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Strong-coupled electron—acoustic-phonon system in one dimension

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A systematic strong-coupling perturbation theory is applied to the one-dimensional model of an electron interacting with acoustic phonons through the deformation potential. The Hamiltonian is diagonalized to the next order in the inverse coupling constant beyond the strong-coupling limit. The energy to this order involves a shift in the density of phonon modes due to the electron-phonon interaction. This shift is analyzed in terms of a phonon Green's function and is found to contain a resonance at phonon frequencies $\sim s/R$ where s is the speed of sound and R is the size of the polaron. There is also a depletion in the density of phonon modes due to the polaron, which iteself appears as a translational mode in the theory. This depletion is related to a form of Levinson's theorem.

In a series of papers[1–3] we have investigated one-dimensional models of an electron coupled strongly to phonons through the deformation potential. In the first of these papers[1] we examined a model with acoustic phonons and determined the ground-state (polaron) energy and wave function analytically in the strong-coupling limit. We also obtained a perturbative correction to the ground-state energy to one additional order in the inverse electron-phonon coupling constant. Because the ground-state wave function is not translationally invariant in the strong-coupling limit, the perturbative correction calculated was incomplete, although it gave the dominant contribution to that order. A translationally invariant variational ground-state wave function was subsequently used[2] but did not lend itself to a systematic development of the desired corrections. A strong-coupling perturbation theory was developed[3] for a model with optical phonons all of frequency ω_0. In addition to the full first-order strong-coupling correction to the polaron energy, we also obtained the leading term in the polaron effective mass and a modified optical-phonon spectrum. It was found that one mode has its frequency reduced from ω_0 to zero and is a translational mode corresponding to the polaron, which demonstrates that the strong-coupling perturbation theory is translationally invariant. Of the remaining lattice vibrational modes only a few have their frequencies altered substantially.

In the present work we develop a similar strong-coupling perturbation theory for the model with acoustic phonons. Because the unperturbed acoustic-phonon spectrum is a continuum, the first-order correction to the polaron energy requires the calculation of a density of phonon modes modified by the electron-phonon interaction. This density of phonon modes can be expressed in terms of a scattering amplitude which describes the mixing of phonon wave vectors through the electron-phonon interaction. In particular, the density of modes can be expressed in terms of an effective scattering phase shift which turns out to exhibit a behavior similar to that in potential scattering when there is a low-energy resonance in the presence of a bound state. In the present case the bound state is the polaron.

In Sec. II we develop the general theory along lines similar to that of Ref. 3. The analysis is presented here mainly for the purpose of completeness. In Sec. III we develop the theory for the density of acoustic-phonon modes and present the results of its computation.

II. GENERAL FORMALISM

In this section we develop the general formalism of the theory which is similar to that of the optical-phonon model[3] and is repeated here to make the work self-contained. If we choose the unit of length to be $\hbar/ms$ and the unit of energy to be ms^2, where m is the electron band mass and s is the speed of sound for the lattice, then the Hamiltonian and momentum operators for an electron interacting with acoustic phonons through the deformation potential are given by

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \sum_k a_k^\dagger a_k |k| + \left[\frac{4\pi\alpha}{l}\right]^{1/2} \sum_k |k|^{1/2}(a_k + a_{-k}^\dagger)e^{ikx} \tag{1}$$

and

$$P = -i\frac{\partial}{\partial x} + \sum_k a_k^\dagger a_k k \ . \tag{2}$$

In these expressions a_k is the phonon annihilation operator for wave vector k, α is the electron-phonon coupling constant, x is the electronic coordinate, and l is the length of the one-dimensional crystal lattice. Next we anticipate the scaling properties inherent in strong coupling by making the changes of variable

$$\begin{aligned} &4\pi\alpha x = x', \quad H/(4\pi\alpha)^2 = H' \\ &4\pi\alpha l = l', \quad P/(4\pi\alpha) = P' \ . \\ &k/4\pi\alpha = k' \ . \end{aligned} \tag{3}$$

Dropping the primes on all of the new variables, we obtain

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{8\pi\alpha}\sum_k (p_k p_{-k} + k^2 q_k q_{-k} - |k|) + \frac{1}{(2\pi\alpha l)^{1/2}}\sum_k |k| q_k e^{ikx} \tag{4}$$

and

$$P = -i\frac{\partial}{\partial x} - i\sum_k q_{-k} p_k k \ , \tag{5}$$

where we have introduced phonon coordinates

$$q_k = \frac{1}{(2|k|)^{1/2}}(a_k + a_{-k}^\dagger) \tag{6}$$

and conjugate momenta

$$p_k = i\left[\frac{|k|}{2}\right]^{1/2}(a_k^\dagger - a_{-k}) \tag{7}$$

with

$$[q_k, p_{k'}] = i\delta_{kk'} \ . \tag{8}$$

According to the physical picture of strong coupling the electron displaces the lattice from its unperturbed equilibrium configuration, and this displaced lattice then serves as a potential well in which the electron becomes bound. In this picture it is essential that the frequencies of lattice waves making up the potential well are much less than the frequency of the electron bound in the well. This adiabatic requirement is necessary if the potential well is to remain static. The potential well is comprised of wave vectors up to some maximum which is comparable to the inverse well size and in the original units is of order $4\pi\alpha ms/\hbar$. The electronic kinetic energy is comparable to the electronic binding energy, and in the original units is of order $(4\pi\alpha)^2 ms^2$. Thus we require

$$4\pi\alpha ms^2 h << (4\pi\alpha)^2 ms^2/\hbar \tag{9}$$

or

$$1 << 4\pi\alpha \ .$$

We conclude that the adiabatic requirement is a strong-coupling requirement.

