TABLE III. The observed sideband peaks in the R_2 transition in KF are listed according to wavelength and also according to the distance in energy from the zero-phonon line. The number of E modes involved in each peak are also shown. The energies are in approximate agreement with the calculations of Karo and Hardy.[a]

Wavelength (Å)	Distance from zero-phonon line (eV)	Number of E modes
5870	0.007	odd
5861	0.011	even
5841	0.020	odd
5832	0.022	even
5820	0.026	odd

[a] A. M. Karo and J. R. Hardy, Phys. Rev. **129**, 2024 (1963).

to below 5700 Å. There is thus no true broad-band dichroism. The decrease is due to the competition between the signals derived from peaks having even and odd numbers of E-symmetry phonons. In the higher-energy part of the band there are many phonons involved and the signals cancel.

V. SUMMARY

Magnetic circular dichroism has been observed with relatively low magnetic fields of about 8 kG in the zero-phonon line and sidebands of the R_2 transition in KCl and KF. The zero-phonon-line data were analyzed by a method of moments. The transition probabilities for circularly polarized light were calculated using vibronic ground-state wave functions appropriate to an E state that is distorted by the Jahn-Teller effect. The first-moment data provided a measure of the reduced orbital angular momentum and hence a measure of the Jahn-Teller coupling strength. The reduced spin-orbit interaction is also determined and is found to be negative in both crystals. The zeroth moment of the zero-phonon line was found to be sensitive to applied stress. The data, taken as a function of applied stress, are interpreted assuming that the interaction of the center with the magnetic field can be treated as a perturbation on the stress interaction. The splitting of the ground state in the internal crystal strain field is estimated. The sideband dichroism yields information about the symmetry of the phonons involved in the sideband peaks. All the experimental results agree well with the theoretical predictions which are based on the Van Doorn model with an E ground state distorted by a dynamic Jahn-Teller interaction.

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Motion of the Piezoelectric Polaron at Zero Temperature

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We analyze a series of theories which are used to obtain the energy-momentum relation for the piezoelectric polaron. Perturbation theory cannot be trusted, because there is a degeneracy in the unperturbed energy levels. The Tamm-Dancoff one-quantum cutoff in this case diagonalizes the degenerate states exactly, but has other shortcomings. The intermediate coupling theory gives what we believe is a reasonable energy-momentum relation, which starts out quadratically and becomes approximately linear as the velocity approaches the speed of sound.

I. INTRODUCTION

INTEREST in the polaron problem has been maintained for many years because it is a simple example of a particle interacting with a field, as well as an integral part of the understanding of electronic motion in ionic crystals.[1] It has recently become clear that the problem of electrons interacting with acoustic phonons in a piezoelectric crystal can be approximated by a Hamiltonian[2] which has the same form as the original polaron problem, and hence it serves as another interesting example of a particle-field interaction.

Whereas the original polaron problem (which we will refer to as the optical polaron) was analogous to a proton interacting with chargeless, spinless mesons, the piezoelectric polaron problem is analogous to quantum electrodynamics.

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[1] A recent review of work on the polaron is contained in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Plenum Press, Inc., New York, 1963).

[2] A. R. Hutson, J. Appl. Phys. **32**, 2287 (1961).

Relative to the transport of electrons in a piezoelectric crystal, there are several difficulties: The lifetime that appears in perturbation theory and Tamm-Dancoff has an infrared divergence at finite temperature, and the polaron energy-momentum relations that have been reported are peculiar and quite varied.[3,4]

All of the above call for a careful investigation of the piezoelectric polaron problem. We hope to begin this in the present paper by considering only the zero-temperature case, weak coupling, and by focusing our attention on the energy-momentum relation, where we believe much of the confusion lies. Another reason for our interest in the energy-momentum relation is that this work is a direct extension of what we have recently done on the optical polaron.[5] With regard to restricting our considerations in this paper to zero temperature, a few comments should be made. First, unfortunately, one cannot assume in the case of the piezoelectric polaron (as one can for the optical polaron) that the zero-temperature properties serve as a good approximation for the behavior of the polarons in some accessible low-temperature range. This is partly due to the fact that the interesting structure takes place for polarons traveling at about the speed of sound, and unless one has heavy band masses, this requires thermal electrons at less than 1°K. The other reason for this difficulty is that there is no separation between the ground state and the excited states with the same momentum. We nevertheless feel justified in considering the zero-temperature case, partly as a first step in understanding the more complicated finite-temperature problem, and also because the zero-temperature problem is the interesting particle-field problem. Some of the results obtained we believe are useful in understanding the finite-temperature problem.

