\,\vec{E}(\vec{x})\cdot\dot{\vec{x}}^{(i)}\delta(\vec{x}-\vec{x}^{(i)})d\tau$$

$$= -\sum_i \left(\frac{1}{m}\right)^{-1}_{rs}\ddot{x}_r^{(i)}\dot{x}_s^{(i)}$$

$$= -\frac{d}{dt}\left(\sum_i \frac{1}{2}\left(\frac{1}{m}\right)^{-1}_{rs}\dot{x}_r^{(i)}\dot{x}_s^{(i)}\right), \tag{20}$$

where the sum is over all the conduction electrons and the effective-mass tensor is symmetric and the same for all the electrons. The right-hand side of Eq. (20) is just the rate at which the kinetic energy of the conduction electrons decreases in the volume V. Therefore

$$\int_V \frac{c}{4\pi}\vec{\nabla}\cdot(\vec{E}\times\vec{H})d\tau = -\frac{d}{dt}\left[\sum_i \tfrac{1}{2}\left(\frac{1}{m}\right)_{rs}p_r^{(i)}p_s^{(i)}\right] - \int_V \frac{du}{dt}d\tau \ ,$$

where u is the energy density (u includes the lattice energy and electron-electron and electron-lattice interaction energies). Taking $\vec{H}=0$, thereby omitting retardation effects, we write

$$\frac{du}{dt} = \frac{1}{4\pi}\vec{E}\cdot\dot{\vec{E}}+\vec{E}\cdot\dot{\vec{P}} = \frac{\vec{E}\cdot\dot{\vec{D}}}{4\pi} \ . \tag{21}$$

In a piezoelectric crystal, where a strain produces an electric field, it is not valid to write $u=\vec{E}\cdot\vec{D}/8\pi$. Instead we must use the more general Eq. (21).

Using Eqs. (3b) and (4) we can write du/dt as

$$\frac{du}{dt} = \frac{d}{dt}\left(\frac{E_i\epsilon_{ij}^S E_j}{8\pi}\right) - \nabla_i\phi\, e_{ijk}^S\nabla_k\dot{\mu}_j \ .$$

We now integrate over the volume of the crystal. If we integrate the second term by parts we have

$$\int_V \frac{du}{dt}d\tau = \frac{d}{dt}\int_V\left(\frac{\nabla_i\phi\,\epsilon_{ij}^S\nabla_j\phi}{8\pi}\right)d\tau$$
$$+\int_V \dot{\mu}_j\,(\nabla_i e_{ijk}^S\nabla_k\phi)\,d\tau \ . \tag{22}$$

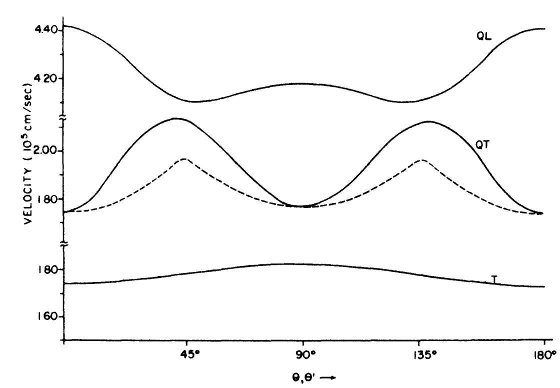

FIG. 2. Sound speeds (CdS) for the transverse mode (T), and the quasimodes (QL and QT). The dotted curve is the velocity to which the polaron asymptotes when it waves in the direction θ' (with $\varphi'=36°$).

Using Eq. (5) in the last term and integrating again by parts, Eq. (22) becomes

$$\frac{d}{dt}\int_V u\,d\tau=\frac{d}{dt}\int_V\left[\frac{\nabla_i\phi\epsilon_{ij}^S\nabla_j\phi}{8\pi}+\frac{\rho\dot{\mu}_i^2}{2}+\frac{\nabla_j\mu_i c_{jilm}^E}{2}\times\nabla_m\mu_l\right]d\tau, \qquad (23)$$

with the integrand on the right-hand side being the energy density u. Thus the polaron Hamiltonian is

$$H=\sum_i\frac{1}{2}\left(\frac{1}{m}\right)_{rs}p_r^{(i)}p_s^{(i)}+\int_V u\,d\tau\ . \qquad (24)$$