To introduce the physical idea of strong coupling we make a canonical redefinition of the phonon coordinates

$$q_k \to q_k + d_k, \quad p_k \to p_k \ , \tag{10}$$

where d_k is a real even c-number function of k. Under the above canonical transformation the Hamiltonian becomes

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{8\pi\alpha}\sum_k (p_k p_{-k} + k^2 q_k q_{-k} - |k|) + \frac{1}{(2\pi\alpha l)^{1/2}}\sum_k |k| q_k e^{ikx} + \frac{1}{4\pi\alpha}\sum_k k^2 d_k q_k + \frac{1}{8\pi\alpha}\sum_k k^2 d_k^2 + \frac{1}{(2\pi\alpha l)^{1/2}}\sum_k |k| d_k e^{ikx} \ . \tag{11}$$

and the momentum becomes

$$P = -i\frac{\partial}{\partial x} - i\sum_k q_{-k} p_k k - i\sum_k d_k k p_k \ . \tag{12}$$

We note at this point that the change of variables does not affect the translational invariance of the system which is stated through the commutation relation

$$[P,H]=0\ . \tag{13}$$

This condition holds for any d_k, and we now determine d_k by making a variational estimate of the system energy. For a trial function we choose

$$|\tau(x)\rangle = u(x)\,|0\rangle\ , \tag{14}$$

where $u(x)$ is an electronic wave function localized about the origin and $|0\rangle$ is the vacuum for the new phonons, i.e., those which are excitations relative to the deformed lattice. The expected value of H gives

$$\begin{aligned}\int_{-\infty}^{\infty} dx\,\langle\tau(x)|H|\tau(x)\rangle &= -\tfrac{1}{2}\int_{-\infty}^{\infty} dx\,u(x)\frac{d^2}{dx^2}u(x)\\ &+\frac{1}{(2\pi\alpha l)^{1/2}}\sum_k |k|\,d_k\int_{-\infty}^{\infty} dx\,u^2(x)e^{ikx}\\ &+\frac{1}{8\pi\alpha}\sum_k k^2 d_k^2\int_{-\infty}^{\infty} dx\,u^2(x)\ ,\end{aligned} \tag{15}$$

where we have assumed that $u(x)$ is real. This quantity is now minimized with respect to the d_k and the functional form of $u(x)$ subject to the constraint

$$\int_{-\infty}^{\infty} dx\,u^2(x)=1\ . \tag{16}$$

This procedure gives

$$\begin{aligned} d_k &= -2\left[\frac{2\pi\alpha}{l}\right]^{1/2}\frac{\rho_k}{|k|}\ ,\\ \rho_k &= \int_{-\infty}^{\infty} dx\,u^2(x)e^{ikx}\ ,\end{aligned} \tag{17}$$

and

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}-2u^2(x)\right]u(x)=\epsilon u(x) \tag{18}$$

which has one bound solution[4,5]

$$u(x)=\frac{1}{\sqrt{2}}\operatorname{sech}x\ ,\quad \epsilon=-\tfrac{1}{2}\ . \tag{19}$$

The quantities ρ_k and d_k of Eq. (17) may then be explicitly evaluated to give

$$\rho_k=\frac{\pi k}{2}\operatorname{csch}\frac{\pi k}{2} \tag{20}$$

and

$$d_k=-\pi\left[\frac{2\pi\alpha}{l}\right]^{1/2}\frac{k}{|k|}\operatorname{csch}\frac{\pi k}{2}\ . \tag{21}$$

This variational expression for the lattice displacements may now be put back into the Hamiltonian of Eq. (11) to give

$$H=H_0+H_1+H_2\ , \tag{22}$$

where

$$H_0=-\frac{1}{2}\frac{d^2}{dx^2}-\operatorname{sech}^2x+\frac{1}{3}\ , \tag{23}$$

$$H_1=\frac{1}{(2\pi\alpha l)^{1/2}}\sum_k |k|\,q_k(e^{ikx}-\rho_k)\ , \tag{24}$$

$$H_2=\frac{1}{8\pi\alpha}\sum_k (p_k p_{-k}+k^2 q_k q_{-k}-|k|)\ . \tag{25}$$

The Hamiltonian in this form serves as the starting point of a strong-coupling perturbation theory. We note here that in addition to the bound state, the Hamiltonian H_0 also has a continuum that was analyzed originally by Yukon.[6] The orthonormal eigenfunctions and eigenvalues of H_0 are

$$\begin{aligned} u(x) &= \frac{1}{\sqrt{2}}\operatorname{sech}x\ ,\quad E_B=-\tfrac{1}{2}+\tfrac{1}{3}=-\tfrac{1}{6}\\ u_p(x) &= \frac{1}{l^{1/2}}e^{ipx}\left[\frac{p+i\tanh x}{p+i}\right]\ ,\quad E_p=\frac{1}{3}+\frac{p^2}{2}\ ,\end{aligned} \tag{26}$$

where the factor of $\frac{1}{3}$ in Eq. (26) is the lattice energy.