The Hamiltonian we will use in this paper is

$$H=\frac{p^2}{2}+\sum_{\mathbf{q}}(a_{\mathbf{q}}{}^\dagger a_{\mathbf{q}}+\tfrac{1}{2})q+\left(\frac{4\pi\alpha}{V}\right)^{1/2}\sum_{\mathbf{q}}\frac{1}{q^{1/2}}(a_{\mathbf{q}}+a^\dagger{}_{-\mathbf{q}})e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (1.1)$$

The unit of energy is ms^2, and the unit of length is $\hbar/ms$, where s is the speed of sound. The operators $a_{\mathbf{q}}{}^\dagger$ and $a_{\mathbf{q}}$ create and annihilate phonons of one mode which replaces the three acoustic modes, and $\mathbf{p}$ and $\mathbf{r}$ are the electron momentum and position.

The coupling constant α can be written

$$\alpha=\frac{\hbar/ms}{\hbar^2\mathcal{E}/me^2}\frac{\langle e^2{}_{ijk}\rangle}{\mathcal{E}C}\frac{1}{2},$$

where $\langle e^2{}_{ijk}\rangle$ is an average[2] of the piezoelectric tensor components, $\mathcal{E}$ is the dielectric constant, and C is an average elastic constant. The term $\langle e^2{}_{ijk}\rangle/\mathcal{E}C$ is the square of what is called the electromechanical coupling constant, and which is referred to as α in some previous works.[2] The first term in the definition of α is the ratio of the unit of length to the Bohr radius in the medium.

Another way of writing the coupling constant which emphasizes the analogy to electromagnetic theory is

$$\alpha=e^{*2}/\hbar s,$$

where the effective charge is

$$e^{*2}=e^2(\langle e^2{}_{ijk}\rangle/\mathcal{E}^2C)\tfrac{1}{2}.$$

In order to see this analogy most clearly, we perform a similarity transformation on H.

$$H'=e^{-S}He^{S},$$

where

$$S=\sum_{\mathbf{q}}\frac{1}{q^{3/2}}\left(\frac{4\pi\alpha}{V}\right)^{1/2}(a_{\mathbf{q}}-a_{-\mathbf{q}}{}^\dagger)e^{i\mathbf{q}\cdot\mathbf{r}},$$

$$H'=\tfrac{1}{2}\left(\mathbf{p}+\frac{1}{i}\nabla S\right)^2+\sum_{\mathbf{q}}(a_{\mathbf{q}}{}^\dagger a_{\mathbf{q}}+\tfrac{1}{2})q-\sum_{\mathbf{q}}\frac{4\pi\alpha}{Vq^2}. \quad (1.2)$$

The last term in (1.2) is a constant and plays no role in the calculation of transition rates, etc.

The first two terms are just the same as the nonrelativistic Hamiltonian for an electron interacting with photons: if one replaces $\alpha\to\alpha=e^2/\hbar c$ and $(1/i)\nabla S\to\mathbf{A}$, the vector potential in the Coulomb gauge, except that $\mathbf{A}$ is transverse and ∇S is longitudinal.

II. PERTURBATION THEORY

The first approach to finding the properties of the Hamiltonian (1.1) in the case where α is small is to apply perturbation theory to the uncoupled electron states, whose energies are $E^{(0)}(p)=\frac{1}{2}p^2$. The first correction to this comes from second-order perturbation theory, which gives

$$E^{(2)}(p)=\tfrac{1}{2}p^2+\Delta E^{(2)}(p), \quad (2.1)$$

$$\Delta E^{(2)}=\sum_{\mathbf{q}}\left(\frac{4\pi\alpha}{Vq}\right)\frac{1}{E^{(0)}(p)-E^{(0)}(p-q)-q} \quad (2.2)$$

$$=-\frac{\alpha}{\pi}\int_0^{q_m}dq\int_{-1}^{+1}dx\frac{1}{(\frac{1}{2}q+1-px)} \quad (2.3)$$

$$=\frac{\alpha}{\pi p}\left[(q_m+2)\ln\left|\frac{q_m+2(1-p)}{q_m+2(1+p)}\right|+2p\ln\frac{4|1-p^2|}{|(q_m+2)^2-4p^2|}-2\ln\left|\frac{1-p}{1+p}\right|\right]. \quad (2.4)$$

[3] Two previous theories that are done at finite temperature neglecting the zero-temperature contribution are G. D. Mahan and J. J. Hopfield, Phys. Rev. Letters **12**, 241 (1964); Yukio Osaka, J. Phys. Soc. Japan **19**, 2347 (1964).