We Fourier analyze the above Hamiltonian according to Eq. (7) and write

$$H=\sum_i\frac{1}{2}\left(\frac{1}{m}\right)_{rs}p_r^{(i)}p_s^{(i)}+\sum_{\vec{k}}\left[\frac{\rho}{2}\dot{\vec{\mu}}(\vec{k})\cdot\dot{\vec{\mu}}(\vec{k})^*+\frac{k^2}{2}\vec{\mu}(\vec{k})\cdot C\cdot\vec{\mu}(\vec{k})^*+\frac{k^2\overline{\epsilon}}{8\pi}\phi(\vec{k})\phi(\vec{k})^*\right], \qquad (25)$$

where C is the tensor whose elements are $\overline{c}_{il}$. Substituting $\phi(\vec{k})$ from Eq. (9) into the above gives

$$H=H_e+H_L+H_{el}\ ,$$

where

$$H_e=\sum_i\frac{1}{2}\left(\frac{1}{m}\right)_{rs}p_r^{(i)}p_s^{(i)}+\sum_{\vec{k}}\frac{2\pi}{k^2\overline{\epsilon}}\rho_0(\vec{k})\rho_0(\vec{k})^*,$$
$$H_L=\frac{1}{2}\sum_{\vec{k}}\left[k^2\vec{\mu}(\vec{k})\cdot d\cdot\vec{\mu}(\vec{k})^*+\rho\dot{\vec{\mu}}(\vec{k})\cdot\dot{\vec{\mu}}(\vec{k})^*\right], \qquad (26)$$

and

$$H_{el}=\sum_{\vec{k}}\frac{2\pi}{\overline{\epsilon}}\left[\rho_0(\vec{k})\vec{e}\cdot\vec{\mu}(\vec{k})^*+\rho_0(\vec{k})^*\vec{e}\cdot\vec{\mu}(\vec{k})\right]\ .$$

d is the previously defined tensor with elements $\overline{d}_{il}$ and $\vec{e}$ is a vector with components $\overline{e}_i$. Introducing again the polarization vectors $\hat{g}$ by writing $\vec{\mu}(\vec{k})=\sum_{\hat{g}}\mu_g(\vec{k})\hat{g}$, Eqs. (26) become

$$H_L=\sum_{\vec{k},\hat{g}}\frac{\rho}{2}\left[\dot{\mu}_g(\vec{k})\dot{\mu}_g(\vec{k})^*+\omega_{kg}^2\mu_g(\vec{k})\mu_g(\vec{k})^*\right]$$

and

$$H_{el}=\sum_{\vec{k},\hat{g}}\frac{2\pi}{\overline{\epsilon}}\vec{e}\cdot\hat{g}\left[\rho_0(\vec{k})\mu_g(\vec{k})^*+\rho_0(\vec{k})^*\mu_g(\vec{k})^*\right], \qquad (27)$$

with H_e unchanged. H_e is the energy of the free electrons described by $\rho_0(\vec{k})$, H_L is the lattice energy, and H_{el} is the energy of interaction between the free electrons and the lattice.

To quantize the system we start with the commutation relation for the displacement and momentum,

$$[\mu_g(\vec{x}),(M/N)\dot{\mu}_{g'}(\vec{x}')]=i\hbar\delta_{gg'}\delta(\vec{x}-\vec{x}') \qquad (28)$$

($\mu_g(\vec{x})$ is the $\hat{g}$ component of $\vec{\mu}(\vec{x})$, where $\hat{g}$ is one of the polarization vectors for an arbitrary $\vec{k}$). M is the total mass and N is the number or atoms. We then define a transformation from the normal coordinates $\mu_g(\vec{k})$ to the operators $a_{kg}^\dagger$ and a_{kg} defined by

$$\mu_g(\vec{k})=(\hbar/2\rho\omega_{kg})^{1/2}(a_{kg}+a_{-kg}^\dagger) \qquad (29a)$$

and

$$\dot{\mu}_g(\vec{k})=i(\hbar\omega_{kg}/2\rho)^{1/2}(a_{-kg}^\dagger-a_{kg})\ , \qquad (29b)$$

with

$$[a_{kg},a_{k'g'}^\dagger]=\delta_{kk'}\delta_{gg'}\ ,\quad [a_{kg},a_{k'g'}]=[a_{kg}^\dagger,a_{k'g'}^\dagger]=0. \qquad (30)$$