We are now in a position to construct the strong-coupling perturbation theory. We expand the eigenstate of H in terms of the complete set $u(x)$ and $u_p(x)$:

$$|\psi(x)\rangle = u(x)\,|\phi\rangle+\sum_p u_p(x)\,|\phi_p\rangle\ , \tag{27}$$

where the "expansion coefficients" $|\phi\rangle$ and $|\phi_p\rangle$ are as yet undetermined phonon-state vectors which are normalized so that

$$\langle\phi|\phi\rangle+\sum_p\langle\phi_p|\phi_p\rangle=1\ . \tag{28}$$

Rather than develop the general method by which $|\phi\rangle$ and $|\phi_p\rangle$ can be determined to arbitrary order in α^{-1} as was done for the optical-phonon model, we solve

$$H\,|\psi(x)\rangle = E\,|\psi(x)\rangle \tag{29}$$

only to one order in α^{-1} beyond the strong-coupling limit. From Eq. (29) we obtain

$$\int_{-\infty}^{\infty} dx\,u(x)H\,|\psi(x)\rangle = E\int_{-\infty}^{\infty} dx\,u(x)\,|\psi(x)\rangle \tag{30}$$

and

$$\int_{-\infty}^{\infty} dx\, u_p^*(x) H\,|\psi(x)\rangle = E\int_{-\infty}^{\infty} dx\, u_p^*(x)\,|\psi(x)\rangle\ . \tag{31}$$

Equation (30) then reduces to

$$(-\tfrac{1}{6}+H_2)\,|\phi\rangle + \sum_p (uH_1u_p)\,|\phi_p\rangle = E\,|\phi\rangle\ , \tag{32}$$

where

$$(uH_1u_p) = \int_{-\infty}^{\infty} dx\, u(x) H_1 u_p(x) \tag{33}$$

and we have used

$$(uH_1u) = (uH_2u_p) = 0\ . \tag{34}$$

From Eq. (31) we also obtain

$$(u_pH_1u)\,|\phi\rangle + \sum_{p'}(u_pH_1u_{p'})\,|\phi_{p'}\rangle = \left[E - \frac{1}{3} - \frac{p^2}{2} - H_2\right]|\phi_p\rangle\ . \tag{35}$$

To the leading order in α^{-1} Eq. (35) becomes

$$|\phi_p\rangle = -\frac{2}{1+p^2}(u_pH_1u)\,|\phi\rangle \tag{36}$$

where we have set E equal to its strong-coupling-limit value of $-\frac{1}{6}$ on the right-hand side of Eq. (35). Putting Eq. (36) back into Eq. (32) we obtain

$$H_{\rm ph}\,|\phi\rangle = E\,|\phi\rangle\ , \tag{37}$$

where $H_{\rm ph}$ is an effective phonon Hamiltonian which involves only the phonon degrees of freedom and is given by

$$H_{\rm ph} = -\tfrac{1}{6} + H_2 - 2\sum_p \frac{(uH_1u_p)(u_pH_1u)}{p^2+1}\ . \tag{38}$$

The solution of Eq. (37) then gives E correctly to order α^{-1}. From Eq. (33) we make the explicit calculation.

$$(u_pH_1u) = \frac{\pi}{l}\frac{1}{(4\pi\alpha)^{1/2}}\frac{1}{p-i} \times \sum_p k\,|k|\,q_k \operatorname{sech}\frac{\pi}{2}(k-p) \tag{39}$$

so that

$$H_{\rm ph} = \frac{1}{6} + \frac{1}{8\pi\alpha}\sum_k \left[p_kp_{-k} + \sum_{k'} R_{kk'}q_kq_{-k'} - |k|\right], \tag{40}$$

where

$$R_{kk'} = |kk'|(\delta_{kk'} - V_{kk'}^{\rm opt}) \tag{41}$$

with

$$V_{kk'}^{\rm opt} = \left[\frac{2\pi}{l}\right]^2 \times \sum_p \frac{kk'}{(p^2+1)^2}\operatorname{sech}\frac{\pi}{2}(p-k)\operatorname{sech}\frac{\pi}{2}(p-k') \tag{42}$$

The quantity $V_{kk'}^{\rm opt}$ is the same matrix element that appears in the optical-phonon model. The form of $H_{\rm ph}$ is similar to that in the optical-phonon model, but the dependence on α^{-1} is quadratic in the optical model and linear in the acoustic model. This difference is a manifestation of the different scaling properties of the two Hamiltonians due to the phonon dispersion relation and k dependence of the electron-phonon interaction.

Although we are interested eventually in the continuum limit, for the present we consider the lattice to consist of a large but finite number, N, of sites separated from neighbors by a lattice constant a. The $R_{kk'}$ can be viewed as an $N\times N$ Hermitian matrix which as N real eigenvalues and N orthonormal eigenvectors with properties

$$\begin{aligned}&\sum_{k'} R_{kk'}g_{k'n} = \Omega_n^2 g_{kn}\ (n=1,\ldots,N),\\ &\sum_k g_{kn}^* g_{kn'} = \delta_{nn'}\ ,\\ &\sum_n g_{kn}^* g_{k'n} = \delta_{kk'}\ (\text{closure})\ .\end{aligned} \tag{43}$$

