PHYSICAL REVIEW B VOLUME 17, NUMBER 4 15 FEBRUARY 1978

Moving acoustical-mode polarons

John Thomchick
Department of Physics and Astronomy, The University of Georgia, Athens, Georgia 30602
(Received 7 October 1977)

A general class of acoustical-phonon mode induced-polaron systems is considered. The electron-phonon interaction for these systems is described by a Fröhlich-interaction Hamiltonian involving Fourier components proportional to q^γ, where γ is an arbitrary real number. The energy versus total momentum (E-P) relations for these polarons are investigated. At weak coupling, in the context of the intermediate coupling theory, it is found that when $-1 < \gamma \leq -1/2$ a linear structure is present in the E-P relations. As γ decreases from $-1/2$ to -1, this linear structure becomes apparent only for larger and larger values of P. For $\gamma > -1/2$, this linear structure is not present, but rather the E-P relations cut off at a critical value of P. When $-1 < \gamma \leq 0$, the polaron mass for these systems grows large as the polaron velocity v approaches the speed of sound s, but for $\gamma > 0$ the polaron mass has a finite value as $v \rightarrow s$. As a function of γ, the self-energy reaches a maximum value for $\gamma \approx -0.73$ and the $v \rightarrow 0$ polaron mass reaches a minimum value for $\gamma \approx -0.25$, independent of coupling strength. From a strong-coupling theory appropriate for moving polarons it is found that a linear structure in the E-P relations is obtained for all $\gamma > -1$. At both weak and strong coupling it is unclear that the E-P relations are meaningful when $\gamma \leq -1$.

I. INTRODUCTION

Both the piezoelectric and the acoustical deformation-potential (ADP) polarons have served as simple, yet interesting, examples of a particle interacting with a nonrelativistic linear field. Although these are the only "acoustical-mode polarons" thought to exist in nature, it was felt that it might be interesting to consider a more general class of electron, acoustical phonon-mode interactions. Aside from the intrinsic academic interest it was thought that it might be worthwhile to investigate some of the properties of the piezoelectric and ADP polarons in relation to this more general class.

The systems we consider are described by a Hamiltonian of the form

$$H = p^2 + \sum \omega(q) a_q^\dagger a_q + \sum Q(q)(a_q - a_{-q}^\dagger) e^{i\vec{q}\cdot\vec{r}}, \quad (1)$$

where

$$\omega(q) = q, \quad (2)$$

$$Q(q) = (4\pi\alpha/V)^{1/2} q^\gamma, \quad (3)$$

and γ is an arbitrary real number. In these equations $\vec{r}$ and $\vec{p}$ are the electron position and momentum operators and $a_q^\dagger$ and a_q are creation and annihilation operators for phonons in an acoustical mode $\vec{q}$. The units $2ms^2$ and $\hbar/2ms$, where m is the band mass and s is the average speed of sound, have been used for energy and length, respectively; the speed of sound is one in these units. The dimensionless quantity α is the coupling constant for the electron-phonon interaction and V is the volume. It is assumed that the prefactor in the expression for $Q(q)$ can always be written in the form given by absorbing any constants into α. For $\gamma = -\frac{1}{2}$, Eqs. (1)–(3) describe the piezoelectric interaction and for $\gamma = +\frac{1}{2}$, the ADP interaction.

In this paper we examine the energy versus total-momentum (E-P) relations for the systems described by Eqs. (1)–(3). Various authors[1–4] have investigated the E-P relation for the piezoelectric polaron. The E-P relation thought to be correct for this polaron is quadratic for very small P, but at large P asymptotes to a straight line with slope equal to the speed of sound. However, Rona and Ayasli[5] recently have investigated the ADP polaron and have indicated that the E-P relation for this polaron should be nearly parabolic. A question arises regarding the type of E-P relations to expect for the more general class of polarons considered here. In Sec. II we briefly review energy-level crossing arguments appropriate for an electron interacting with acoustical phonons. From these arguments it is found that a linear structure is expected in the E-P relations for any acoustical-mode interaction. In Sec. III we consider the E-P relations at weak coupling in the context of the intermediate-coupling theory and find that a linear structure in the E-P relations is predicted only for a limited range of γ. Finally, in Sec. IV we consider the above systems in a strong-coupling theory appropriate for moving polarons. From this theory we find that at strong coupling a linear structure in the E-P relations is predicted for any acoustical-mode interaction for which $\gamma > -1$.

