PHYSICAL REVIEW B VOLUME 14, NUMBER 8 15 OCTOBER 1976

Interaction of electrons with acoustic phonons via the deformation potential in one dimension

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(Received 14 June 1976)

We investigate the one-dimensional polaron in the case where the electron couples to the acoustic phonons via the deformation potential. In addition to the fact that this model may apply for some quasi-one-dimensional systems, it has several interesting features. The model exhibits the same type of divergence as the piezoelectric polaron but in a mathematically more tractable form. Realistic values of the deformation potential suggest that strong coupling applies. We show that in the strong-coupling limit the theory reduces to another polaron model that Gross has shown to be exactly solvable. We also obtain a soliton-like model for the moving polaron. The first correction to the strong-coupling limit has an ultraviolet divergence which is caused by the fact that the short-wavelength phonons follow the motion of the electron in its self-trapped state. This situation is also analogous to the piezoelectric polaron.

I. INTRODUCTION

In every crystal where there is band conduction the electrons are coupled to the phonons via the deformation potential.[1] In ionic crystals electrostatic coupling usually is more important, but even in these the deformation potential scattering often dominates in some temperature region. Electron-phonon interaction in metals can generally be thought of as deformation-potential coupling, and it dominates transport phenomena in nonpolar semiconductors over a wide range of temperatures. In almost all cases where deformation-potential coupling is important it is thought to be sufficiently weak to be treated by the lowest order of perturbation theory.

It was, however, suggested some time ago by Toyozawa[2,3] that in some instances the strong-coupling theory may apply. We will first present a very simple heuristic version of Toyozawa's theory, and show that the same theory in one dimension is not only much more manageable but that reasonable values of the parameters suggest that strong coupling should apply in quasi-one-dimensional systems. In the strong-coupling polaron theory[4] the electron causes the lattice to deform in such a way that an attractive potential is set up for the electron. The electron then becomes trapped in this potential well and its presence in turn maintains the lattice deformation. Let us assume that this has happened and calculate the energy. We assume that the electron is trapped in a region of radius R giving rise to an electronic kinetic energy of $\hbar^2/2mR^2$. Since the electron-phonon interaction is short range (see Sec. III) the lattice will deform primarily where the electron is, and hence we assume a constant dilation Δ in a sphere of radius R. This gives rise to an elastic energy of $(C\Delta^2/2)(4\pi/3)R^3$ where C is an average elastic constant[5] (i.e., $C\Delta^2/2$ is the energy per unit volume). The electron-phonon interaction contributes a term $-D\Delta$, where D is the deformation potential. Dropping all numerical factors, we have for the energy

$$E=\hbar^2/mR^2+C\Delta^2R^3-D\Delta\ . \qquad (1)$$

If we set $\partial E/\partial\Delta=0$, we then find that

$$\Delta=D/2CR^3 \qquad (2)$$

and

$$E=\hbar^2/mR^2-D^2/4CR^3\ . \qquad (3)$$

If we next minimize this energy with respect to R, we see that for R small enough the negative term must dominate and $E\to-\infty$ as $R\to 0$. Hence when we treat the crystal as an elastic continuum the solution is unstable. However, in a real crystal R is limited by the lattice constant a, and then if the deformation potential is large enough, we can have a stable bound solution if

$$0>E=\hbar^2/ma^2-D^2/4Ca^3$$

or

$$D^2m/\hbar^2 4Ca>1\ . \qquad (4)$$

In addition to this requirement, which is peculiar to this type of polaron, there is the usual requirement for the validity of the strong-coupling polaron theory, namely that in order for Eq. (1) to be correct is necessary that the electron in its bound state move faster than the lattice can respond, or else the lattice well will start to follow the electron in its internal motion and the bound state will break up. In the bound state the electron moves with a frequency $\simeq\hbar/ma^2$ and the lattice well is made of phonons whose approximate wave vector is $q_m=\pi/a$ and whose frequency is $s\pi/a$. So we need for the consistency of Eq. (1)

$$\hbar/ma^2 \gg s/a$$

or (5)

$$\hbar/ms \gg a\,.$$

This condition is usually satisfied. $\hbar/ms$ is the analogy of the Compton wavelength for an electron interacting with acoustic phonons instead of photons. For the band effective mass m equal to the free-electron mass $\hbar/ms \simeq 2\times 10^{-6}$ cm.

More elaborate versions or variations of this theory have received alot of attention in the literature.[6] In the present paper we want to consider a one-dimensional version. The heuristic theory proceeds in much the same way as the above except for the calculation of the energy stored in the strain field. The term $C\Delta^2$ (with C an appropriate elastic parameter) is the energy stored per unit length and hence the total elastic energy is $C\Delta^2R$ rather than $C\Delta^2R^3$, which completely changes the character of the solution. The analogy of Eq. (1) in one dimension is

$$E=\hbar^2/mR^2+C\Delta^2R-D\Delta\,. \tag{6}$$

We set

$$\frac{\partial E}{\partial\Delta}=0$$

and get that

$$\Delta=D/2CR\,,$$

and for this value of Δ we have

$$E=\hbar^2/mR^2-D^2/4CR\,,$$

which unlike the three-dimensional case has a minimum for any D at

$$R_{\min}=8\hbar^2C/mD^2. \tag{7}$$

We then always have that the minimum energy is

$$E_{\min}=-D^4/64C^2\hbar^2. \tag{8}$$

Hence there is always a stable bound state like the original polaron problem,[4] providing the adiabatic condition is satisfied. In this case, as in three dimensions, we need that the electron moves faster in its bound state than the phonons that make up the lattice well. The frequency of the electron is $\hbar/mR_{\min}^2$ while the most important phonons in the lattice distortion have wavelength $R_{\min}$ and hence frequency $s\pi/R_{\min}$. Therefore we need that

$$\hbar/mR_{\min}^2 \gg s/R_{\min}\,,$$

hence

$$\hbar/ms \gg R_{\min}$$

or

$$D^2/8\hbar sC \gg 1. \tag{9}$$

In Sec. II we will show that this is essentially the condition that the coupling constant α be large in comparison to one. Hence this is the standard strong-coupling theory which has stable solutions for all coupling in one dimension without the complexities that beset the three-dimensional theory.