Furthermore, because

$$R_{kk'} = R_{kk'}^* = R_{-k-k'} \tag{44}$$

we can choose the g_{kn} to satisfy

$$g_{-kn}^* = g_{kn}\ . \tag{45}$$

We then introduce Hermitian operators

$$\begin{aligned}\eta_n &= \sum_k g_{kn}q_k\ ,\\ \xi_n &= \sum_k g_{kn}^* p_k\ ,\end{aligned} \tag{46}$$

with inverse transformations

$$q_k = \sum_n g^*_{kn}\eta_n \ , \qquad p_k = \sum_n g_{kn}\xi_n \ . \tag{47}$$

By putting Eq. (47) into Eq. (40) and using the properties of Eq. (43) we find that the effective Hamiltonian is diagonalized by the linear transformation Eq. (47):

$$H_{\rm ph} = -\frac{1}{6} + \frac{1}{8\pi\alpha}\left[\sum_n(\xi_n^2 + \Omega_n^2\eta_n^2) - \sum|k|\right] . \tag{48}$$

As in the optical-phonon model we can show that one of the eigenfrequencies, say Ω_1, vanishes by translational invariance. In an appendix we repeat the proof that the translational invariance of the effective Hamiltonian is expressed through the condition

$$[\Pi, H_{\rm ph}] = 0 \tag{49}$$

where

$$\Pi = -i\sum_k k d_k p_k \ . \tag{50}$$

We note here that Eq. (49) is reasonable since the momentum operator Eq. (12) becomes the operator Π in the strong-coupling limit because $d_k \sim (\alpha)^{1/2}$. When Eq. (40) is used in Eq. (49) we obtain

$$\sum_{k'} R_{kk'}k' d_{k'} = 0 \tag{51}$$

which indicates that kd_k is an eigenvector of $R_{kk'}$ with zero eigenfrequency. When normalized and given a phase to make ξ_1 and η_1 Hermitian, the eigenfunction for the translational mode is

$$g_{k1} = ikd_k\left[\sum_k k^2 d_k^2\right]^{-1/2} , \tag{52}$$

with

$$\eta_1 = i\sum_k k d_k q_k \left[\sum_{k'} k'^2 d_{k'}^2\right]^{-1/2} \tag{53}$$

and

$$\xi_1 = -i\sum_k d_k p_k \left[\sum_{k'} k'^2 d_{k'}^2\right]^{-1/2} . \tag{54}$$

The effective Hamiltonian is then given by

$$H_{\rm ph} = -\frac{1}{6} + \frac{1}{8\pi\alpha}\left[\xi_1^2 + \sum_{n\neq 1}(\xi_n^2 + \Omega_n^2\eta_n^2) - \sum_k |k|\right] . \tag{55}$$

Finally, we introduce phonon annihilation operators

$$A_n = (2\Omega_n)^{-1/2}(\Omega_n\eta_n + i\xi_n) \quad (n \neq 1)$$
$$[A_n, A_m^\dagger] = \delta_{nm} \tag{56}$$

and obtain

$$H_{\rm ph} = -\frac{1}{6} + \frac{\Pi^2}{2m_*} + \frac{1}{4\pi\alpha}\left[\sum_{n\neq 1} A_n^\dagger A_n\Omega_n + \frac{1}{2}\sum_n - \frac{1}{2}\sum_k |k|\right] . \tag{57}$$

In this final version of the effective Hamiltonian we have expressed ξ_1 in terms of the generator of translations Π through Eqs. (50) and (54).

The quantity m_* is the polaron effective mass which is given in terms of the electron band mass by

$$m_* = 4\pi\alpha\sum_k k^2 d_k^2 m = \tfrac{2}{3}(4\pi\alpha)^2 m \ . \tag{58}$$

The effective Hamiltonian describes a free polaron of mass m_* and free phonons of frequencies Ω_n. The state $|\phi\rangle$ is then specified by the momentum eigenvalues of Π and a set of occupation numbers N_n. The last two terms in Eq. (57) give the shift in the vibrational zero-point energy due to the electron-phonon interaction. To calculate this shift we must determine the shift in the density of phonon modes brought about by the electron-phonon interaction.

III. DENSITY OF PHONON MODES

In the optical-phonon model the analog of the eigenvalue problem stated in Eq. (43) was solved for the phonon frequencies and eigenvectors. For the acoustic model in the continuum limit we must proceed in a different manner, since the spectrum is actually known and is the same as the unperturbed continuum. The relevant quantity for the acoustic-phonon model is the *density* of vibrational modes. If the number of phonon modes between frequency

ω and $\omega + d\omega$ is $\Delta(\omega)d\omega$, then any quantity involving a sum over phonon modes can be expressed as an integral over $\Delta(\omega)$. In particular, the shift in zero-point energy in Eq. (57) is proportional to

$$\tfrac{1}{2}\sum_{n\neq 1}\Omega_n - \tfrac{1}{2}\sum_k |k| = \tfrac{1}{2}\int_0^\infty d\omega[\Delta(\omega)-\Delta_0(\omega)]\omega , \tag{59}$$

where $\Delta_0(\omega)$ is the density of phonon modes in the absence of the electron-phonon interaction. These densities of modes can be written as

$$\Delta_0(\omega) = \sum_k \delta(\omega - |k|) \qquad \Delta(\omega) = \sum_{n\neq 1}\delta(\omega-\Omega_n) , \quad \Omega_n \geq 0 . \tag{60}$$