II. REVIEW OF ENERGY-LEVEL CROSSING ARGUMENTS

In the energy-level crossing arguments[1] the degeneracy inherent in a noninteracting system of

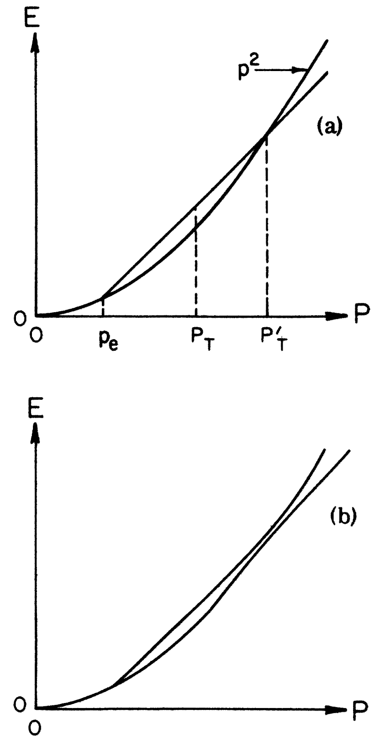

FIG. 1. (a) Crossing of an electron state and a one-phonon state at momentum P'_T. (b) Crossing of the electron state and the one-phonon state eliminated by the perturbation.

conduction-band electron plus acoustical phonons is considered.[6] Of particular interest is the situation where a state involving an electron with no phonons present and a state consisting of an electron plus a free phonon have identical energies. We then turn on the electron-phonon interaction and try to determine the type of E-P relation which might result from the splitting of the degeneracy by this perturbation.

The situation is depicted in Fig. 1(a), where any point on the parabolic curve corresponds to a state of definite momentum for a conduction-band electron. A straight line with slope equal to s can be added to this curve at any momentum p_e. This straight line represents a free-acoustical phonon, and at momentum P_T, for example, there are two possible states, one consisting simply of the conduction-band electron with no phonons present and the other consisting of an electron with momentum p_e plus a phonon with momentum $P_T - p_e$. At P_T these two states have distinct energies, but at P'_T the energies of two similar states are identical. If the electron-phonon interaction is now introduced, one might expect that the states with momentum P'_T would be split by the perturbation [cf. Fig. 1(b)] and, furthermore, that the resulting states near P'_T would be linear combinations of the zero-phonon state and the one-phonon state (i.e., the resulting states near P'_T would be something resembling a polaron).

More generally, the curves for a state involving a free phonon can cross the zero-phonon curve at any point for which the slope of the latter curve is $\geq s$. Applying degenerate perturbation theory to each of these points one obtains a curve which is quadratic at small P (when the slope of the zero-phonon curve is $<s$) and linear with slope s for large P. Any other possible states involving a free phonon must lie in the continuum above this curve.

These energy-crossing arguments are intuitively appealing but in using them there is no consideration given to the mechanism producing the electron-phonon interaction. Thus, these arguments might lead one to believe that the linear structure should be expected regardless of the type of acoustical-mode interaction involved. Indeed, the type of E-P relation predicted for the piezoelectric polaron agrees, at least qualitatively, with that suggested from the above arguments. However, as pointed out above, the E-P relation for the ADP polaron is thought to be nearly parabolic. On the other hand, it seems reasonable that there are other polaron systems (other values of γ) for which the linear structure should be expected. Thus, it seems interesting to pursue further a study of the E-P relations for the more general class of polarons described above.

III. E-P RELATIONS AT WEAK COUPLING

In considering the E-P relations for the systems described by Eqs. (1)–(3) we will first focus attention on the intermediate-coupling theory.[7] This theory is regarded as being appropriate in describing the weak-coupling regime and, in particular, is *not* an interpolation theory as the name might suggest.