[4] A calculation of the self-energy in a degenerate semiconductor by G. D. Mahan and C. B. Duke [Phys. Rev. **149**, 705 (1966)] neglects the contribution that remains when there is only one electron present.

[5] George Whitfield and Robert Puff, Phys. Rev. **139**, A338 (1965).

The maximum wave vector is q_m, which is about 300 in these units. Note that in the limit $q_m \to \infty$ the second term in (2.4) diverges logarithmically. This is a slower divergence than in quantum electrodynamics because the nonrelativistic $E^{(0)}(\mathbf{p}) \propto p^2$ rather than p, and the integrals are cut off faster at large q.

Although there is no actual difficulty with ultraviolet divergences here, we like to work with the approximation $q_m = \infty$ whenever we can because any quantity which depends on q_m has been very poorly calculated by the type of theory that we are doing here. The reasons for this are that the Hamiltonian applies best for small q and we have not taken the shape of the Brillouin zone boundaries into account in the integrals of q.

Note that the integral in (2.3) is proper when $p<1$. In the region $p>1$, we have given the principal value of the integral. Therefore, below $p=1$ we are calculating the properties of an eigenstate of H, but above $p=1$ we are discussing a quasiparticle which has a finite width Γ.

$$\begin{aligned} \Gamma &= 0, & p&<1 \\ &= (2\alpha/p)(p-1), & p&>1. \end{aligned} \tag{2.5}$$

For small values of p

$$\begin{aligned} E^{(2)}(\mathbf{p}) &\simeq E(0) + p^2/2m^*, \\ E(0) &= -(4\alpha/\pi)\ln(\tfrac{1}{2}q_m+1), \\ \frac{1}{m^*} &= 1 - \frac{4\alpha}{3\pi} + \frac{4\alpha}{3\pi}\frac{1}{(\frac{1}{2}q_m+1)^2}. \end{aligned} \tag{2.6}$$

It is interesting to note that although $E(0)$ diverges in the limit $q_m \to \infty$, the effective mass does not. In fact, the cutoff dependent term in m^* is negligible for any reasonable α and q_m.

We note further that at $\alpha \sim 3$ the effective mass becomes negative. A clear view of the situation is obtained from Fig. 1, where we plot $E^{(2)}(p)$ for two values of α. Note the peculiar structure around $p=1$, where the velocity first becomes zero, then negative, then $-\infty$, and a new minimum occurs away from $p=0$. A similar sort of structure is obtained from perturbation theory for the optical polaron,[5] and we identified it there as being due to a degeneracy in the unperturbed energy levels, which leads to a distortion when treated by nondegenerate perturbation theory. By investigating the structure of unperturbed energy levels, we were able to get some insight into what the correct energy-momentum relations should be, and we will follow the same approach in Sec. III. It is also clear from Fig. 1 that the negative mass at $p=0$ is associated with the effects of this degeneracy extending back to $p=0$.

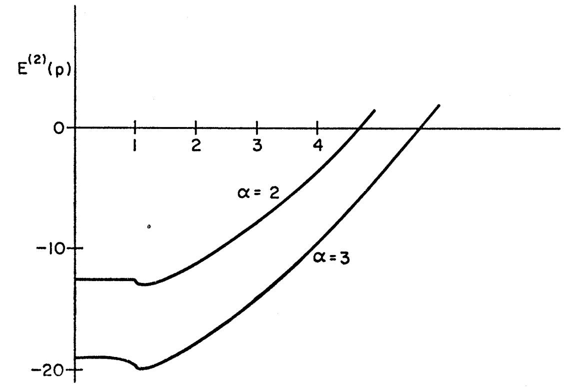

FIG. 1. Energy versus momentum according to the second perturbation theory. At $P=1$, the slope is $-\infty$.