This expression for $\Delta(\omega)$ is inconvenient since it is given in terms of the unknown mode designation described by the index n. To express $\Delta(\omega)$ in terms of the noninteracting phonon wave vectors, k, we first note that

$$\Delta(\omega) = 2i\sum_{n\neq 1}\int_{-\infty}^{\infty} dt\,\langle 0|\xi_n(t)\eta_n|0\rangle e^{i\omega t} , \tag{61}$$

where η_n and ξ_n are the modified phonon coordinates and conjugate momenta, respectively, and $\xi_n(t)$ is the Heisenberg operator

$$\xi_n(t) = e^{i\bar{H}t}\xi_n e^{-i\bar{H}t} . \tag{62}$$

Here $\bar{H}$ is the effective Hamiltonian of Eq. (57) without the constant polaron self energy and with an additional convenient change of energy scale

$$\bar{H} = \sum_{n\neq 1} A_n^\dagger A_n \Omega_n + \frac{4\pi\alpha\Pi^2}{2m_*} + \tfrac{1}{2}\sum_n \Omega_n - \tfrac{1}{2}\sum_k |k| \tag{63}$$

with

$$H_{\rm ph} = -\frac{1}{6} + \frac{1}{4\pi\alpha}\bar{H} . \tag{64}$$

With this new scale, time is measured in units of $(4\pi\alpha m s^2/\hbar)^{-1}$ and hence frequency in units of $(4\pi\alpha m s^2/\hbar)$. The state $|0\rangle$ is simultaneously the phonon vacuum defined by

$$A_n|0\rangle = 0 \tag{65}$$

and the polaron zero-momentum eigenstate

$$\Pi|0\rangle = \xi_1|0\rangle = 0 . \tag{66}$$

The equality of Eqs. (60) and (61) follows from Eq. (56). Then through the linear transformation Eq. (46), the closure relation Eq. (43), and the polaron momentum eigenvalue property

$$\sum_k \langle 0|g_{k1}^* p_k = \langle 0|\xi_1 = 0 , \tag{67}$$

we arrive at

$$\Delta(\omega) = 2i\sum_k \int_{-\infty}^{\infty}\frac{dt}{2\pi}\langle 0|p_k(t)q_k|0\rangle . \tag{68}$$

We define a retarded-phonon Green's function by

$$D_{kk'}(t) = -i\Theta(t)\langle 0|[q_{-k}(t),q_{k'}]|0\rangle , \tag{69}$$

where $\Theta(t)$ is the Heaviside function

$$\Theta(t) = i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{e^{i\omega t}}{\omega - i\eta} = \begin{cases} 1, & t>0 \\ 0, & t<0 \end{cases} \qquad \eta = 0+ , \tag{70}$$

and note that its Fourier transform

$$G_{kk'}(\omega) = \int_{-\infty}^{\infty} dt\, D_{kk'}(t)e^{i\omega t} \tag{71}$$

has a spectral representation

$$G_{kk'}(\omega) = \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\left[\frac{A_{kk'}(\omega')}{\omega'-\omega-i\eta} + \frac{A_{-k',-k}(\omega')}{\omega'+\omega+i\eta}\right. \tag{72}$$

where the spectral function $A_{kk'}(\omega')$ is given by

$$A_{kk'}(\omega) = \int_{-\infty}^{\infty} dt\,\langle 0|q_{-k}(t)q_{k'}|0\rangle e^{i\omega t} \tag{73}$$

$$\langle 0|q_{-k}(t)q_{k'}|0\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A_{kk'}(\omega)e^{i\omega t} .$$

By writing the Hamiltonian Eq.(63) in terms of the q_k and p_k,

$$\bar{H} = \tfrac{1}{2}\sum_k\left[p_k p_{-k} + k^2 q_k q_{-k} - |k| - \sum_{k'}(V_{kk'}q_k q_{-k'}\right] , \tag{74}$$

where

$$V_{kk'} = |kk'|V_{kk'}^{\rm opt} \tag{75}$$

and $V_{kk'}^{\rm opt}$ is defined by Eq. (42), we determine that

$$\begin{aligned} 2i\langle 0|p_k(t)q_{k'}|0\rangle &= 2\langle 0[q_{-k}(t),\bar{H}(t)q_{k'}]0\rangle \\ &= 2i\langle 0|\dot{q}_{-k}(t)q_{k'}|0\rangle \\ &= \int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega A_{kk'}(\omega)e^{-i\omega t} . \end{aligned} \tag{76}$$

From Eq. (73) it also follows that

$$A^{*}_{kk'}(\omega) = A_{-k-k'}(\omega) \tag{77}$$

and thus from Eq. (72) we obtain

$$2\,\mathrm{Im}\sum_k G_{kk}(\omega) = \sum_k A_{kk}(\omega),\ \omega > 0\ . \tag{78}$$

Finally, from Eqs. (68), (76), and (78) we make a connection between the density of phonon modes and the retarded Green's function:

$$\Delta(\omega) = \begin{cases} \dfrac{2\omega}{\pi}\sum_k \mathrm{Im}G_{kk}(\omega), & \omega > 0 \\ 0, & \omega < 0\ . \end{cases} \tag{79}$$