The two-dimensional theory has a lattice energy $C\Delta^2R^2$ and

$$E=\hbar^2/mR^2+C\Delta^2R^2-D\Delta\,.$$

Then

$$\frac{\partial E}{\partial\Delta}=0$$

gives that

$$\Delta=D/2CR^2$$

and

$$E=\hbar^2/mR^2-D^2/4CR^2\,.$$

This result is qualitatively like the three-dimensional theory in that it requires a minimum D for a bound state with the binding energy becoming deeper as R gets smaller. We will not discuss two dimensions further in this paper.

II. HAMILTONIAN

Since the deformation potential interaction is usually used only to calculate transition rates in first-order perturbation theory, the Hamiltonian has not been cast in the standard dimensionless form of polaron theory,[3]

$$H_p=-\tfrac{1}{2}\nabla_r^2+\sum_q a_q^\dagger a_q\,\omega(q)+\left(\frac{4\pi\alpha}{V}\right)^{1/2}\sum_q Q(q)(a_q+a_{-q}^\dagger)e^{i\vec{q}\cdot\vec{r}}\,. \tag{10}$$

We will show that the Hamiltonian for an electron interacting with acoustic phonons via the deformation potential can be put in the form of Eq. (10) by an appropriate choice of units and identification of the coupling constant α. We will see later that α is not the only parameter in the theory but that the cutoff wave vector q_m plays an essential role. Once we have the form for three dimensions, that for one dimension will follow immediately.

Consider an electron moving in an energy band whose energy momentum relation is $\epsilon(\vec{k})=\hbar^2k^2/2m$. Then in the effective mass approximation we write an effective Hamiltonian

$$H=-(\hbar^2/2m)\nabla^2+D\vec{\nabla}\cdot\vec{u}+H_{\text{lattice}}\,.$$

We will consider a wide band with one electron of effective mass m in it. [In the case of a narrow band which might be appropriate for some quasi-one-dimensional system of interest we would have to use a more complicated function for $\epsilon(\vec{k})$ and also for the interaction term $D\vec{\nabla}\cdot\vec{u}$.] The deformation potential D is the constant of proportionality for the shift of the bottom of the band with lattice dilation $(\vec{\nabla}\cdot\vec{u})$.

The displacement of the lattice[1] at the point $\vec{r}$ is $\vec{u}(\vec{r})$.

$$\vec{u}(\vec{r}) = \sum_{q,\sigma}\left(\frac{\hbar}{2NM\omega(q,\sigma)}\right)^{1/2} \hat{e}(q\sigma) \times (a'^{\dagger}_{-q,\sigma} + a'_{q,\sigma})e^{i\vec{q}\cdot\vec{r}} . \tag{11}$$

The phonon wave vector is $\vec{q}$, and σ is the polarization index which runs from 1 to 3 for acoustic phonons. We assume that $\sigma = 1$ is a longitudinal wave and $\sigma = 2, 3$ are transverse waves. We choose $\hat{e}(q,1) = i\hat{q}$ insuring that $\hat{e}^*(q,1) = \hat{e}(-q,1)$ and $\hat{e}^*(q,1)\cdot\hat{e}(q,1) = 1$. The number of unit cells is N and the mass of an ion core is M. The phonon frequency $\omega(q1) \equiv \omega(q) = s|q|$. Hence the interaction term is the Hamiltonian involves only the longitudinal phonons and is given by

$$H_{\text{int}} = D\vec{\nabla}\cdot\vec{u} = -\sum_q D\left(\frac{\hbar}{2NMs}\right)^{1/2}(|q|)^{1/2} \times (a'_{q,1} + a'^{\dagger}_{-q,1})e^{\vec{q}\cdot\vec{r}} . \tag{12}$$

Since the interaction in the polaron problem traditionally has a positive sign we make the substitution $a'_{q,1} = -a_q$ and obtain for the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla_r^2 + \sum_q a_q^\dagger a_q\,\omega(\vec{q}) + \sum_q D\left(\frac{\hbar}{2NMs}\right)^{1/2}(|q|)^{1/2}(a^\dagger_{-q} + a_q)e^{i\vec{q}\cdot\vec{r}} . \tag{13}$$

If we use ms^2 as a unit of energy and $\hbar/ms$ as a unit of length, we have $H' = H/ms^2$, $x' = xms/\hbar$, $q' = \hbar q/ms$, and hence

$$H' = -\tfrac{1}{2}\nabla^2_{r'} + \sum_{q'} a^\dagger_{q'}a_{q'}|q'| + \sum_{q'}\frac{D}{ms^2}\left(\frac{m|q'|}{2NM}\right)^{1/2}(a_{q'} + a^\dagger_{-q'})e^{i\vec{q}'\cdot\vec{r}'} . \tag{14}$$