The intermediate-coupling theory is felt to be an improvement over perturbation theory and the Tamm-Dancoff one-phonon cutoff approximation. For the piezoelectric polaron one finds from both perturbation theory and the Tamm-Dancoff approximation an indication that structure other than the usual quadratic behavior should be present in the E-P relation.[1] However, the E-P relations obtained using these methods are not fully believable, whereas the intermediate-coupling theory gives essentially the same type of curve as predicted from the energy-crossing arguments. For the ADP polaron, perturbation theory, the Tamm-Dancoff approximation, and the intermediate-coupling theory all give essentially the same qualitative results for the E-P relation with no indication of any linear structure.[5]

The intermediate-coupling theory is also useful in that it yields an upper bound to the energy for each value of the total momentum. Thus, if a linear curve is obtained from this theory it will always be lower in energy than a parabolic curve for sufficiently high P. In addition, for the piezoelectric polaron, the present author and Whitfield have shown that the states corresponding to the asymptotic part of the E-P relation obtained from the intermediate-coupling theory correspond to those expected for a polaron (i.e., an electron plus concomitant lattice distortion) rather than to a state involving a free phonon.[8] We have also shown, at least for a small range of coupling, that the lowest state at high P for the piezoelectric polaron Hamiltonian [Eqs. (1)–(3) with $\gamma=-\frac{1}{2}$] is not one containing a free phonon but is very likely a polaron state as described by the intermediate-coupling theory.[9]

The state vectors used in the intermediate-coupling theory are given by

$$|\psi_{ic}\rangle = U_1 U_2 |0\rangle \,, \tag{4}$$

where

$$U_1 = \exp\left[-i\left(\sum \vec{q}\, a_q^\dagger a_q\right)\cdot \vec{r}\right], \tag{5}$$

and

$$U_2 = \exp\left(\sum f_q (a_q^\dagger - a_q)\right). \tag{6}$$

The f_q are determined from the condition

$$\frac{\partial E}{\partial f_q} = \frac{\partial \langle \psi_{ic}|H|\psi_{ic}\rangle}{\partial f_q} = 0 \,, \tag{7}$$

and are given by

$$f_q = -Q(q)/[q^2 + \omega(q) - \vec{q}\cdot\vec{v}] \,, \tag{8}$$

where

$$\vec{v} = \frac{\partial E}{\partial \vec{P}} \,. \tag{9}$$

The state vectors given by Eq. (4) are eigenstates of the total-momentum operator

$$\vec{\mathcal{P}} = \vec{p} + \sum \vec{q}\, a_q^\dagger a_q \,, \tag{10}$$

and the eigenvalues of $\vec{\mathcal{P}}$ are denoted by $\vec{P}$ {note $[\vec{\mathcal{P}}, H] = 0$}.

For the Hamiltonian, Eq. (1), the energy and momentum are given by

$$E = P^2 - (\vec{P} - \tfrac{1}{2}\vec{v})^2 - \frac{4\pi\alpha}{V} \sum \frac{q^{2\gamma}}{q^2 + \omega(q) - \vec{q}\cdot\vec{v}} \tag{11}$$

and

$$\vec{P} = \tfrac{1}{2}\vec{v} + \frac{4\pi\alpha}{V} \sum \frac{\vec{q}\, q^{2\gamma}}{[q^2 + \omega(q) - \vec{q}\cdot\vec{v}]^2} \,. \tag{12}$$

In these expressions it is assumed that $\vec{P}$ and $\vec{v}$ point in the same direction. The integrals appearing in Eqs. (11) and (12) can easily be performed for a number of values of γ (an upper cutoff q_m is used; $q_m \approx 150$ in the units used here). They can also be computed numerically for a wide range of γ. The following results emerge. For $\gamma \leqslant -1$ both E and P diverge for any v so that it is not clear that an E-P relation is meaningful in this case. This occurs because of the long-range nature of the interaction for these values of γ. It is possible that we could patch up this difficulty by introducing a lower cutoff into the interaction, such as was done by Rona and Whitfield[10] who investigated the effect of introducing a cutoff into the piezoelectric interaction. However, this would take us somewhat afield of the simpler problems we wish to consider here. When $-1 < \gamma < -\frac{1}{2}$ one finds at large P that the E-P relation asymptotes to a straight line with slope s. The E-P relations for some representative values of γ in this range are shown in Fig. 2 (in each case $\alpha = 1.0$). For $\gamma = -\frac{1}{2}$ the slope of the E-P curve is already 0.99 when $P \approx 1.5$ (in units $2ms$). For $\gamma = -\frac{3}{4}$ the slope is 0.99 only when P is as large as ≈ 8.0. For $\gamma = -\frac{9}{10}$ the slope does not reach 0.99 until $P \approx 40.0$ (in the figure the slope is ≈ 0.94 for $P \approx 10.0$). The reason that as γ decreases from $-\frac{1}{2}$ to -1 larger and larger momenta are required before the slope approaches its limiting value of 1.0 can be seen from the expression for P, Eq. (12). The linear structure occurs when $-1 < \gamma \leqslant -\frac{1}{2}$ because for this range of γ the total momentum becomes unbounded as $v \to 1$. For larger negative values of γ in this range the divergence is stronger and, thus, larger