To determine $G_{kk'}(\omega)$ we note that $D_{kk'}(t)$ obeys the differential equation

$$\left[k^2 + \frac{\partial^2}{\partial t^2}\right] D_{kk'}(t) = \delta_{kk'}\delta(t) + \sum_k V_{kk_1} D_{k_1 k'}(t) \tag{80}$$

which follows from the definition Eq. (69), the usual Heisenberg equations of motion, and Eq. (74) which gives $\bar{H}$ in terms of the q_k and p_k. By Fourier-transforming Eq. (80) we obtain

$$G_{kk'}(\omega) = G^0_k(\omega)\delta_{kk'} + G^0_k(\omega)\sum_{k_1} V_{kk} G_{k_1 k'}(\omega) \tag{81}$$

where

$$G^0_k(\omega) = \frac{1}{k^2 - (\omega + i\eta)^2}\ . \tag{82}$$

In the continuum limit Eq. (81) becomes an inhomogeneous linear integral equation for $G_{kk'}(\omega)$, but it is more advantageous to first introduce a scattering amplitude $T_{kk'}(\omega)$ defined by

$$T_{kk'}(\omega)G^0_{k'}(\omega) = \sum_{k_1} V_{kk_1} G_{k_1 k'}(\omega)\ . \tag{83}$$

By inserting Eq. (81) into the right-hand side of Eq. (83) we obtain the Lippman-Schwinger equation

$$T_{kk'}(\omega) = V_{kk'} + \sum_{k_1} V_{kk_1} G^0_{k_1}(\omega) T_{k_1 k'}(\omega)\ . \tag{84}$$

On the other hand, by substituting the right-hand side of Eq. (83) into Eq. (81) we obtain

$$G_{kk}(\omega) = G^0_k(\omega) + [G^0_k(\omega)]^2 T_{kk}(\omega) \tag{85}$$

which then relates the density of phonon modes to the scattering amplitude through

$$\Delta(\omega) = \frac{2\omega}{\pi}\mathrm{Im}\sum_k G^0_k(\omega)\ , + \frac{2\omega}{\pi}\mathrm{Im}\sum_k [G^0_k(\omega)]^2 T_{kk}(\omega)\ . \tag{86}$$

At this point we pass to the continuum limit by defining

$$T_{kk'}(\omega) = \frac{2\pi}{l} T(k,k';\omega)\ ,$$

$$V_{kk'} = \frac{2\pi}{l} V(k,k')\ , \tag{87}$$

where from definitions Eqs. (42), (76), and the prescription $2\pi l^{-1}\sum_p(\ ) \rightarrow \int_{-\infty}^{\infty} dp(\ )$ we find

$$V(k,k') = |kk'|kk' \times \int_{-\infty}^{\infty} dp\ \frac{\mathrm{sech}\frac{\pi}{2}(p-k)\mathrm{sech}\frac{\pi}{2}(p-k')}{(p^2+1)^2}\ . \tag{88}$$

The density of phonon modes may now be written as

$$\Delta(\omega) = \Delta_0(\omega) + \bar{\Delta}(\omega)\ , \tag{89}$$

where $\Delta_0(\omega)$ is the unperturbed value

$$\Delta_0(\omega) = \frac{2\omega}{2\pi} l \int_{-\infty}^{\infty} \frac{dk}{2\pi}\ \mathrm{Im}\ \frac{1}{k^2 - (\omega + i\eta)^2} = \frac{l}{\pi} \tag{90}$$

and $\bar{\Delta}(\omega)$ is the shift generated by the electron-phonon interaction

$$\bar{\Delta}(\omega) = \frac{1}{\pi}\int_{-\infty}^{\infty} dk \times \mathrm{Im}\left[T(k,k;\omega)\frac{\partial}{\partial\omega}\frac{1}{k^2 - (\omega + i\eta)^2}\right]. \tag{91}$$

The scattering amplitude $T(k,k';\omega)$ in Eq. (91) is determined from the continuum Lippman-Schwinger equation

$$T(k,k';\omega) = V(k,k') + \int_{-\infty}^{\infty} dk_1 \frac{V(k,k_1)T(k_1,k';\omega)}{k_1^2 - (\omega + i\eta)^2}\ . \tag{92}$$

The interpretation of the scattering described by this amplitude arises from the last term in the Hamiltonian Eq. (74) which can be viewed as an external phonon potential well from which a phonon of

wave vector k is scattered into a new wave vector k'. It might appear that this interpretation violates momentum conservation and hence translational invariance. However, to the order of approximation considered here, the *polaron* carries momentum but the phonons do not.

In the Born approximation we replace $T(k,k';\omega)$ by $V(k,k')$, and Eq. (91) reduces to

$$\bar{\Delta}(\omega) = \bar{\Delta}_B(\omega) \equiv \frac{d}{d\omega}\left[\frac{V(\omega,\omega)}{\omega}\right] . \tag{93}$$

From the explicit form of $V(\omega,\omega)$ given in Eq. (88) we note that $\bar{\Delta}_B(\omega)$ has the properties

$$\bar{\Delta}_B(\omega) \rightarrow \begin{cases} O(\omega^{-2}), & \omega \rightarrow \infty \\ O(\omega^2), & \omega \rightarrow 0 \end{cases} \tag{94}$$

$$\int_0^\infty d\omega\, \bar{\Delta}_B(\omega) = 0 .$$

As we will see, only the first of these properties is retained by $\bar{\Delta}(\omega)$ when the full scattering amplitude is used. In Fig. 1 we have plotted $\bar{\Delta}_B(\omega)$ as a function of frequency. Because of the behavior of $\bar{\Delta}_B(\omega)$ at high frequency, the shift in the zero-point energy diverges. Using the explicit form of $V(\omega,\omega)$ and cutting off the integral at $\omega = \omega_{\max}$ we find that the divergent and hence dominant contribution to the energy in dimensional units is

$$E_{\text{div}} = -8\alpha ms^2 \ln(\hbar\omega_{\max}/ms^2) , \tag{95}$$

which is the result of Ref. 1. In fact the perturbation theory used there is essentially equivalent to the use of the Born approximation here. Physically, the divergence appears because the high-frequency phonons cannot be treated adiabatically and should be treated by weak coupling. It is reassuring that E_{div} also appears in weak-coupling perturbation theory.[1]