The Hamiltonian now becomes

$$H=H_e+\sum_{\vec{k},\hat{g}}\hbar\omega_{kg}(a_{kg}^\dagger a_{kg}+\tfrac{1}{2})+\sum_{\vec{k},\hat{g}}\frac{4\pi}{\overline{\epsilon}}\vec{e}\cdot\hat{g}\left(\frac{\hbar}{2\rho\omega_{kg}}\right)^{1/2}\times\rho_0^*(\vec{k})(a_{kg}+a_{-kg}^\dagger). \qquad (31)$$

To write the Hamiltonian corresponding to a single electron interacting with the acoustic modes of the lattice vibrations, let $\omega_{kg}=v_g k$ and $\rho_0(\vec{k})=-e\,e^{-i\vec{k}\cdot\vec{x}}/V^{1/2}$. We now have the final anisotropic polaron Hamiltonian:

$$H=\frac{1}{2}\left(\frac{1}{m}\right)_{rs}p_r p_s+\sum_{\vec{k},\hat{g}}\hbar v_g k(a_{kg}^\dagger a_{kg}+\tfrac{1}{2})+\sum_{\vec{k},\hat{g}}V_g(\vec{k})(a_{kg}e^{i\vec{k}\cdot\vec{x}}+a_{kg}^\dagger e^{-i\vec{k}\cdot\vec{x}})\ , \qquad (32)$$

where[26]

$$V_g(\vec{k})=-\frac{4\pi e}{\overline{\epsilon}}\vec{e}\cdot\hat{g}\left(\frac{\hbar}{2M\omega_{kg}}\right)^{1/2}. \qquad (33)$$

The polaron Hamiltonian thus retains the simple form of the isotropic case, as in Ref. 3, but the terms of Eq. (32) all contain the anisotropy of the crystal as shown, for example, in Eq. (33) for $V_g(\vec{k})$ and in the mass tensor $(1/m)_{rs}$. In Eq. (32) we have neglected the electron's electrostatic self-energy (not to be confused with the "self-energy" or lowering of the electron's energy at $\vec{k}=0$ owing to its interaction with the phonons).

IV. INTERMEDIATE COUPLING THEORY

The intermediate-coupling theory[19] is a variational theory using a trial wave function $\psi(\vec{x})$ given by

$$\psi(\vec{x})=\exp\left[\frac{i}{\hbar}\left(\vec{P}-\sum_{\vec{k},\hat{g}}a_{kg}^\dagger a_{kg}\hbar\vec{k}\right)\cdot\vec{x}\right]\times\exp\left[\sum_{\vec{k},\hat{g}}f_{kg}(a_{kg}^\dagger-a_{kg})\right]|0\rangle\ . \qquad (34)$$

Since the Hamiltonian commutes with the total momemtum operator $\vec{P}$ given by

$$\vec{\mathbf{P}}=\vec{\mathbf{p}}+\sum_{\vec{\mathbf{k}},\hat{\epsilon}} a^{\dagger}_{k\epsilon} a_{k\epsilon}\hbar\vec{\mathbf{k}}\ , \tag{35}$$

and since $\psi(\vec{\mathbf{x}})$ is an eigenfunction of $\vec{\mathbf{P}}$, the total momentum is a constant of the motion and can be regarded as a "c" number. We form the expectation value of the Hamiltonian in the state $\psi(\vec{\mathbf{x}})$ and minimize it with respect to the $f_{k\epsilon}$. The minimum value thus obtained is an upper bound to the true ground-state energy and is given by

$$E_0=\frac{1}{2}\left(\frac{1}{m}\right)_{rs}P_rP_s-\sum_{\vec{\mathbf{k}},\hat{\epsilon}}\left\{2V^2_\epsilon(\vec{\mathbf{k}})\Big/\left[\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar\left(\frac{1}{m}\right)_{rs}k_r\left(P_s-\sum_{\vec{\mathbf{k}}',\hat{\epsilon}'}f^2_{k'\epsilon'}\hbar k'_s\right)\right]\right\}$$
$$+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}\left(\sum_{\vec{\mathbf{k}},\hat{\epsilon}}\left\{V^2_\epsilon(\vec{\mathbf{k}})\vec{\mathbf{k}}\Big/\left[\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar\left(\frac{1}{m}\right)_{rs}k_r\left(P_s-\sum_{\vec{\mathbf{k}}',\hat{\epsilon}'}f^2_{k'\epsilon'}\hbar k'_s\right)\right]^2\right\}\right)^2$$
$$+\sum_{\vec{\mathbf{k}},\hat{\epsilon}}\left\{V^2_\epsilon(\vec{\mathbf{k}})\left(\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar\left(\frac{1}{m}\right)_{rs}k_rP_s\right)\Big/\left[\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar\left(\frac{1}{m}\right)_{rs}k_r\left(P_s-\sum_{\vec{\mathbf{k}}',\hat{\epsilon}'}f^2_{k'\epsilon'}\hbar k'_s\right)\right]^2\right\}. \tag{36}$$