Comparing these with the last term in Eq. (10), we see that $Q(q') = (|q'|)^{1/2}$ and that

$$\alpha_3 = D^2m^2/8\pi\rho\hbar^3 s , \tag{15}$$

where $\rho = MN/V$ is the mass density of the crystal and α_3 is the coupling constant for three dimensions. This expression can also be written, by use of the relation $C = \rho s^2$, as

$$\alpha_3 = D'^2/C' ,$$

where D' and C' are the deformation potential and the elastic constant in our dimensionless units. In terms of this coupling constant we see that the condition, Eq. (4), for the existence of the stable bound solutions in three dimensions discussed in the introduction is

$$D^2m/\hbar^2 4Ca = 2\alpha_3 q'_m > 1 .$$

Here we have defined $q'_m = \hbar\pi/msa$ and the adiabatic condition Eq. (5) reads

$$q'_m \gg 1 .$$

Hence we have the peculiar situation that the condition for the strong-coupling theory depends not only on α but also on the cutoff wave vector q_m. This has been realized by Toyozawa and Sumi[6] but we have repeated it here in the present form to put in the context of the polaron problem.

Our main purpose in the present paper is to discuss the one-dimensional problem where the equation correponding to Eq. (14) is

$$H' = -\frac{1}{2}\frac{\partial^2}{\partial x'^2} + \sum_{q'} a^\dagger_{q'}a_{q'}|q'| + \sum_{q'}\frac{D}{ms^2}\left(\frac{m|q'|}{2NM}\right)^{1/2}(a^\dagger_{-q'} + a_{q'})e^{iq'x'} . \tag{16}$$

Again putting this in the standard form for a polaron [Eq. (10)], when we replace the volume by the length $L' = L/(\hbar/ms)$ we have

$$H' = -\frac{1}{2}\frac{\partial^2}{\partial x'^2} + \sum_{q'} a^\dagger_{q'}a_{q'}|q'| + \left(\frac{4\pi\alpha}{L'}\right)^{1/2}\sum_{q'}(|q'|)^{1/2}(a^\dagger_{-q'} + a_{q'})e^{iq'x'} , \tag{17}$$

where

$$\alpha = \frac{1}{8\pi}\frac{D^2a}{\hbar m s^3} = \alpha_3\left(\frac{\hbar/ms}{a}\right)^2 . \tag{18}$$

It is interesting to note that $\alpha \gg 1$ for most reasonable values of the parameters. In these terms the result of the heuristic theory [Eqs. (7) and (8)] with $C = \rho s^2 = (M/a)s^2$ becomes

$$R_{\min} = (1/\pi\alpha)\hbar/ms \tag{19}$$

and

$$E_{\min} = -\pi^2\alpha^2 ms^2 . \tag{20}$$

We will see in Sec. IV that this is very close to the exact answer for the strong-coupling theory. The adiabatic condition Eq. (9) is that $\alpha \gg 1$. We note that the cutoff wave vector q'_m plays no essential role in the one dimensional strong-coupling limit, however, we will see in Sec. VI that the first corrections to the theory are cutoff dependent.

III. WEAK COUPLING

Although the value of $\alpha \gg 1$ for most quasi-one-dimensional systems, we will investigate the weak-coupling theory for two reasons. First, we are interested in this problem partly for academic reasons, and therefore we want a complete view of it. And second, we will see in Sec. VI that the short-wavelength phonons couple to the electron essentially by perturbation theory even when $\alpha \gg 1$.

A. Perturbation theory

Starting with the Hamiltonian given in Eq. (17), and treating the last term in second-order perturbation theory, we obtain for the energy of a polaron with wave vector P

$$E_p(P) = \frac{P^2}{2} + \frac{4\pi\alpha}{L} \sum_q \frac{|q|}{\frac{1}{2}P^2 - \frac{1}{2}(P-q)^2 - |q|}, \quad (21)$$

$$E_p(P) = \frac{P^2}{2} - 4\alpha \ln\left(\frac{q_m^2 + 4q_m + 4(1-P^2)}{4(1-P^2)}\right), \quad P<1. \quad (22)$$

For convenience we have dropped the primes that we used in Sec. II to indicate that all quantities are dimensionless. For small P we write

$$E_p(P) = E_p(0) + P^2/2m^*, \quad (23)$$

where

$$E_p(0) = -8\alpha \ln(\tfrac{1}{2}q_m + 1), \quad (24)$$

$$1/m^* = 1 - 8\alpha + 8\alpha/(\tfrac{1}{2}q_m + 1)^2. \quad (25)$$

It is interesting to note that in the $q_m \to \infty$ limit the self energy diverges but the effective mass is finite. Also these results are essentially the same as those obtained for the three-dimensional piezoelectric polaron.[7]

For larger P we see that as $P \to 1$ the energy [Eq. (22)] diverges. See Fig. 1. This is typical of the unphysical behavior that we have come to expect from nondegenerate perturbation theory near the threshold for emission of phonons.[7,8] For $P \gg 1$ we would again expect reasonable results from perturbation theory by taking the principal value of the sum in (21).

In the analogous three-dimensional piezoelectric polaron problem we found[7] that the behavior below the phonon emission threshold was more reasonable in the intermediate-coupling theory. Therefore we consider that theory now.

B. Intermediate-coupling theory

We will next consider a well known polaron theory first devised by Lee, Low, and Pines,[9] and also by Gurari,[10] which although it is called intermediate coupling applies primarily in the weak-coupling range, and is in some respects an improvement on perturbation theory.