In the Born approximation $\bar{\Delta}(\omega)$ has the convenient form given in Eq. (93), and when $\bar{\Delta}(\omega)$ is given without approximation it is possible to express it in a similar form. We first note that $V(k,k')$ can be written as

$$V(k,k') = \int_{-\infty}^{\infty} dp\, B(k,p)B(k',p) , \tag{96}$$

where

$$B(k,p) = k\,|k|\,(p^2+1)^{-1}\operatorname{sech}\frac{\pi}{2}(k-p) . \tag{97}$$

To facilitate the following analysis we write Eq. (96) in matrix notation

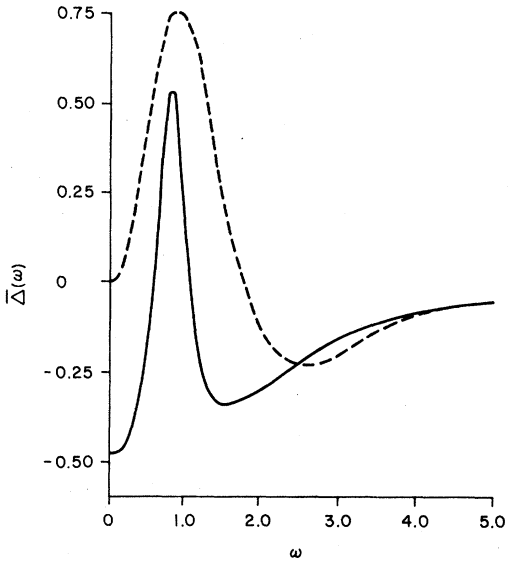

FIG 1. The shift in the density of phonon modes as a function of frequency. Dashed curve is for Born approximation. Solid curve is without approximation. Frequency is in units of $4\pi\alpha ms^2/\hbar$.

$$V = BB^T , \tag{98}$$

where the superscript T is the transpose, and similarly the Lippman-Schwinger equation Eq. (92)

$$T(\omega) = BB^T + BB^T G_0(\omega)T(\omega) , \tag{99}$$

where $G_0(\omega)$ is a diagonal matrix. As a practical matter the integrals implied by the matrix multiplication can be approximated by finite sums in a variety of numerical integration schemes and the matrix multiplication can be interpreted accordingly. Since B^{-1} exists we may define

$$R(\omega) = B^{-1}T(\omega)(B^T)^{-1} \tag{100}$$

and hence Eq. (99) can be solved for

$$R(\omega) = [1 - C(\omega)]^{-1} , \tag{101}$$

where

$$C(\omega) = B^T G_0(\omega) B . \tag{102}$$

The shift in the density of modes is then given by

$$\bar{\Delta}(\omega) = \frac{1}{\pi}\operatorname{Im}\operatorname{Tr}\left[BR(\omega)B^T\frac{\partial}{\partial\omega}G_0(\omega)\right]$$

$$= \frac{1}{\pi}\operatorname{Im}\operatorname{Tr}\left[R^{-1}(\omega)\frac{\partial}{\partial\omega}R(\omega)\right] . \tag{103}$$

Because $R(\omega)$ is symmetric (but not Hermitian) it can be diagonalized by an orthogonal transformation for which the trace in Eq. (103) is invariant. In this way we can obtain

$$\bar{\Delta}(\omega) = \frac{1}{\pi}\frac{d}{d\omega}\delta(\omega) , \tag{104}$$

where $\delta(\omega)$ is defined through

$$\det R(\omega) = r(\omega)e^{i\delta(\omega)} \tag{105}$$

[$r(\omega)$ and $\delta(\omega)$ real] and we have made use of the invariance of $\det R(\omega)$ under the orthogonal transformation. In potential theory the connection between scattering phase shifts and the shift in the density of states due to interaction is well known and finds an application in the quantum-mechanical theory of the second virial coefficient.[7] Note that in the Born approximation we can make the identification

$$\delta_B(\omega) = \pi V(\omega,\omega)/\omega . \tag{106}$$

We have computed $\delta(\omega)$ from Eqs. (101), (102), and (105) by Gaussian quadrature and there are several interesting features of the results which are plotted in Fig. 2. Unlike its Born approximation, $\delta(\omega)$ does not vanish as $\omega \to 0$ but approaches π instead. Since $\delta(\omega) \to 0$ as $\omega \to \infty$, we then obtain

$$\int_{\infty}^{\infty} d\omega\, \bar{\Delta}(\omega) = \frac{[\delta(\infty) - \delta(0)]}{\pi} = -1 \tag{107}$$

which is analogous to Levinson's theorem[8] in potential theory when a bound state is present. The significance of Eq. (107) is that one vibrational mode becomes a translational mode in the presence of the electron-phonon interaction, as was indicated previously in Eq. (51) by the occurrence of a vanishing eigenfrequency. The translational state was also identified previously with the polaron which is the bound state of the system. The absence of one vibrational mode is shared by all wave vectors, and the extent to which each value of k (and hence ω in our units) participates is given approximately by $g_{\omega 1}^2 \propto (\omega \operatorname{csch}\omega\pi/2)^2$, where g_{k_1} is the eigenfunction for the translational mode. Hence the shift in the density of states is depleted more at zero frequency. From Eq. (104) we may calculare $\Delta(\omega)$ which has been plotted in Fig. 1, and the depletion has this qualitative feature.