III. ENERGY CROSSING AND THE TAMM-DANCOFF APPROXIMATION

Using the same type of argument[6] that we applied to the optical-polaron problem,[5] we consider the exact eigenvalues $\mathcal{E}^0(P)$ of the noninteracting Hamiltonian [the first two terms in (1.1)]. Here P is the total momentum of the state. In Fig. 2(a), we plot the energy of these states as functions of P. The curve $\frac{1}{2}p^2$ represents the no-phonon states. To obtain the one-phonon states, we start at any point on $\frac{1}{2}p^2$ and draw a straight line with slope ± 1 (the speed of sound in these units). The resulting curves represent the one-phonon states, and a moment's reflection shows that they represent the multiphonon states as well. We see then that for $P<1$ the lowest state is the no-phonon state $\frac{1}{2}p^2$ and for $P>1$ the lowest state contains phonons and has the energy $P-\frac{1}{2}$. Above this lowest state, we have a continuum. For $P<1$, the no-phonon state lies on the bottom of the continuum, but at $P=1$ (when the electron has the speed of sound), it crosses into the continuum.

Now let us consider what happens when we include the interaction term as a perturbation. Since the interaction is translationally invariant, it connects only those unperturbed states which have the same total momentum. In Fig. 2(b), we redraw a few of the states in Fig. 2(a). We include the no-phonon states and the states which include an electron with momentum p' and any phonon. [Note: Although many phonon states also lie along this line, they are not coupled to the no-phonon state directly by the Hamiltonian (1.1).] We see that somewhat above $P=1$ the two sets of energy levels cross and at the point of crossing the matrix element connecting the two degenerate states is not zero. We know that we must diagonalize these two degenerate states exactly, and that when we do the energy levels no longer cross and the curves should

[6] This type of energy crossing argument was first used by T. D. Schultz, Solid State and Molecular Theory Group, MIT Technical Report No. 9, 1956 (unpublished).

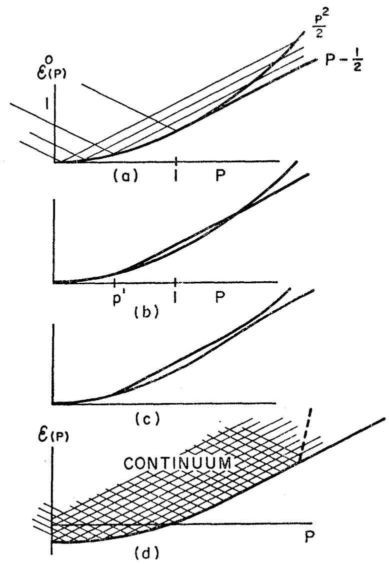

FIG. 2. (a) The energy of the exact eigenstates of the unperturbed Hamiltonian $\mathcal{E}^0(P)$ versus the total momentum of the state P; (b) free-electron energies crossing a set of one-phonon states; (c) level crossing is eliminated by a perturbation which couples the two degenerate states; (d) expected form for the polaron energy-momentum relation. The bottom curve asymptotes to the speed of sound. The dashed curve indicates a quasiparticle crossing into the continuum.

look something like those shown in Fig. 2(c). If we add more of the one-phonon states and repeat the above argument, we expect the final curve $\mathcal{E}(P)$ to look like that shown in Fig. 2(d). Note that this curve has been shifted at $P=0$ to account for the polaron self-energy. We expect a continuum of states to lie immediately above this curve composed of polaron and phonon states. (We do not expect the inclusion of one electron in the crystal to shift the phonon energies appreciably.) It is important in carrying out this argument to remember that whenever the polaron has velocity <1 it lies on the bottom of the continuum, but if its velocity is >1 then it is in the continuum. Thus the energy-crossing argument leads to a curve like $\mathcal{E}(P)$, where $\partial\mathcal{E}(P)/\partial P<1$ and approaches unity as P increases. Our previous experience suggests that at some finite P a quasiparticle will cross into the continuum and subsequently approach the free-electron curve. This is indicated by a dashed line in Fig. 2(d). We should note that in Fig. 2(b) there is actually another point of degeneracy where the electrons have momentum P_1 involving a zero-momentum phonon. But owing to the density of such states, this degeneracy does not lead to an infinity of the integrand in Eq. (2.3), whereas the degeneracy that sets in at $P=1$ does.

