Theory of Superconducting Semiconductors and Semimetals

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(Received 20 May 1968)

A Green's-function method is used to derive a superconducting energy-gap equation without the assumption that the Fermi energy is much larger than phonon energies. This equation is then approximated using two separate methods. The first method applies when the screened electron-phonon interaction is almost independent of wave vector and the Fermi energy is of the order of, or larger than, phonon energies. The gap equation obtained in this way takes account of the variation in the density of electron states with energy. The second approximation method applies when the screened electron-phonon interaction depends strongly on wavelength or when the Fermi energy is small compared to phonon energies. In this case, the gap equation takes account of the wave-vector dependence of the interaction, the wave-vector and frequency dependence of the electronic screening, the energy dependence of the density of states, and the wave-vector dependence of the superconducting energy gap. In addition, the effects of the retardation of the electron-electron interaction are included.

I. INTRODUCTION

MOST known superconductors are metallic, and have Fermi energies and plasma frequencies much larger than phonon frequencies in the material. However, the prediction[1] and verification that GeTe,[2] $SrTiO_3$,[3] and SnTe,[4] all degenerate semiconductors, were superconductors has led to a study of superconductivity in systems in which the phonon energies $\hbar\omega_{ph}$ are of the same order of magnitude or even larger than the Fermi energy ϵ_F and the plasma energy $\hbar\omega_p$.

One of the first considerations of the possibility of superconductivity in semiconductors was made by Gurevich, Larkin, and Firsov,[5] who began with the superconducting gap equation derived by Eliashberg.[6] Although these authors did not use the integration procedure of Eliashberg which is valid only in the limit of $\epsilon_F \gg \hbar\omega_{ph}$, they did make approximations such as the neglect of the variation in the density of electron states times the electron-phonon coupling over energies of the order of the phonon frequency, and the use of frequency-independent electronic screening. These approximations are valid only when $\hbar\omega_{ph} \ll \epsilon_F$ and $\omega_{ph} \ll \omega_p$.

The next investigation of superconducting semiconductors was made by one of the authors[1] who included the intervalley interaction for the first time. The equation used in Ref. 1 to determine the transition temperature is essentially that of Bardeen, Cooper, and Schrieffer[7] generalized to the case of many valleys and taking account of the density of states variation. This equation may be derived using the Nambu-Gor'kov formulation[8,9] extended to finite temperatures[10] if the interaction is taken to be nonretarded, that is, independent of frequency.[11] The use of a nonretarded interaction is a good approximation only if $\hbar\omega_{ph} \gg \epsilon_F$ and $\hbar\omega_p \gg \epsilon_F$.

While the use of a nonretarded interaction has led to a good agreement between theory and experiment for $SrTiO_3$,[12–14] where, in fact, the Fermi energy is small compared to important phonon energies, the application of the theory to SnTe and GeTe, which have $\epsilon_F > \hbar\omega_{ph}$, may cause discrepancies in quantitative comparisons of theoretical predictions with experiment.

The equations necessary to determine the superconducting energy gap as a function of temperature have been obtained for the case $\epsilon_F \gg \hbar\omega_{ph}$ and $\hbar\omega_p \gg \hbar\omega_{ph}$, and good agreement with tunneling experiments has

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* A. P. Sloan Foundation Fellow. Supported by the National Science Foundation.

[1] Marvin L. Cohen, Phys. Rev. **134**, A511 (1964).

[2] R. A. Hein, J. W. Gibson, R. Mazelsky, R. C. Miller, and J. K. Hulm, Phys. Rev. Letters **12**, 320 (1964).

[3] J. F. Schooley, W. R. Hosler, and M. L. Cohen, Phys. Rev. Letters **12**, 474 (1964).

[4] R. A. Hein, J. W. Gibson, R. S. Allgaier, B. B. Houston, Jr., R. L. Mazelsky, and R. C. Miller, in *Proceedings of the Ninth International Conference on Low-Temperature Physics*, edited by J. A. Daunt *et al.* (Plenum Press, Inc., New York, 1965), p. 604.

[5] V. L. Gurevich, A. I. Larkin, and Yu. A. Firson, Fiz. Tverd. Tela **4**, 185 (1962) [English transl: Soviet Phys.—Solid State **4**, 131 (1962)].

[6] G. M. Eliashberg, Zh. Experim. i Teor. Fiz. **38**, 966 (1960) [English transl.: Soviet Phys.—JETP, **11**, 696 (1960)].

[7] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[8] Y. Nambu, Phys. Rev. **117**, 648 (1960).

[9] L. P. Gor'kov Zh. Experim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].