If we assume the crystal to be isotropic there is only one preferred direction, that of $\vec{\mathbf{P}}$. Hence, we can write $\sum_{\vec{\mathbf{k}},\hat{\epsilon}}f^2_{k\epsilon}\hbar\vec{\mathbf{k}}=\eta(P)\vec{\mathbf{P}}$. In the anisotropic case discussed here we write instead

$$\sum_{\vec{\mathbf{k}},\hat{\epsilon}}f^2_{k\epsilon}\hbar k_r=\eta_{rs}P_s\ , \tag{37}$$

noting that this will still give us an upper bound to the true ground-state energy. The form of the second-rank tensor η_{rs} reflects the symmetry of the crystal. Looking again at CdS, which is of crystal class $6mm$ (dihexagonal polar), η_{rs} takes on the form

$$\begin{pmatrix}\eta_1 & 0 & 0\\ 0 & \eta_1 & 0\\ 0 & 0 & \eta_3\end{pmatrix}. \tag{38}$$

Using Eq. (37) and rearranging and combining the terms of Eq. (36) we can write E_0 as

$$E_0=\frac{1}{2}\left(\frac{1}{m}\right)_{rs}P_rP_s-\sum_{\vec{\mathbf{k}},\hat{\epsilon}}\left\{V^2_\epsilon(\vec{\mathbf{k}})\Big/\left[\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar\left(\frac{1}{m}\right)_{rs}k_r(P_s-\eta_{sl}P_l)\right]\right\}$$
$$-\frac{\hbar}{2}\left(\frac{1}{m}\right)_{rs}\sum_{\vec{\mathbf{k}},\hat{\epsilon}}\left\{V^2_\epsilon(\vec{\mathbf{k}})(k_r\eta_{sl}P_l)\Big/\left[\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar\left(\frac{1}{m}\right)_{rs}k_r(P_s-\eta_{sl}P_l)\right]^2\right\}. \tag{39}$$

Since the polaron velocity is given by $v_r(\vec{\mathbf{P}})=\partial E_0/\partial P_r$, we can write

$$v_r(\vec{\mathbf{P}})=\left(\frac{1}{m}\right)_{rs}(P_s-\eta_{sl}P_l) \tag{40}$$

and

$$E_0=\frac{1}{2}\left(\frac{1}{m}\right)_{rs}P_rP_s-\frac{1}{2}\left(\frac{1}{m}\right)_{rs}\left[P_r-\left(\frac{1}{m}\right)^{-1}_{rl}v_l(\vec{\mathbf{P}})\right]\left[P_s-\left(\frac{1}{m}\right)^{-1}_{sm}v_m(\vec{\mathbf{P}})\right]$$
$$-\sum_{\vec{\mathbf{k}},\hat{\epsilon}}\left\{V^2_\epsilon(\vec{\mathbf{k}})\Big/\left[\hbar v_\epsilon k+\frac{\hbar^2}{2}\left(\frac{1}{m}\right)_{rs}k_rk_s-\hbar k_rv_r(\vec{\mathbf{P}})\right]\right\}. \tag{41}$$

E_0 is here written in a form analogous to that of the isotropic case. However, we must remember that our $v_r(\vec{\mathbf{P}})$ contains the anisotropy of the crystal through $(1/m)_{rs}$ and η_{sl}.

V. POLARON VELOCITY AND COUPLING CONSTANT

The polaron velocity, Eq. (40), is given by

$$v_r(\vec{\mathbf{P}})=\left(\frac{1}{m}\right)_{rs}P_s-\frac{V}{8\pi^3}\left(\frac{1}{m}\right)_{rs}\sum_{\hat{\epsilon}}\int d^3k\,\frac{V^2_\epsilon(\vec{\mathbf{k}})k_s/k^2}{\hbar[v_\epsilon+\frac{1}{2}\hbar(1/m)_{rs}\alpha_rk_s-\alpha_iv_i(\vec{\mathbf{P}})]^2}\ ,$$

where in the denominator v_g is the sound speed and $v_i(\vec{P})$ is the polaron velocity. The last term in the denominator of the integral can be written