Energy-crossing arguments usually involve only two states, whereas here we are concerned about degeneracy between one set of states and a continuum. This difficulty, as we have seen in the case of the optical polaron,[5] can be resolved by using the Tamm-Dancoff one-quantum cutoff. If we consider the matrix obtained by representing the Hamiltonian (1.1) in the unperturbed eigenstates, we note that the submatrix which involves only the zero- and one-phonon states can be diagonalized exactly. (In doing this we must hold the volume finite so that the matrix will be discrete.) The lowest eigenvalue is given by

$$E_T(P)=\tfrac{1}{2}P^2+\Sigma(P,E_T(P)),\tag{3.1}$$

$$\Sigma(P,\omega)=\sum_q\left(\frac{4\pi\alpha}{Vq}\right)\frac{1}{\omega-E^0(P-q)-q}.\tag{3.2}$$

The integral in (3.2) is given in Appendix A, and the function $E_T(P)$ is plotted in Fig. 3 for several values of α. Equations (3.1) and (3.2) are called the Tamm-Dancoff one-quantum cutoff approximation. Remember that in the energy-crossing argument we had to consider a degeneracy involving only the zero- and one-phonon states and this is just the part of the Hamiltonian which is exactly diagonalized in the Tamm-Dancoff. Hence the Tamm-Dancoff should handle the effects of this degeneracy correctly. We note that there is a place where the energy-momentum relations bend over and become tangent to the line $P-\frac{1}{2}$. After they reach this line, the integral in (3.2) is no longer proper and the polaron becomes a quasiparticle with finite lifetime and energy given by the real part of (3.1). This part of the curve is indicated by a dotted line in Fig. 3. The over-all shape of the curve is, however, very different from the one that the energy-crossing argument led us to expect [Fig. 2(d)]. This situation is again similar to that in the optical polaron,[5] where we realized that although the Tamm-Dancoff analyzed the degeneracy exactly the theory puts the continuum at the wrong place and in this sense gives wrong results. This is easily understood when we recall that the continuum should be composed of a polaron and some free phonons, but since the polaron contains some phonons, the expected value of the phonon number in a continuum state must be greater than one, and hence these states

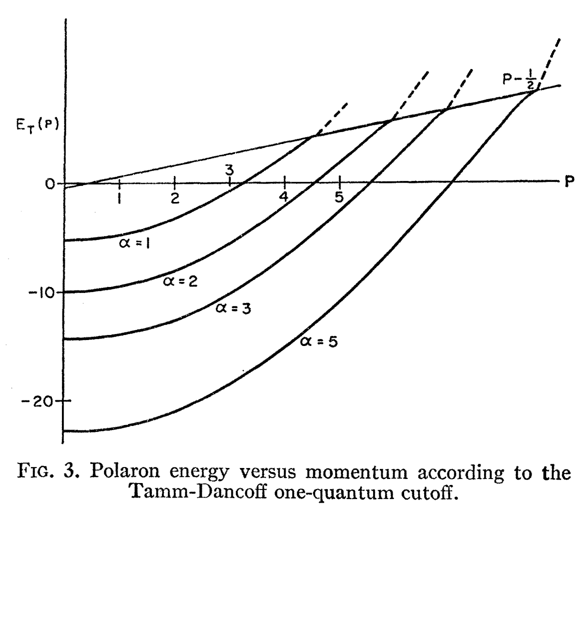

FIG. 3. Polaron energy versus momentum according to the Tamm-Dancoff one-quantum cutoff.

cannot occur in the Tamm-Dancoff. The only continuum states which can occur are the free electron and phonons (i.e., the unperturbed continuum). We see then that the Tamm-Dancoff gives a solution which tends to stay below this incorrectly placed continuum. In order for the polaron energy-momentum relation to stay below the correct continuum, we require only that its velocity stay below unity. Hence we return to the conclusion that we expect the correct energy-momentum relation to be like that in Fig. 2(d).