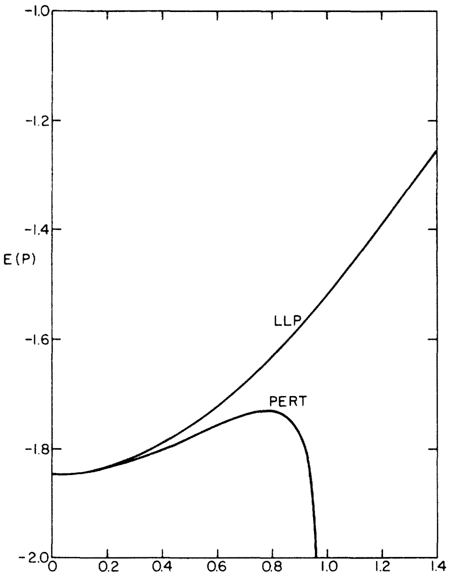

FIG. 1. Energy-momentum relation for perturbation theory and the intermediate-coupling theory of Lee, Low, and Pines (LLP). Curves are for $q_m = 200$ and $\alpha = 0.05$.

This theory is an upper bound to the ground-state energy for each value of P (the total momentum), because it can be formulated variationally using a trial state which is an eigenstate of total momentum.[9]

The energy is given by[11]

$$E_L(P) = \tfrac{1}{2} P^2 - \tfrac{1}{2}[P - v(P)]^2 - \frac{4\pi\alpha}{L} \sum_q \frac{|q|}{|q| - qv(P) + \frac{1}{2}q^2}, \quad (26)$$

and $v(P)$ is given by the equation

$$v(P) = P - \frac{4\pi\alpha}{L} \sum_q \frac{|q|q}{[qv(P) - \frac{1}{2}q^2 - |q|]^2}. \quad (27)$$

By differentiating Eq. (26) and using Eq. (27) we can show that $v(P) = \partial E/\partial P$, and hence it is the polaron velocity. By replacing $\sum_q$ by $(L/2\pi)\int_{-q_m}^{q_m}$ in Eqs. (26) and (27) we get that

$$E_L(P) = \tfrac{1}{2} P^2 - \tfrac{1}{2}(P-v)^2 - 4\alpha \ln\left(\frac{(1+\frac{1}{2}q_m)^2 - v^2}{1-v^2}\right), \quad v<1, \quad (28)$$

and that

$$(P - v) = 8\alpha v\{(1-v^2)^{-1} - [(1+\tfrac{1}{2}q_m)^2 - v^2]^{-1}\}, \quad v<1. \quad (29)$$

Note that the integral that leads to Eq. (29) does not even have a principal value when $v > 1$. For small P, Eqs. (28) and (29) give a self energy

$$E_L(0) = E_p(0) = -8\alpha \ln(\tfrac{1}{2}q_m + 1)$$

and an effective mass

$$1/m^* = [1 + 8\alpha - 8\alpha/(\tfrac{1}{2}q_m + 1)^2]^{-1},$$

which are essentially the same results as perturbation theory, as is always the case with this theory. However for larger P the theories are strikingly different. $E_p(P)$ goes to $-\infty$ as $P \to 1$, but

$$E_L(P) \to 8\alpha \ln \tfrac{1}{2}q_m + P - 4\alpha \ln P/4\alpha \tag{30}$$

and $v(P) \to 1 - 4\alpha/P$ for $q_m \gg 1$. These curves are compared in Fig. 1.

As we have discussed at length in connection with the piezoelectric polaron,[7,11] we feel that the intermediate coupling gives the more plausible result. At least for some region of P space the polaron should be locked below the speed of sound. We will see below that the exactly soluble strong coupling has the same qualitative behavior.

IV. STRONG-COUPLING–STATIONARY POLARON

A. Three dimensions

The strong-coupling theory was first done by Pekar[4] in a variational form. He uses a trial wave function of the form

$$|T\rangle = \phi(\vec{r} - \vec{R}) e^{S(\vec{R})}|0\rangle, \tag{31}$$

where

$$S(\vec{R}) = \sum_q d_q (a_q e^{i\vec{q}\cdot\vec{R}} - a_q^\dagger e^{-i\vec{q}\cdot\vec{R}}). \tag{32}$$

The operator $e^{S(\vec{R})}$ makes a deformation of the lattice centered around the arbitrary point $\vec{R}$. The shape of the deformation is determined by the variational parameters d_q. The electron is then put in a bound state $\phi(\vec{r} - \vec{R})$ in the potential caused by the lattice deformation. We determine ϕ and d_q by minimizing the expected value of the Hamiltonian, Eq. (10),

$$\langle T|H_p|T\rangle = \int d^3r\, \phi^*(\vec{r} - \vec{R}) H_0 \phi(\vec{r} - \vec{R}),$$

where

$$H_0 = \frac{p^2}{2} + \sum_q d_q^2 \omega(q) - \sum_q d_q Q(q) \left(\frac{4\pi\alpha}{V}\right)^{1/2} \times (e^{-i\vec{q}\cdot(\vec{r}-\vec{R})} + e^{i\vec{q}\cdot(\vec{r}-\vec{R})}).$$

Setting

$$\frac{\partial}{\partial d_q}\langle T|H_p|T\rangle = 0,$$

gives that

$$d_q = \left(\frac{4\pi\alpha}{V}\right)^{1/2} \frac{Q(q)}{\omega(q)} \frac{(\rho_q + \rho_{-q})}{2}, \tag{33}$$

where

$$\rho_q \equiv \int d^3r\, |\phi(\vec{r} - \vec{R})|^2 e^{i\vec{q}\cdot(\vec{r}-\vec{R})}. \tag{34}$$