In the absence of any further structure the phase shift would fall monotonically to zero as $\omega \to \infty$. However, at $\omega \sim 0.5$ the phase shift rises abruptly and reaches a maximum at $\omega \gtrsim 1$ after which it falls monotonically to zero as $\omega \to \infty$. In potential theory a resonance is indicated by a phase shift which starts at zero for zero energy, *rises rapidly through* $\pi/2$, ans then falls slowly to zero at high energy. The behavior of the phase shift $\delta(\omega)$ in Fig. 2 *suggests* the presence of both a bound state and a resonance. We point out, however, that we have made no attempt to decompose the phase shift $\delta(\omega)$ into contributions from different "channels" (e.g., parity) as is done in the analogous potential-scattering density of states referred to above.[7] In that case the analog of $\delta(\omega)$ is a sum of phase shifts for various angular momentum states. Consequently, in our case it is not clear that there is a resonance in the traditional sense. But there is clearly an enhancement in the phonon density of states at $\omega \approx 1$, and this serves as the analog of the localized modes which were first discussed for the optical-phonon case by Melnikov and Rashba,[9] and subequently by Gross[10] and Shaw and Whitfield [3] along the lines of the present work. That the enhancement occurs at $\omega \approx 1$ can be understood when it is noted that in our units this corresponds to wavelengths comparable to the size of the polaron. The electron-phonon interaction tends to lower the phonon frequencies, and phonons "resonating" with the polaron would interact most strongly and hence be lowered the most. This would cause a bunching of phonon modes slightly below $\omega = 1$.

Finally, the shift in the zero-point energy can be calculated numerically in terms of the shift in the phonon density of states, and the ground-state energy for a polaron of low momentum p is given by

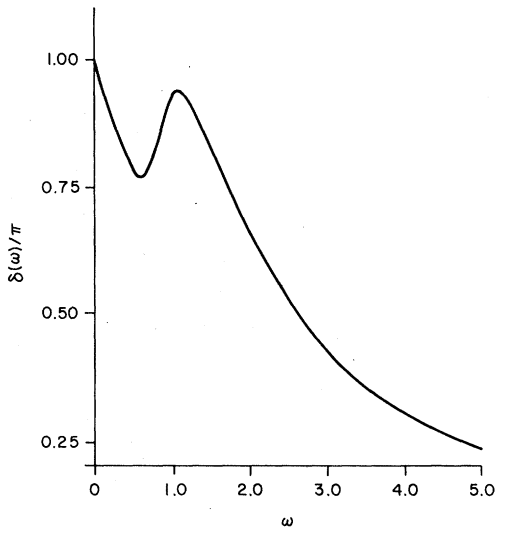

FIG 2. The phase shift $\delta(\omega)/\pi$ as a function of frequency measured in units of $4\pi\alpha ms^2/\hbar$.

$$E_G(p) = -(4\pi\alpha)^2\frac{ms^2}{6} + \frac{p^2}{2m_*} + 0.178\ 4\pi\alpha ms^2 - 8\alpha ms^2 \ln\left[\frac{\hbar\omega_{\max}}{4\pi\alpha ms^2}\right], \tag{108}$$

where

$$\hbar\omega_{\max} >> 4\pi\alpha ms^2, \tag{109}$$

$$p << m_* s,$$

and we have restored all dimensional units.

We wish to thank G. Whitfield for helpful discussions.

APPENDIX

We show that

$$[\Pi, H_{\rm ph}] = 0. \tag{A1}$$

The proof is essentially that given in Ref. 3 for optical phonons. The translational invariance of the system is contained in the statement.

$$[P, H] = 0. \tag{A2}$$

In Eqs. (22)—(25) the Hamiltonian H is written as a polynomial in $\alpha^{-1/2}$, and in a similar manner we may decompose the momentum as

$$P = P_0 + P_{-1}, \tag{A3}$$

where

$$P_0 = -i\frac{\partial}{\partial x} - i\sum_k q_{-k} p_k k \tag{A4}$$

and

$$P_{-1} = \Pi = -i\sum_k k d_k p_k. \tag{A5}$$

By separating $[P,H]$ into terms with the same power of $\alpha^{-1/2}$ we obtain four identities:

$$[\Pi, H_0] = 0, \tag{A6}$$

$$[P_0, H_0] + [\Pi, H_1] = 0, \tag{A7}$$

$$[P_0, H_1] + [\Pi, H_2] = 0, \tag{A8}$$

$$[P_0, H_2] = 0. \tag{A9}$$

Only Eqs. (A7) and (A8) are nontrivial. Now from Eq. (36) we obtain

$$[\Pi, H_{\rm ph}] = [\Pi, H_2] - 2\sum_p \frac{(u[\Pi, H_1]u_p)(u_p H_1 u) + (uH_2 u_p)(u_p[\Pi, H_1]u)}{p^2 + 1}. \tag{A10}$$

By using Eq. (A7), Eq. (34), and the completeness of $u(x)$ and $u_p(x)$ we find

$$[\Pi, H_{\rm ph}] = [\Pi, H_2] + (u[P_0, H_1]u). \tag{A11}$$

Finally, by using Eq. (A8) we prove Eq. (A1).

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