$$\begin{aligned}\alpha_i v_i(\vec{P}) &= \alpha_1 v_1(\vec{P}) + \alpha_2 v_2(\vec{P}) + \alpha_3 v_3(\vec{P}) \\ &= \sin\theta\cos\phi\, v(\vec{P})\sin\theta'\cos\phi' + \sin\theta\sin\phi\, v(\vec{P})\sin\theta'\sin\phi' + \cos\theta\, v(\vec{P})\cos\theta' \\ &= v(\vec{P})[\sin\theta\sin\theta'(\cos\phi\cos\phi' + \sin\phi\sin\phi') + \cos\theta\cos\theta'] \\ &= v(\vec{P}) f(\theta, \phi, \theta', \phi') ,\end{aligned}$$

where θ' and ϕ' give the direction of the polaron velocity. Thus, the above expression for the velocity becomes

$$v_r(\vec{P}) = \left(\frac{1}{m}\right)_{rs} P_s - \frac{V}{8\pi^3}\left(\frac{1}{m}\right)_{rs} \sum_{\hat{g}} \int d^3k \, \frac{V_g^2(\vec{k})\,\alpha_s/k}{\hbar[v_g + \frac{1}{2}\hbar(1/m)_{rs}\,\alpha_r k_s - v(\vec{P}) f(\theta, \phi, \theta', \phi')]^2} \, . \tag{42}$$

Since $(v_g + \frac{1}{2}\hbar(1/m)_{rs}\,\alpha_r k_s)$ is positive we expect that as we increase $v(\vec{P})$ from zero the denominator may vanish for some $v(\vec{P})$ and cause a divergence in the integral, blowing up as $1/x^2$. In this case the momentum approaches infinity as the polaron velocity approaches this $v(\vec{P})$, and so this is a limiting velocity for the polaron. Below this velocity intermediate-coupling theory approximates an eigenstate of energy and momentum, but we are unable to extend this statement above this $v(\vec{P})$. This limiting velocity was found for CdS and is plotted in Fig. 2 (dotted line) as a function of θ', with ϕ' chosen to be 36°.

Since we are interested in finding the effect of the theory on the electron's mass we will assume an isotropic-band mass of $m^* = 0.20\, m_0$, where m_0 is the free-electron mass. With this approximation the polaron velocity is written as

$$v_r(\vec{P}) = \frac{P_r}{m^*} - \frac{V}{8\pi^3}\frac{1}{m^*}\sum_{\hat{g}}\int d^3k \times \frac{V_g^2(\vec{k})\,\alpha_r/k}{\hbar[v_g + \hbar k/2m^* - v(\vec{P}) f(\theta, \phi, \theta', \phi')]^2} \, . \tag{43}$$

Equation (43) has been solved numerically (arbitrarily choosing $\theta' = 18°$) for the three components of $\vec{v}(\vec{P})$ and $v_y(\vec{P})$ has been plotted in Fig. 3 as a function of P_y. The asymptotic nature of the velocity is clearly seen here. In performing the integrations in this paper we have used a maximum wave vector of $k_{max} = 10^8\ \text{cm}^{-1}$, corresponding to a phonon wavelength comparable with the lattice spacing. We have also approximated the polarization vectors $\hat{g}$ by vectors longitudinal and transverse to $\vec{k}$. This does not affect our conclusions qualitatively and should have only a slight effect on our numerical results. From the linear portions of the $v_i(\vec{P})$ vs P_i curves we have obtained the polaron mass at small P and find

$$m_1^p = m_2^p = 0.30\, m_0$$

and

$$m_3^p = 0.38\, m_0 .$$

The polaron effect on the mass at 0 °K is thus seen to be quite large, and increase of 50% for m_1^p and m_2^p and almost 100% for m_3^p.

The polaron energy $E_0(P)$ in the isotropic-band-mass approximation becomes

$$E_0(P) = \frac{\vec{P}^2}{2m^*} - \frac{[\vec{P} - m^*\vec{v}(\vec{P})]^2}{2m^*} - \sum_{\vec{k},\hat{g}} \frac{V_g^2(\vec{k})}{[\hbar v_g k + \hbar^2 k^2/2m^* - \hbar\vec{k}\cdot\vec{v}(\vec{P})]} \, . \tag{44}$$

Integrating this numerically we obtain $E(P)$ as a function of P in Fig. 4. This curve is quadratic for small P and becomes linear at large P indicating the limiting velocity, and gives 7.7×10^{-5} eV for the self-energy, $E(0)$, corresponding to a little less than 1 °K.