For the stationary polaron we expect $\phi(\vec{r} - \vec{R})$ to be spherically symmetric and real, which gives that

$$d_q = \left(\frac{4\pi\alpha}{V}\right)^{1/2} \frac{Q(q)}{q} \rho_q. \tag{35}$$

If we now vary $\langle T|H_p|T\rangle$ with respect to $\phi(\vec{r} - \vec{R})$ subject to the constraint that

$$\int |\phi(\vec{r} - \vec{R})|^2 d^3r = 1,$$

we obtain a nonlinear Schrödinger-like equation for the best $\phi(\vec{r} - \vec{R})$:

$$\left(-\tfrac{1}{2}\nabla_r^2 - \frac{4\pi\alpha}{V}\sum_q \frac{2Q^2(q)}{(\omega)q}\rho(q) e^{i\vec{q}\cdot(\vec{r}-\vec{R})} + \sum_q \frac{4\pi\alpha}{V}\frac{Q^2(q)\rho^2(q)}{\omega(q)}\right)\phi(\vec{r} - \vec{R}) = E\phi(\vec{r} - \vec{R}) \tag{36}$$

and

$$\langle T|H|T\rangle_{\min} = E.$$

The equation is nonlinear because $\rho(q)$ given by Eq. (34) depends on the solution $\phi(\vec{r} - \vec{R})$. Although we arrive at Eq. (36) variationally its solution has been shown to be the correct strong-coupling limit for the polaron problem by several authors.[12-15]

We would like to point out that the physical properties of the system enter this theory only through the factor

$$(4\pi\alpha/V)Q^2(q)/\omega(q).$$

The dimensionless volume V is cancelled in any calculation by the volume factor that appears when we replace $\sum_q$ by $V\int d^3q/(2\pi)^3$, and we will show below that α appears only as a scale factor. Hence the character of the solution is determined entirely by the factor $Q^2(q)/\omega(q)$. For the original polaron problem[16] (coupling to the longitudinal optical mode in an ionic crystal) $Q^2(q) = q^{-2}$ and $\omega(q) = 1$, hence $Q^2(q)/\omega(q) = q^{-2}$. For the coupling to acoustic phonons in a piezoelectric crystal $Q^2(q) = q^{-1}$ and $\omega(q) = q$, hence again $Q^2(q)/\omega(q) = q^{-2}$. Therefore as we have pointed out before[14] the strong-coupling limit is identical for these two otherwise different systems. There is another pair of systems that are identical in strong coupling. The first involves the interaction with optical modes via the deformation potential. For this case $Q(q)=\omega(q)=1$, and hence $Q^2/\omega=1$. This case is often used as the simplest form for the H_p with no reference to deformation potentials. It was in this spirit that Gross[15] introduced it when he showed that the strong coupling could be solved exactly in one dimension. However for the very common case of an electron interacting with acoustic phonons via deformation potential, $Q(q)=(|q|)^{1/2}$ and $\omega(q)=q$, so $Q^2(q)/\omega(q)=1$. Therefore the strong-coupling limit of this system, which may have considerable practical application, can also be solved exactly in one dimension.

The reason why these pairs of systems reduce to the same strong-coupling limit[14] (as we have explained in detail before) is that in the strong coupling one considers only a static deformation of the lattice, and hence the dynamics of the lattice play no role. It is only the shape of the static lattice deformation that counts. In the two examples when $Q^2/\omega=q^{-2}$ the mechanism of coupling is through lattice polarization, and hence it is essentially Coulombic where as the deformation potential is essentially short range. This is most clearly seen by putting Eq. (36) in position space. When $Q^2/\omega=q^{-2}$ Eq. (36) becomes

$$\left(-\tfrac{1}{2}\nabla_r^2-2\alpha\int d^3r'\,\frac{|\phi(\vec{r}'-\vec{R})|^2}{|\vec{r}-\vec{r}'|}\right)\phi(\vec{r}-\vec{R})=\epsilon\phi(\vec{r}-\vec{R})\,. \quad (37)$$

When $Q^2/\omega=1$, Eq. (36) becomes

$$[-\tfrac{1}{2}\nabla_r^2-8\pi\alpha|\phi(\vec{r}-\vec{R})|^2]\phi(\vec{r}-\vec{R})=\epsilon\phi(\vec{r}-\vec{R})\,. \quad (38)$$

In each of the above the constant term in the effective Hamiltonian has been combined with the eigenvalue E to give $\epsilon=E-C$, where

$$C=\sum_q \frac{4\pi\alpha}{V}\,\frac{Q^2}{\omega}\rho^2\,. \quad (39)$$

B. One dimension

Following the same procedure as in Sec. IV A, but starting from Eq. (17), we get

$$|T_1\rangle=\phi(x-R)e^{S(R)}|0\rangle\,, \quad (40)$$

$$S(R)=\sum_q d_q(a_q e^{iqR}-a_q^\dagger e^{-iqR})\,, \quad (41)$$

$$d_q=(4\pi\alpha/L\sqrt{q})\rho_q\,, \quad (42)$$

$$\rho_q=\int dx\,|\phi(x-R)|^2 e^{iq(x-R)}\,, \quad (43)$$

$$\int_{-\infty}^{\infty} dx\,|\phi(x-R)|^2=1\,. \quad (44)$$

ϕ is the solution of the nonlinear eigenvalue problem

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}-\frac{8\pi\alpha}{L}\sum_q \rho_q e^{iq(x-R)}+\sum_q \frac{4\pi\alpha}{L}\rho_q^2\right)\phi(x-R)=\epsilon\phi(x-R) \quad (45)$$