IV. INTERMEDIATE COUPLING THEORY

The next well-known polaron theory which applies in the weak-coupling region was devised by Lee, Low, and Pines and also by Gurari[7] (LLPG), and is often called the intermediate coupling theory. This theory, which is an upper bound to the ground state with momentum P because it can be formulated variationally, gives

$$E_L(P)=\tfrac{1}{2}P^2-\tfrac{1}{2}[\mathbf{P}-\mathbf{v}(\mathbf{P})]^2-\sum_q\left(\frac{4\pi\alpha}{Vq}\right)\frac{1}{q-\mathbf{q}\cdot\mathbf{v}(\mathbf{P})+\frac{1}{2}q^2}, \quad (4.1)$$

where $\mathbf{v}(\mathbf{P})$ is determined by the transcendental equation

$$\mathbf{v}(\mathbf{P})=\mathbf{P}-\sum_q\left(\frac{4\pi\alpha}{Vq}\right)\frac{\mathbf{q}}{(\mathbf{q}\cdot\mathbf{v}(\mathbf{P})-\frac{1}{2}q^2-q)^2}. \quad (4.2)$$

The results of these integrations are recorded in Appendix B. It follows directly from (4.1) and (4.2) that $v(P)=\partial E_L/\partial P$, and hence is the polaron velocity.

$E_L(P)$ can be determined numerically and is plotted in Fig. 4. We see that the result is very close to what the energy-crossing arguments predicted, but there is no indication of a quasiparticle crossing into the continuum. In fact, we can see from Eq. (4.2) that as $v\rightarrow 1$, $p\rightarrow\infty$. The fact that $E_L(P)$ is an upper bound to the ground state of H with momentum P does not necessarily mean that the polaron must stay below $E_L(P)$ for all P. Remember that in both perturbation theory and the Tamm-Dancoff the polaron was described by an eigenstate of H for momenta below a certain $P\approx 1$, and above this momentum the polaron was a quasiparticle which had no simple relation to the eigenstates of H. The low eigenstates for large P could easily be composed of a polaron of $P\approx 1$ plus a free phonon of large momentum. Therefore, an energy-momentum relation like that shown in Fig. 2(d) is quite compatible with the predictions of the LLPG theory.

[7] T. D. Lee, F. Low, and D. Pines, Phys. Rev. **90**, 297 (1953); M. Gurari, Phil. Mag. **44**, 329 (1953).

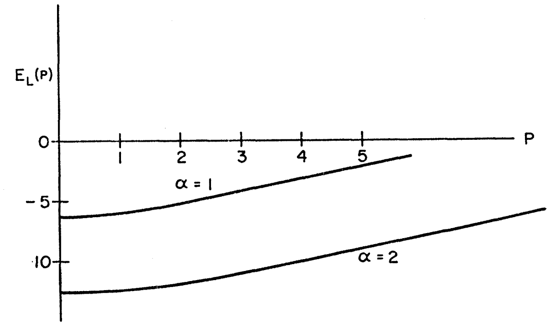

FIG. 4. Polaron energy versus momentum according to intermediate coupling theory.

In order to understand why the LLPG theory gives essentially the result predicted by the energy-crossing arguments, we note that the Tamm-Dancoff, Eqs. (3.1) and (3.2), is essentially the same as perturbation theory, Eqs. (2.1) and (2.2), except that one of the unperturbed energies in the energy denominator is replaced by a corrected energy which is then solved for self-consistently. Now Eq. (4.2) is essentially the derivative of these equations, but here a corrected velocity is put in the energy denominator and solved for self-consistently. Since, as we have pointed out many times, it is the polaron velocity and not the energy which is the important function near the point of degeneracy, this result is not surprising.

We should comment that the LLPG theory gives a linear energy momentum relation at high P even for the optical polaron. This fact does not affect our conclusions here. We believe that for the piezoelectric polaron the LLPG theory gives a good energy-momentum relation because it agrees with the energy-crossing arguments. For the optical polaron, it does not agree with the energy-crossing arguments; therefore, we think it is a poor approximation in this case.

V. DISCUSSION

It is clear from the considerations above that the energy-momentum relation given by perturbation theory and the Tamm-Dancoff theory are qualitatively incorrect. For the same reasons that these theories are wrong at zero temperature,[8] they are also wrong at finite temperature.[3] At zero temperature, the energy-momentum relation should look like Fig. 2(d), with Fig. 4 giving a good quantitative version of it up to the

[8] At finite temperature, the self-energy for these two theories is the sum of two terms. One is the one we have considered above, and the second is a term which disappears when $T=0$. This second term involves the same energy denominator as the first and, like the first, structure in the finite-temperature term occurs when this denominator is zero.

momentum where it no longer describes the polaron. We cannot be sure that such a break will occur, but the fact that it does in the Tamm-Dancoff we regard as a strong argument for it.