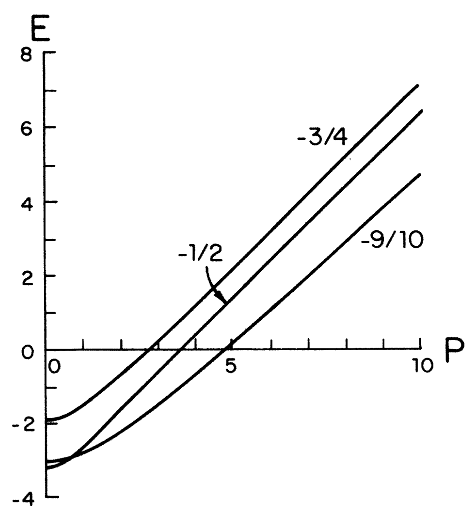

FIG. 2. E-P relations in the intermediate-coupling theory for the cases $\gamma = -\frac{1}{2}$, $-\frac{3}{4}$, and $-\frac{9}{10}$. In each case $\alpha = 1.0$.

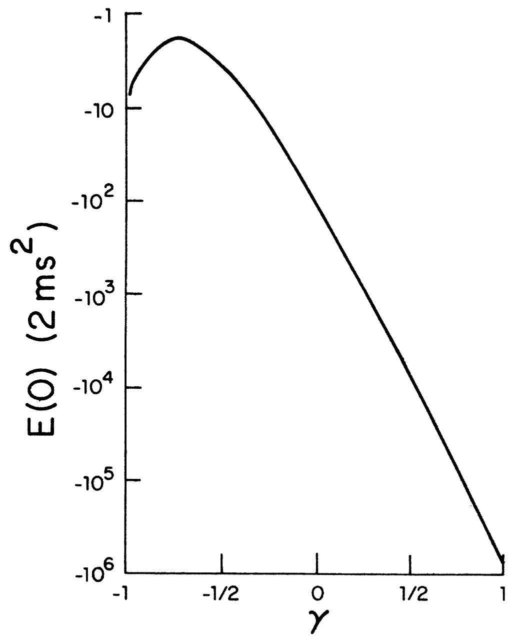

FIG. 3. Self-energy in the intermediate-coupling theory as a function of γ for $\alpha = 1.0$. There is a maximum at $\gamma \approx -0.73$ and the curve diverges logarithmically as $\gamma \to -1$.

values of P are obtained for a given value of v close to 1.0. It is interesting to note that the divergence which occurs as $v \to 1$ is weakest (logarithmic) for the piezoelectric case ($\gamma = -\frac{1}{2}$).

We should also point out that the self-energy $E(0)$ is larger for $\gamma = -\frac{3}{4}$ than for either of the cases $\gamma = -\frac{1}{2}$ or $\gamma = -\frac{9}{10}$. As a function of γ the self-energy in this theory reaches a maximum value for $\gamma \approx -0.73$. The value of γ at which this maximum occurs is independent of coupling strength. This behavior of the self-energy results because of the relative importance of the small-wave-vector contribution versus the large-wave-vector contribution to the integrands in Eqs. (11) and (12). As γ decreases ($\gamma \to -1$) small q values give the dominant contribution to the integrals in Eqs. (11) and (12), but as γ increases and becomes positive the large wave vectors assume increased importance. In each limit the self-energy is a large negative number. The self-energy as a function of γ is plotted in Fig. 3 for the case $\alpha = 1.0$.

For $\gamma > -\frac{1}{2}$ the expression for P does not become unbounded even as $v \to 1$. Thus, there is no linear structure in the E-P relations for these values of γ. In fact, for these values of γ the E-P relations given by the intermediate-coupling theory stop at a critical value of P beyond which there are no solutions. Thus, it seems that a better theory could be found to describe the systems corresponding to this range of γ.