or

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}-8\pi\alpha\phi^2(x-R)\right)\phi(x-R)=\epsilon\phi(x-R)\,, \quad (46)$$

where $\epsilon=E-C$ and

$$C=\sum_q \frac{4\pi\alpha}{L}\rho_q^2\,. \quad (47)$$

This is exactly the same equation that was obtained by Gross[15] for deformation-potential optical-type coupling [i.e., $\omega(q)=Q(q)=1$], and which he showed is solved by

$$\phi(x-R)=(2\pi\alpha)^{1/2}\,\mathrm{sech}4\pi\alpha(x-R)\,, \quad (48)$$

with

$$\epsilon=E-C=-8\pi^2\alpha^2 \quad (49)$$

and

$$C=\tfrac{1}{3}(4\pi\alpha)^2\,, \quad (50)$$

giving

$$\langle T_1|H|T_1\rangle=E=-\tfrac{8}{3}\pi^2\alpha^2\,. \quad (51)$$

Restoring units and substituting Eq. (18) for α we get

$$E=-\tfrac{1}{24}D^4/\hbar^2C^2\,. \quad (52)$$

We see by comparing with Eq. (8) that except for the numerical factor this is the same result as that obtained from the heuristic theory.

This one-dimensional model is very convenient and most of its properties are easily calculated in closed form. For instance, the lattice displacements are

$$d_q=\left(\frac{4\pi\alpha|q|}{L}\right)^{1/2}\frac{1}{8\alpha\sinh(|q|/8\alpha)}\,, \quad (53)$$

and the Fourier transform of the electronic charge density is

$$\rho_q=q/8\alpha\sinh(q/8\alpha)\,, \quad (54)$$

and the lattice displacement in position space, in cgs units is

$$\langle T_1|u(x)|T_1\rangle=-(mD/2\hbar\rho s)\times\tanh[(4\pi\alpha m\,s/\hbar)(x-R)]\,. \quad (55)$$

Before we proceed to corrections to this theory we would like to show that the α dependence in the above equation can be essentially removed by a scale transformation. If we write

$$y = 4\pi\alpha(x - R)\,, \tag{56}$$

$$(4\pi\alpha)^{1/2}\chi(4\pi\alpha(x-R)) = \phi(x - R)\,, \tag{57}$$

then

$$\chi(y) = (1/\sqrt{2})\,\mathrm{sech}\,y\,, \tag{58}$$

which is normalized to unity. Equation (46) then becomes

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial y^2} - 2\chi^2(y)\right)\chi(y) = \epsilon'\chi(y)\,, \tag{59}$$

where

$$\epsilon' = \epsilon/(4\pi\alpha)^2\,, \tag{60}$$

is clearly independent of α because it is determined by Eq. (59) which contains no α.

If we multiply Eq. (59) by $\partial\chi/\partial y$, it becomes a perfect differential, and from this we can easily see that $(1/\sqrt{2})\,\mathrm{sech}\,y$ is the only solution for which $\chi(y) \to 0$ as $y \to \pm\infty$.

V. STRONG COUPLING–MOVING POLARON

We can extend the analysis in Sec. IV to a moving polaron by replacing the trial wave function Eq. (40) by

$$|T_w\rangle = e^{iwx}\,\phi_w(x - R)e^{S_w(R)}|0\rangle\,, \tag{61}$$

where

$$S_w(R) = \sum_q d_q(w)(a_q e^{iqR} - a_q^\dagger e^{-iqR}) \tag{62}$$

and

$$\phi_w(x) = \phi_w(-x)\,.$$

Although Eq. (61) is not an eigenfunction of the total momentum

$$\mathcal{P} = \frac{1}{i}\frac{\partial}{\partial x} + \sum_q a_q^\dagger a_q q\,,$$

we will require that

$$\langle T_w|\mathcal{P}|T_w\rangle = P\,, \tag{63}$$

and then minimize the expected value of the Hamiltonian Eq. (17) subject to the momentum constraint Eq. (63) and the normalization constraint

$$\langle T_w|T_w\rangle = \int_{-\infty}^{\infty}\phi^*\phi\,dx = 1\,. \tag{64}$$

This procedure requires minimizing

$$I = \langle T, w|H - v\mathcal{P} - \lambda|T, w\rangle$$

with respect to w, ϕ, and d_q. The Lagrange multipliers v and λ are then determined by the constraint Eqs. (63) and (64).

Setting

$$\frac{\partial I}{\partial w} = 0$$

gives $w = v$, and

$$\delta I/\delta\phi^* = 0$$

leads to the eigenvalue problem

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} - \left(\frac{4\pi\alpha}{L}\right)^{1/2}\sum_q (|q|)^{1/2}(d_q + d_{-q})\,e^{iq(x-R)}\right] \times\phi_v(x - R) = \epsilon_v\phi_v(x - R)\,, \tag{65}$$

where

$$\epsilon_v = \tfrac{1}{2}v^2 - \sum_q d_q^2(|q| - qv) + \lambda\,.$$

Setting

$$\frac{\partial I}{\partial d_q} = 0$$

gives

$$d_q = \left(\frac{4\pi\alpha}{L}\right)^{1/2}\frac{(|q|)^{1/2}\rho_q(v)}{|q| - qv}\,, \tag{66}$$

where

$$\rho_q(v) = \rho_{-q}(v) = \int_{-\infty}^{\infty}|\phi_v(x)|^2 e^{iqx}dx\,.$$

Using these expressions for the d_q in Eq. (65) gives

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{8\pi\alpha}{1 - v^2}\phi_v^2(x - R)\right)\phi_v(x - R) = \epsilon_v\phi_v(x - R)\,. \tag{67}$$