It is common to measure the strength of the elec-

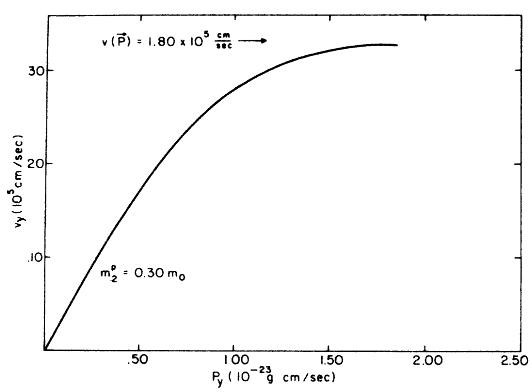

FIG. 3. Polaron's y component of velocity as a function of the y component of its momentum. The polaron mass m_2^p is given for small P, i.e., over the linear portion of the curve. The velocity is clearly seen to have an asymptote.

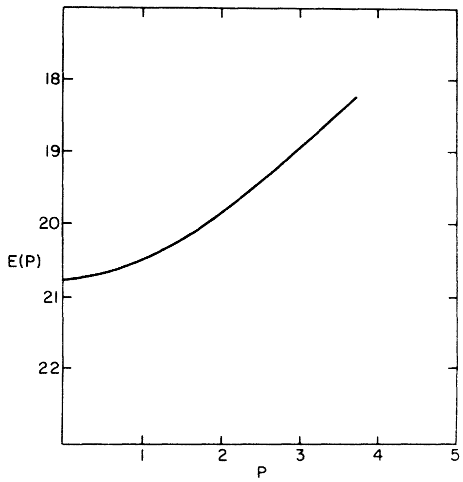

FIG. 4. Polaron energy vs momentum. The units of energy and momentum are m^*s^2 and m^*s, respectively, where $m^* = 1.82\times10^{-28}$ g and $s = 1.80\times10^5$ cm/sec.

tron-phonon interaction by the dimensionless quantity α, the coupling constant. Usually some sort of average over all directions is used and we call this average coupling constant $\langle\alpha\rangle$. In the anisotropic case α depends on the direction of $\vec{k}$. By comparing the interaction term in the anisotropic theory with that of the isotropic theory, we see that the effective coupling constant is

$$\alpha_g(\theta) = \frac{2\pi e^2}{\rho\hbar}\frac{(\vec{e}\cdot\hat{g})^2}{\bar{\epsilon}^2(\theta)v_g^3(\theta)}, \quad (45)$$

where we have indicated the θ dependence of $\bar{\epsilon}$ and v_g and the mode to which the electron is coupled by the subscript g. Again we point out our approximation of longitudinal and transverse polarization vectors.

If we take the spherical average of Eq. (45), i.e.,

$$\langle\alpha\rangle = \frac{2\pi e^2}{\rho\hbar}\frac{1}{2}\int_0^\pi \frac{(\vec{e}\cdot\hat{g})^2}{\bar{\epsilon}^2(\theta)v_g^3(\theta)}\sin\theta\, d\theta,$$

we obtain $\langle\alpha\rangle_{QL} = 0.11$ and $\langle\alpha\rangle_{QT} = 1.5$, for the quasilongitudinal and quasitransverse modes, respectively. If we take the spherical average of each term in the integrand separately and then find $\langle\alpha\rangle$, we get roughly the same result. The values we use are $\langle(\vec{e}\cdot\hat{g})^2\rangle_{QL} = 0.25\times10^{10}$ statcoul/cm^2, $\langle(\vec{e}\cdot\hat{g})^2\rangle_{QT} = 0.33\times10^{10}$ statcoul/cm^2, $\langle\bar{\epsilon}\rangle = 9.17$, $\langle v_{QT}\rangle = 1.95\times10^5$ cm/sec, and $\langle v_{QL}\rangle = 4.17\times10^5$ cm/sec. Mahan[27] has recently reported values for $\langle\alpha\rangle$ which differ slightly from those we have obtained. After we divide his values by 2 to account for a difference in the definition of α, they become $\langle\alpha\rangle_{QL} = 0.105$ and $\langle\alpha\rangle_{QT} = 1.85$. The disagreement in $\langle\alpha\rangle_{QT}$ is accounted for by the fact that he used $\langle v_{QT}\rangle = 1.78\times10^5$ cm/sec and $\langle\bar{\epsilon}\rangle = 9.28$ rather than the spherical averages we calculated for these quantities.