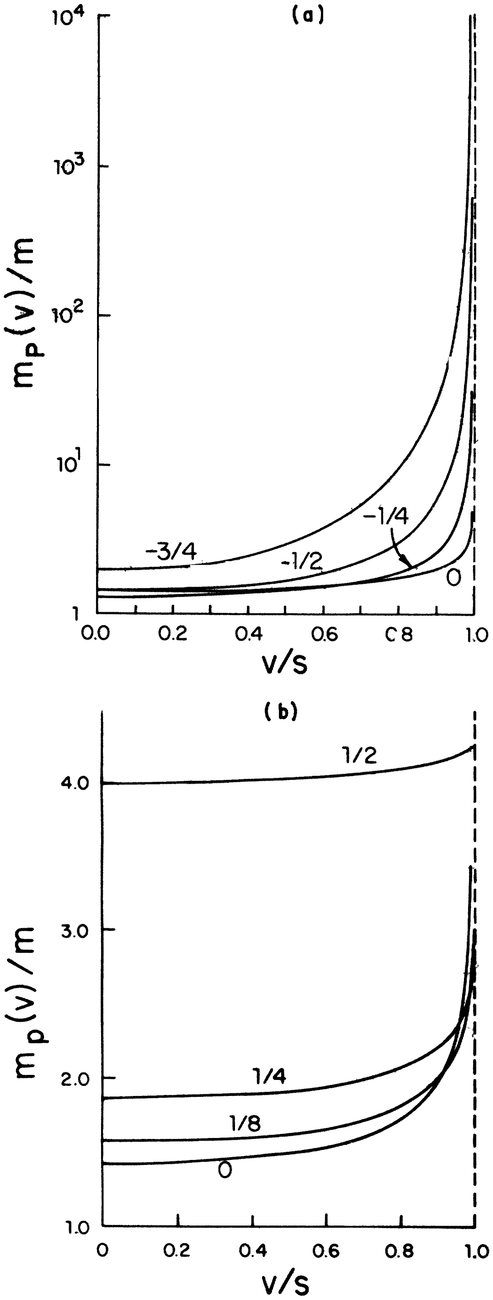

FIG. 4. (a) Polaron mass vs polaron velocity in the intermediate coupling theory for several values of $\gamma \leq 0$ ($\alpha = 1.0$). The curve for $\gamma = 0$ diverges logarithmically as $v \to 1$. (b) Polaron mass vs polaron velocity in the intermediate-coupling theory for several values of $\gamma \geq 0$ ($\alpha = 1.0$). When $\gamma > 0$, there are finite values of the mass for $v = 1.0$.

The mass in this theory is most easily calculated by using $m_p = \partial \vec{P} / \partial \vec{v}$ and is given (in units of m) by

$$m_p(v) = 1 + \frac{16\pi\alpha}{V} \sum \frac{q^{2\gamma+2}}{[q^2 + \omega(q) - \vec{q} \cdot \vec{v}]^3} \cdot \quad (13)$$

Just as for E and P, when $\gamma \leq -1$ the integral in Eq. (13) diverges for any v. However, we find that even though the asymptotic linear behavior in this theory occurs only for $-1<\gamma\leq-\frac{1}{2}$, the mass becomes unbounded in the limit $v\to 1$ for $-1<\gamma\leq 0$. Thus, the large mass in the limit $v\to 1$ is not sufficient to cause the linear structure as might be concluded from a study of the piezoelectric polaron. The mass as a function of the polaron velocity is shown in Fig. 4(a) for several values of γ in the range $-1<\gamma\leq 0$ (in each case $\alpha=1.0$). For the $\gamma=0$ curve the divergence as $v\to 1$ is logarithmic. In Fig. 4(b) the mass is plotted as a function of velocity for several values of $\gamma>0$ and these curves are compared with the $\gamma=0$ case. Even for $\gamma>0$ it is noted that the mass increases slightly as $v\to 1$. However, in each case for $\gamma>0$ there is a finite value for the mass at $v=1.0$.

In Fig. 4(a) the curve for $\gamma=0$ lies above that for $\gamma=-\frac{1}{4}$ for small v even though the strength of the divergence as $v\to 1$ is much greater for the $\gamma=-\frac{1}{4}$ curve. For the same reason that the self-energy as a function of γ reached a maximum value, the $v\to 0$ polaron mass as a function of γ reaches a minimum value in this theory. This minimum occurs for $\gamma\approx-0.25$, independent of coupling strength. The curve $m_p(v\to 0)$ vs γ is plotted in Fig. 5 for the case $\alpha=1.0$.