This is just the same as Eq. (46) except that

$$\alpha \to \alpha/(1 - v^2)\,.$$

The only bound-state solution is then

$$\phi_v(x - R) = \left(\frac{2\pi\alpha}{1 - v^2}\right)^{1/2}\mathrm{sech}\left(\frac{4\pi\alpha}{1 - v^2}(x - R)\right) \tag{68}$$

and

$$\epsilon_v = -8\pi^2\alpha^2/(1 - v^2)^2\,. \tag{69}$$

Hence the only effect of the motion on the electronic wave function is a scale change. Note that in this form it is particularly clear that the effective electron-phonon coupling increases as $v \to 1$. The energy of the system

$$E_s = \langle Tv|H|Tv\rangle$$

becomes

$$E_s = \tfrac{1}{2}v^2 + \epsilon_v + \sum_q d_q^2|q| = \tfrac{1}{2}v^2 - \tfrac{1}{6}(4\pi\alpha)^2\frac{(1 - 5v^2)}{(1 - v^2)^3}\,. \tag{70}$$

Note that it is only the electronic wave function not E_s that scales with a factor $(1-v^2)^{-1}$.

The constraint equation for eliminating v is

$$P - v = \sum_q d_q^2 q = \frac{2}{3}\frac{(4\pi\alpha)^2 v}{(1-v^2)^3} . \qquad (71)$$

The dependence of E_s on the momentum P is given parametrically by Eqs. (70) and (71), and is shown explicity in Fig. 2. One can check from Eqs. (70) and (71) that

$$v = \frac{\partial E_s}{\partial P},$$

and hence v is the polaron velocity.

In limiting cases, we first note that for $P \to 0$

$$E_s(P) \approx -\tfrac{8}{3}\pi^2\alpha^2 + p^2/2m^*, \quad m^* = 1 + \tfrac{32}{3}\pi^2\alpha^2 ,$$

where we note that the effective mass is proportional to α^2 as in the piezoelectric polaron.[14] On the other hand, for $P \to \infty$ we see that

$$v \to 1 \text{ and } E_s \to +P - \tfrac{1}{2}[\tfrac{1}{3}(2\pi\alpha)^2]^{1/3} P^{2/3} - \tfrac{1}{2}. \quad (72)$$

At large P the energy becomes increasingly below the unperturbed continuum $(P - \frac{1}{2})$. In fact comparing Eq. (72) to the corresponding expression for weak coupling Eq. (30) we see that for sufficiently large P the strong coupling will become lower. Although E_L is an upper bound for each value of P unfortunately E_s is not. Nevertheless this suggests[17] that as $v \to 1$ the strong coupling is

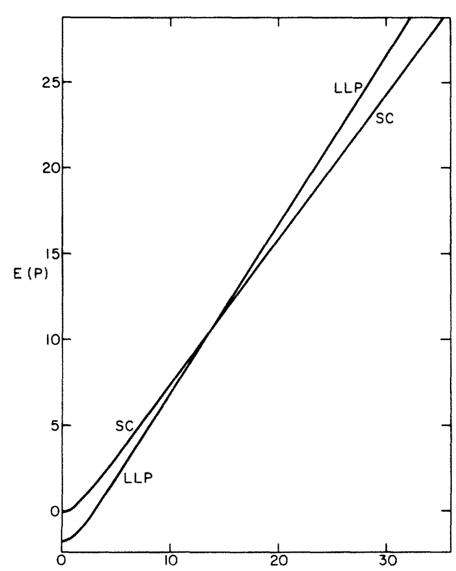

FIG. 2. Energy-momentum relation for the strong-coupling moving polaron and the intermeditate-coupling theory of Lee, Low, and Pines. Curves are for q_m =200 and α =0.05. The slope of the LLP curve has already approached very close to the speed of sound. The slope of the strong-coupling curve will also approach unity at higher P.

the preferred theory. However in order to make this inference binding we should use a strong-coupling trial function which is an eigenfunction of $\mathcal{P}$, such as that used by Höhler.[18]

VI. CORRECTION TO STRONG COUPLING

The first corrections to strong coupling are usually broken into two terms, one called the localization energy and the second called the fluctuation energy.[13] In order to estimate the localization energy we would have to use a trial function which is an eigenfunction of momentum, or utilize one of the extremely involved versions of polaron theory[12–15] that maintain translational invariance from the begining. Although both of these projects are feasible, they are very involved and we have not undertaken them here. The other part of the first correction (the fluctuation energy) can be calculated easily and has the interesting property that it depends on the high-momentum cutoff q_m. Since all of the calculations for the adiabatic limit of the one-dimensional deformation-potential coupling are cutoff independent, it would be natural to assume that the whole theory is. However since the high-momentum phonons have a large frequency they can follow the electron in its fluctuations in the bound state, suggesting that these phonons should be treated by perturbation theory. In Sec. III we showed that perturbation theory is cutoff dependent, and hence we are not surprised to find cutoff-dependent corrections to the strong-coupling theory.