We can also find an average α from the polaron self-energy. In order to arrive at the polaron energies obtained in this paper using a completely isotropic theory one would use $\langle\alpha\rangle_{QT} = 1.4$ and $\langle\alpha\rangle_{QL} = 0.11$. This is obtained by using

$$E_g(0) = -\frac{4\langle\alpha\rangle_g}{\pi} m^* v_g^2 \ln\left(\frac{\hbar k_{max}}{2m^* v_g} + 1\right), \quad (46)$$

from the isotropic theory[15] (we have inserted units). In calculating these $\langle\alpha\rangle$ we used the spherical averages above for the sound speeds, and -0.303×10^{-16} ergs for $E_{QL}(0)$ and -0.922×10^{-16} ergs for $E_{QT}(0)$, the contributions to the polaron self-energy due to coupling with the QL and QT modes, respectively. The agreement between this method of finding α and that of shperically averaging $\alpha_g(\theta)$ gives further weight to our results.

VI. CONCLUSIONS

The anisotropic piezoelectric polaron Hamiltonian has been derived from the phenomenological equations (1) and (2) and Maxwell's equations. The intermediate-coupling theory was then applied to the problem giving the result that the polaron energy-momentum relation becomes linear at large P (Fig. 4). For small P the polaron masses are $m_1^p = m_2^p = 0.30\, m_0$ and $m_3^p = 0.38 m_0$ and become very large at larger P.

We give 0.11 and 1.5 for $\langle\alpha\rangle_{QL}$ and $\langle\alpha\rangle_{QT}$, the average coupling constants for coupling of the electron to the QL and QT acoustic-phonon modes. These values are obtained by spherically averaging the complete anisotropic expression for α and also by fitting α to our $E(0)$ using the isotropic theory.

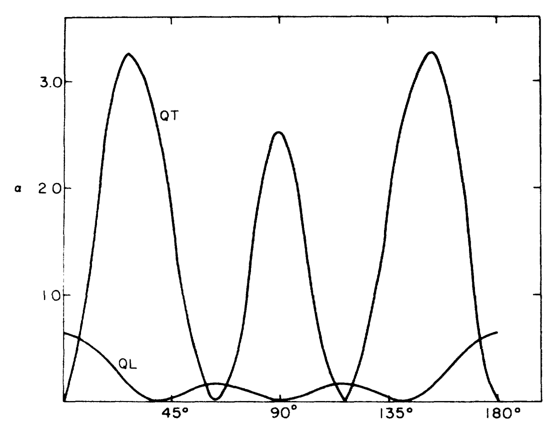

FIG. 5. Electron-phonon coupling constant, quasitransverse (QT) and quasilongitudinal (QL) modes. θ is the angle measured from the $\hat{c}$ axis.

ACKNOWLEDGMENTS

We are grateful to C. H. Henry for sending us his notes on the derivation of the anisotropic piezoelectric polaron Hamiltonian. We would also like to thank Emanuel Feuchtwang for a helpful suggestion and John Thomchick for comments and aid in the computer programming.

APPENDIX

Solving the two-dimensional eigenvalue problem for the quasimodes, the velocities of the quasilongitudinal and quasitransverse modes are given by

$$\rho v^2 = (b \pm \Delta^{1/2})/2,$$

where

$$b = c_{11}\sin^2\theta + c_{33}\cos^2\theta + c_{44} + (4\pi/\bar{\epsilon})\left[(e_{15}+e_{31})^2\sin^2\theta\cos^2\theta + (e_{15}\sin^2\theta + e_{33}\cos^2\theta)^2\right],$$

and

$$\Delta = (c_{11}^2 - 4c_{11}c_{44})\sin^4\theta + (c_{33}^2 - 4c_{33}c_{44})\cos^4\theta + 2c_{11}c_{44}\sin^2\theta + 2c_{33}c_{44}\cos^2\theta + c_{44}^2$$
$$+ (4c_{13}^2 + 8c_{13}c_{44} - 2c_{11}c_{33})\sin^2\theta\cos^2\theta$$
$$+ (4\pi/\bar{\epsilon})\{(e_{15}\sin^2\theta + e_{33}\cos^2\theta)^2 \times (2c_{44} + 2c_{33}\cos^2\theta - 2c_{11}\sin^2\theta - 4c_{44}\cos^2\theta)$$
$$+ (e_{15}+e_{31})^2(2c_{44} + 2c_{11}\sin^2\theta - 2c_{33}\cos^2\theta - 4c_{44}\sin^2\theta)\sin^2\theta\cos^2\theta$$
$$+ 8(c_{13}+c_{44})(e_{15}+e_{31})(e_{15}\sin^2\theta + e_{33}\cos^2\theta) \times \sin^2\theta\cos^2\theta$$
$$+ (4\pi/\bar{\epsilon})\left[(e_{15}+e_{31})^2\sin^2\theta\cos^2\theta + (e_{15}\sin^2\theta + e_{33}\cos^2\theta)^2\right]^2\}.$$