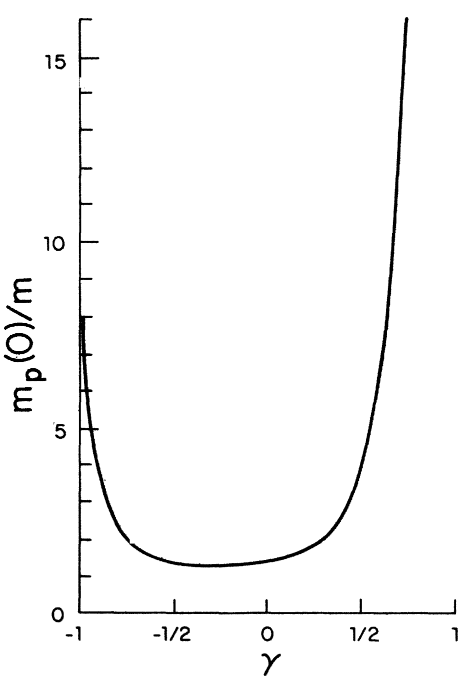

FIG. 5. $v\to 0$ polaron mass vs γ in the intermediate-coupling theory for $\alpha=1.0$. There is a minimum for $\gamma\approx-0.25$ and the curve diverges logarithmically as $\gamma\to-1$.

IV. *E-P* RELATIONS AT STRONG COUPLING

A version of strong-coupling theory appropriate for moving polarons[11] also gives a linear E-P relation for the piezoelectric polaron.[12] We briefly consider the application of this theory to the general class of polarons described in Eqs. (1)–(3).

The state vectors used in this theory are given by

$$|\psi_{sc}\rangle = e^{i\vec{w}\cdot\vec{r}_e}\Phi(\vec{r}_e-\vec{r})\,e^{S(\vec{r})}|0\rangle\,, \tag{14}$$

where

$$S(\vec{r})=\sum d_q(a_q e^{i\vec{q}\cdot\vec{r}}-a_q^\dagger e^{-i\vec{q}\cdot\vec{r}})\,, \tag{15}$$

and where $\Phi(\vec{r})$ is a bound-state electronic wave function whose exact form may vary depending on the range of the electron-phonon interaction.[13] The parameters d_q are determined variationally to be

$$d_q=\tfrac{1}{2}Q(q)(\rho_q+\rho_{-q})/[\omega(q)-\vec{v}\cdot\vec{q}]\,, \tag{16}$$

where

$$\rho_q=\int d^3r\,\Phi^\dagger(\vec{r})\,e^{i\vec{q}\cdot\vec{r}}\Phi(\vec{r})\,. \tag{17}$$

The factor $e^{i\vec{w}\cdot\vec{r}_e}$ allows the entire system to move, with $\vec{w}$ also determined variationally and given by

$$\vec{w}=\frac{\vec{v}}{2}-\int d^3r\,\Phi^\dagger(\vec{r})\vec{p}\Phi(\vec{r})\,. \tag{18}$$

The state vectors, Eq. (14), are not eigenstates of $\vec{\mathcal{P}}$. The E-P relations in this theory are obtained in terms of the expected value of $\vec{\mathcal{P}}$ which is introduced as a constraint

$$\vec{P}=\langle\psi_{sc}|\vec{\mathcal{P}}|\psi_{sc}\rangle\,. \tag{19}$$

The Lagrange multiplier associated with this constraint is proportional to the polaron velocity.

The energy and the equation relating the momentum and velocity are given by

$$E=P^2-(\vec{P}-\tfrac{1}{2}\vec{v})^2+\int d^3r\,\Phi^\dagger p^2\Phi - \frac{4\pi\alpha}{V}\sum\frac{q^{2\gamma}|\rho_q|^2}{\omega(q)-\vec{v}\cdot\vec{q}}\,, \tag{20}$$

and

$$\vec{P}=\frac{\vec{v}}{2}+\frac{4\pi\alpha}{V}\sum\frac{\vec{q}q^{2\gamma}|\rho_q|^2}{[\omega(q)-\vec{v}\cdot\vec{q}]^2}\,. \tag{21}$$

The structure we are concerned with here is not affected by a reasonable choice of the electronic wave function. As in the weak-coupling case, it again is not clear whether the E-P relations are meaningful for $\gamma\leq-1$. However, for all $\gamma>-1$ one finds that as $v\to 1$ the momentum grows large. Thus, from this theory an asymptotic linear behavior is predicted at strong coupling for all acoustical-mode polarons ($\gamma>-1$) including the deformation-potential case. Unfortunately, since the E-P relations are calculated in terms of the expected value of $\vec{\mathcal{P}}$ rather than in terms of an eigenvalue of $\vec{\mathcal{P}}$ it is not clear how meaningful these relations are.