We start with the Hamiltonian Eq. (17) and apply the unitary displaced oscillator transformation

$$H' = e^{-S} H e^{S} , \qquad (73)$$

where S is the operator given by Eq. (41):

$$S(R) = \sum_q d_q (a_q e^{iqR} - a_q^\dagger e^{-iqR}) . \qquad (41)$$

The transformed Hamiltonian can be written

$$H' = H_0 + H_{\text{ph}} + H_{\text{int}} , \qquad (74)$$

where

$$H_0 = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \left(\frac{4\pi\alpha}{L}\right)^{1/2} \sum_q (d_q + d_{-q}) Q_q + \sum_q d_q^2 |q| , \qquad (75)$$

$$H_{\text{ph}} = \sum_q a_q^\dagger a_q |q| , \qquad (76)$$

$$H_{\text{int}} = \left(\frac{4\pi\alpha}{L}\right)^{1/2} \sum_q (|q|)^{1/2} (a_q + a_{-q}^\dagger) e^{iqx} + \sum_q |q| d_q (a_q e^{iqR} + a_q^\dagger e^{-iqR}) . \qquad (77)$$

We note that d_q is at this point arbitrary. We now *choose* d_q according to the variational analysis of Sec. IV on the static polaron in which we found

$$d_q = \left(\frac{4\pi\alpha|q|}{L}\right)^{1/2} \frac{1}{8\alpha \sinh(|q|/8\alpha)} . \tag{53}$$

With this value of d_q, the various parts of the Hamiltonian H' become

$$H_0 = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - (4\pi\alpha)^2 \operatorname{sech}^2 4\pi\alpha(x-R) + \tfrac{1}{3}(4\pi\alpha)^2 , \tag{78}$$

$$H_{\rm ph} = \sum_q a_q^\dagger a_q |q| , \tag{76}$$

$$H_{\rm int} = \sum_q \left(\frac{4\pi\alpha|q|}{L}\right)^{1/2} (a_q + a_{-q}^\dagger) \times (e^{iqx} - \rho_q e^{iqR}) , \tag{79}$$

where

$$\rho_q = q/8\alpha \sinh(q/8\alpha) . \tag{54}$$

We would like to emphasize that there is no approximation in going from H to this final form of H'. We further note that with the above choice of d_q the lowest eigenvalue of $H_0 + H_{\rm ph}$ is, by design, that obtained from the previous static variational calculation.

We now treat $H_{\rm int}$ as a perturbation on $H_0 + H_{\rm ph}$. This approach, which we call "adiabatic perturbation theory," was first derived by Höhler and has been used extensively.[19] The aspect that is unique about the present application is that the eigenfunctions of H_0 can be found exactly. We have already noted that the bound-state solution is given by

$$\phi(x) = (2\pi\alpha)^{1/2} \operatorname{sech}(4\pi\alpha x) , \tag{48}$$

with eigenvalue

$$E = -8\pi^2\alpha^2 + (4\pi\alpha)^2/3 , \tag{51}$$

and this is the only bound state. It has been shown by Yukon[20] that the continuum eigenfunctions of H_0 are

$$\phi_k(x) = \left(\frac{4\pi\alpha}{L}\right)^{1/2} e^{ik4\pi\alpha x} \frac{(k + i\tanh 4\pi\alpha x)}{k+i} , \tag{80}$$

with eigenvalue

$$E_k = (4\pi\alpha)^2 \tfrac{1}{2}k^2 + (4\pi\alpha)^2/3 . \tag{81}$$

We now apply Rayleigh-Schrödinger perturbation theory to the ground-state energy E. From Eq. (79) it is easy to see that $H_{\rm int}$ has a zero expectation value in the ground state of H_0, and hence there is no first-order correction. In second-order perturbation theory there will be intermediate states of the type

$$\phi(x-R)a_q^\dagger|0\rangle . \tag{82}$$

However, we again see from Eq. (79) and the definition of ρ_q that states of the type in Eq. (82) do not contribute to the energy shift. The lowest correction to the ground state is then

$$\Delta E^{(2)} = \sum_{k,q} \frac{|\langle 0|\phi H_{\rm int}\phi_k a_q^\dagger|0\rangle|^2}{E - (4\pi\alpha)^2\frac{1}{2}k^2 - \frac{1}{3}(4\pi\alpha)^2 - |q|} \tag{83}$$

$$\Delta E^{(2)} = -\frac{1}{4(4\pi\alpha)^3} \times \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dq\,dk}{(k^2+1)} \frac{|q|^3 \operatorname{sech}^2(q/8\alpha - \frac{1}{2}\pi k)}{[1+k^2+2|q|/(4\pi\alpha)^2]} . \tag{84}$$

We next make a scale change $q' = q/8\alpha$ and obtain for the energy shift

$$\Delta E^{(2)} = -\frac{16\alpha}{\pi^3} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq'\,dk \times \frac{|q'|^3 \operatorname{sech}^2(q' - \frac{1}{2}\pi k)}{(k^2+1)(k^2+1+|q'|/\pi^2\alpha)} . \tag{85}$$

If the integrand falls off sufficiently rapidly for large q' we can expand the energy denominator in powers of $q'/\pi^2\alpha$ thereby generating a series in $1/\alpha$, with the first term in $\Delta E^{(2)}$ being proportional to α as we would expect in analogy with the piezoelectric case.[19] However, we can see that as both q' and k become large, with $q' - \frac{1}{2}\pi k$ fixed, the integrand behaves as $1/k$ and then the integral diverges logarithmically. If we set the maximum value of q' and k as q_m, then the leading term in the case $q_m \gg 8\alpha$ is

$$\Delta E^{(2)} \simeq -8\alpha \ln q_m , \tag{86}$$

which is just the leading term in perturbation theory, Eq. (24). This analysis suggests[19] (as we have pointed out at length in connection with the piezoelectric polaron) that whenever $\alpha \gg 1$ we have strong coupling for the long-wavelength phonons and weak coupling for the short-wavelength phonons.

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