For $\theta = 0$ the above reduces to

$$\rho v_{QL}^2 = c_{33} + (4\pi/\bar{\epsilon})e_{33}^2$$

and

$$\rho v_{QT}^2 = c_{44}.$$

For $\theta = \pi/2$ we have

$$\rho v_{QL}^2 = c_{11}$$

and

$$\rho v_{QT}^2 = c_{44} + (4\pi/\bar{\epsilon})e_{15}^2.$$

---

[1]A. R. Hutson, J. Appl. Phys. 32, 2287 (1961).
[2]W. S. Baer and R. N. Dexter, Phys. Rev. 135, A 1388 (1964).
[3]K. Sawamoto, J. Phys. Soc. Jap. 18, 1224 (1963).
[4]W. W. Piper and R. E. Halsted, in *Proceedings of the International Conference on Semiconductor Physics, Prague*, 1960 (Academic, New York, 1961), p. 1046.
[5]J. J. Hopfield and D. G. Thomas, Phys. Rev. 122, 35 (1961).
[6]M. Balkanski and J. J. Hopfield, Phys. Status Solidi 2, 623 (1962).
[7]J. D. Zook and R. N. Dexter, Phys. Rev. 129, 1980 (1963).
[8]W. W. Piper and D. T. F. Marple, J. Appl. Phys. 32, 2237 (1961).
[9]G. D. Mahan and J. J. Hopfield, Phys. Rev. Lett. 12, 241 (1964).
[10]David M. Larsen, Phys. Rev. 142, 428 (1966).
[11]M. Saitoh and A. Kawabata, J. Phys. Soc. Jap. 23, 1006 (1967).
[12]S. J. Miyake, Phys. Rev. 170, 726 (1968).
[13]K. J. Button, B. Lax, D. R. Cohn, and W. Dreybrodt, in *Proceedings of the Tenth International Conference on the Physics of Semiconductors, Cambridge, Massachusetts*, 1970 (U.S. Atomic Energy Commission, National Technical Information Service, Springfield, Virginia, 1970), p. 153. Also S. Narita, K. Nagasaka, and G. Kido, *ibid.*, p. 158.
[14]Y. Osaka, J. Phys. Soc. Jap. 19, 2347 (1964).
[15]G. D. Whitfield, J. Gerstner, and K. Tharmalingam, Phys. Rev. 165, 993 (1968).
[16]K. Okamoto, J. Phys. Soc. Jap. 32, 46 (1972).
[17]M. Engineer and G. D. Whitfield, J. Phys. Soc. Jap. 34, 564 (1973).
[18]M. Rona and G. D. Whitfield, Phys. Rev. B 7, 2727 (1973).
[19]T. D. Lee, F. Low, and D. Pines, Phys. Rev. 90, 297 (1953).
[20]M. Gurari, Philos. Mag. 44, 329 (1953).
[21]This derivation of the anisotropic Hamiltonian follows an unpublished set of notes by Charles Henry of the Bell Telephone Laboratories.
[22]The material leading up to Eqs. (1c) and (3b) and much of the notation follow that of W. P. Mason, *Piezoelectric Crystals and their Application to Ultrasonics* (Van Nostrand, Princeton, N.J., 1950), pp. 32–36.
[23]Max Born and Kun Huang, *Dynamical Theory of Crystal Lattices* (Oxford U. P., London, 1954), p. 82.
[24]Mason, in Ref. 22, p. 27. We also use the fact that $T_{ij} = T_{ji}$ and $S_{ij} = S_{ji}$.
[25]Born and Huang, in Ref. 23, pp. 96–99.
[26]G. D. Mahan has recently derived the expression $V_g(\vec{k})$ and the polaron Hamiltonian via a different approach, in *Polarons in Ionic Crystals and Polar Semiconductors*, edited by Jozef T. Devreese (Elsevier, New York, 1972).
[27]Mahan uses the spherical average of $(\vec{e}\cdot\hat{g})$ as first performed by Hutson in Ref. 1.