In order to determine the limits of the LLPG theory we should develop a theory which explicitly allows for a complex self-energy. The most natural way that we know to do this is to start with the Green's-function formulation,[9] and look for an approximation which gives the LLPG theory. However, attempts to derive the LLPG theory from Green's functions have been largely unsuccessful in the past.[10]

APPENDIX A

$$\Sigma(P,\omega)\frac{\pi P}{\alpha}=q_m\ln\left|\frac{(q_m-P+1)^2+(2P-2\omega-1)}{(q_m+P+1)^2-(2P+2\omega+1)}\right|+(1-P)\ln\left|\frac{(q_m-P+1)^2+(2P-2\omega-1)}{(1-P)^2+(2P-2\omega-1)}\right|$$
$$-(1+P)\ln\left|\frac{(q_m+P+1)^2-(1+2P+2\omega)}{(1+P)^2-(1+2P+2\omega)}\right|+J.$$

If $\omega<-\frac{1}{2}-P$,

$$J=2(2P-2\omega-1)^{1/2}\left\{\tan^{-1}\left[\frac{q_m+1-P}{(2P-2\omega-1)^{1/2}}\right]-\tan^{-1}\left[\frac{1-P}{(2P-2\omega-1)^{1/2}}\right]\right\}$$
$$-2(-(1+2P+2\omega))^{1/2}\left\{\tan^{-1}\left[\frac{(q_m+1+P)}{(-(1+2P+2\omega))^{1/2}}\right]-\tan^{-1}\left[\frac{1+P}{(-(1+2P+2\omega))^{1/2}}\right]\right\}.$$

If $-\frac{1}{2}-P<\omega<-\frac{1}{2}+P$,

$$J=2(2P-2\omega-1)^{1/2}\left\{\tan^{-1}\left[\frac{q_m+1-k}{(2P-2\omega-1)^{1/2}}\right]-\tan^{-1}\left[\frac{1-P}{(2P-2\omega-1)^{1/2}}\right]\right\}$$
$$-(1+2P+2\omega)^{1/2}\ln\left|\frac{[q_m+1+P+(1+2P+2\omega)^{1/2}][1+P-(1+2P+2\omega)^{1/2}]}{[q_m+1+P-(1+2P+2\omega)^{1/2}][1+P+(1-2P+2\omega)^{1/2}]}\right|.$$

If $\omega>-\frac{1}{2}+P$,

$$J=(1-2P+2\omega)^{1/2}\ln\left|\frac{[q_m+1-P+(1-2P+2\omega)^{1/2}][1-P-(1-2P+2\omega)^{1/2}]}{[q_m+1-P-(1-2P+2\omega)^{1/2}][1-P+(1-2P+2\omega)^{1/2}]}\right|$$
$$-(1+2P+2\omega)^{1/2}\ln\left|\frac{1+q_m/[1+P+(1+2P+2\omega)^{1/2}]}{1+q_m/[1+P-(1+2P+2\omega)^{1/2}]}\right|.$$

APPENDIX B

After integration, Eqs. (4.1) and (4.2) become

$$P-v=\frac{2\alpha}{\pi v^2}\left[\ln\left(\frac{1+v}{1-v}\right)+(1+\tfrac{1}{2}q_m)\ln\left(\frac{1+\frac{1}{2}q_m-v}{1+\frac{1}{2}q_m+v}\right)\right],$$

and

$$E_L(P)=\tfrac{1}{2}P^2-\tfrac{1}{2}(P-v)^2+\frac{\alpha}{\pi v}\left\{(q_m+2)\ln\left[\frac{q_m+2(1-v)}{q_m+2(1+v)}\right]-2v\ln[(q_m+2)^2-4v^2]-2\ln\left(\frac{1-v}{1+v}\right)+2v\ln[4(1-v^2)]\right\}.$$

[9] G. Whitfield and R. Puff, in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Plenum Press, Inc., New York, 1963).

[10] D. Pines, in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Plenum Press, Inc., New York, 1963), p. 170.