V. CONCLUDING REMARKS

We have considered a general class of acoustical-phonon mode induced-polaron systems characterized by a Fröhlich interaction Hamiltonian involving Fourier components proportional to q^γ. The energy-momentum relations for these systems were investigated. From energy-level crossing arguments we were led to expect that the E-P relations for these systems should be quadratic for small P, but linear for large values of P. For the weak-coupling limit, in the context of the intermediate-coupling theory, we found for the range $-1<\gamma\leqslant-\frac{1}{2}$ qualitatively the type of E-P relation suggested from the energy-level crossing arguments. This relation is quadratic for small P and asymptotes to a straight line with slope equal to the speed of sound for large P. For $\gamma>-\frac{1}{2}$ there was no indication of linear structure in the E-P relations and, in fact, the E-P relations cutoff for a critical value of P beyond which there are no solutions. From a strong-coupling theory appropriate for moving polarons we found that the linear structure was expected in each case for $\gamma>-1$. However, in this theory the E-P relations are given in terms of the expected value of P and, thus, it is not clear that they can be fully trusted. In both weak and strong coupling the E-P relations are not meaningful when $\gamma\leqslant-1$; this resulted because of the very long-range nature of the interactions for these values of γ.

There need be no inconsistency concerning the fact that the linear structure at weak coupling appears for only a limited range of $\gamma>-1$, while at strong coupling the linear structure is present for all $\gamma>-1$. Although the weak-coupling results do not agree with the energy-level crossing arguments, in these arguments one considers only the degeneracy in the electron-phonon system, not the range of the interaction. In the weak-coupling limit, if the range of the interaction is not sufficiently long, then, apparently, as $v\rightarrow1$ there are not enough (long-wavelength) phonons collecting in the "phonon cloud" around the electron in order to trap the electron at the speed of sound. However, at strong coupling this situation does not arise since in this limit the electron is always much more deeply bound.

ACKNOWLEDGMENT

The author wishes to thank Claud F. Elliott, Jr. for aid with some of the computer programming.

[1] G. Whitfield, G. Gerstner, and K. Tharmalingam, Phys. Rev. 165, 993 (1968).
[2] K. Okamoto, J. Phys. Soc. Jpn. 32, 46 (1972).
[3] G. E. Volovik and V. M. Edel'shtein, Sov. Phys-JETP 40, 147 (1975).
[4] V. I. Sheka, L. Khazen, and E. V. Mozdor, Phys. Status Solidi B 72, 883 (1975).
[5] M. Rona and S. Ayasli, Phys. Rev. B 15, 4822 (1977).
[6] Similar energy level crossing arguments have been used previously for optical-phonon systems. See T. D. Schultz, Solid State and Molecular Theory Group, MIT Tech. Rep. No. 7 (1956) (unpublished), and G. Whitfield and R. Puff, Phys. Rev. 139, A338 (1965).
[7] T. D. Lee, F. Low, and D. Pines, Phys. Rev. 90, 297 (1953); M. Gurari, Philos. Mag. 44, 324 (1953).
[8] J. Thomchick and G. Whitfield, Phys. Rev. B 10, 3458 (1974).
[9] J. Thomchick and G. Whitfield, Phys. Rev. B 9, 1506 (1974).
[10] M. Rona and G. Whitfield, Phys. Rev. B 7, 2727 (1973).
[11] S. I. Pekar, *Research in Electron Theory of Crystals*, AEC (U.S. GPO, Washington, D.C., 1963).
[12] R. Parker, G. Whitfield and M. Rona, Phys. Rev. B 10, 698 (1974).
[13] For example, for the piezoelectric case a Gaussian wave function has been used (cf. Ref. 12), but for the ADP case it is thought that the wavefunctions corresponding to something like a spherical square-well potential may be more appropriate.