[10] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, Zh. Experim. i Teor. Fiz. **36**, 900 (1959) [English transl.: Soviet Phys.—JETP **9**, 636 (1959)].

[11] J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964).

[12] C. S. Koonce, Marvin L. Cohen, J. F. Schooley, W. R. Hosler, and E. R. Pfeiffer, Phys. Rev. **163**, 380 (1967).

[13] J. F. Schooley, W. R. Hosler, E. Ambler, J. G. Becker, M. L. Cohen, and C. S. Koonce, Phys. Rev. Letters **14**, 305 (1965).

[14] For a general review of this approach to the calculation of superconducting properties of low-density systems see Marvin L. Cohen, in Superconductivity, edited by R. D. Parks (to be published).

been obtained.[15] In the case $\hbar\omega_p \gg \hbar\omega_{ph}$ and $\epsilon_F \gg \hbar\omega_{ph}$ the interaction through phonons may be greatly simplified, but the Coulomb interaction still poses a problem since $\hbar\omega_p$ is greater than ϵ_F, and additional approximations must be made.[16] These approximations are not critical for most metals, however, since the importance of the Coulomb interaction decreases as the ratio ω_{ph}/ω_p decreases.

This paper will attempt to fill the gap between the theories valid in the limit $\epsilon_F \gg \hbar\omega_{ph}$ and $\omega_p \gg \omega_{ph}$ and those valid when $\hbar\omega_{ph} \gg \epsilon_F$ and $\omega_{ph} \gg \omega_p$. We will first derive general equations using the Nambu-Gor'kov formulation which will be valid over the range from $\epsilon_F \gg \hbar\omega_{ph}$ to $\epsilon_F \gg \hbar\omega_{ph}$. These equations are quite difficult to solve in practice and two separate sets of approximations will be made in order to solve them.

First, we will consider the case $\epsilon_F \gtrsim \hbar\omega_{ph}$ and the electron-phonon coupling independent of wave vector, and obtain an energy-gap equation which includes the variation in the density of states over the energy range of interest. These equations should always be more accurate than the corresponding equations derived in the limit $\epsilon_F \gg \hbar\omega_{ph}$, but for most metals the difference is negligible.

Next we will consider the case $\epsilon_F \lesssim \hbar\omega_{ph}$, and derive equations which should be more accurate for all materials than equations derived using an instantaneous interaction.

II. DERIVATION OF THE SUPERCONDUCTING-GAP EQUATION

We will use the Nambu-Gor'kov formalism to calculate the equation for the superconducting energy gap at zero temperature $\Delta(\epsilon,p_0)$, the renormalization $Z(\epsilon,p_0)$, and the Hartree-Fock energy $\chi(\epsilon,p_0)$. The energy ϵ is the quasiparticle energy for electrons in the normal state in the absence of renormalization arising from phonons or other electrons in the conduction band measured from ϵ_F and p_0 is the energy variable conjugate to time. Our development will follow that of Schreiffer.[11]

We may write the zero-order Hamiltonian

$$H_0=\sum_k \epsilon_k(C_{k\uparrow}^\dagger C_{k\uparrow}+C_{-k\downarrow}^\dagger C_{-k\downarrow}) \tag{1}$$

using the spinor fields introduced by Nambu, namely,

$$\psi_k=\begin{pmatrix} C_{k\uparrow} \\ C_{-k\downarrow}^\dagger \end{pmatrix} \quad \text{as} \quad H_0=\sum_k \psi_k^\dagger \epsilon_k \tau_3 \psi_k+\sum_k \epsilon_k, \tag{2}$$

where $C_k^\dagger$ is the creation operator for electrons in the conduction band, $\epsilon_k=\epsilon$, and

$$\tau_1=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2=\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_3=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{I}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

[15] D. J. Scalapino, J. R. Schrieffer, and J. W. Wilkins, Phys. Rev. 148, 263 (1966).
[16] J. W. Garland, Phys. Rev. 153, 460 (1967).

The Green's function for the system described by H_0 is

$$\mathbf{G}_0(\mathbf{p},p_0)=e^{i\eta p_0\tau_3}/[p_0\mathbf{I}-\epsilon(\mathbf{p})\tau_3+i\eta], \tag{3}$$

where $p=(\mathbf{p},p_0)$ and $\eta>0$. $\mathbf{G}_0$ is now a matrix with off-diagonal elements equal to zero.

We will proceed by using self-consistent perturbation theory and allowing the off-diagonal elements of $\mathbf{G}(\mathbf{p},p_0)$ to be nonzero. The most general form for the self-energy is

$$\mathbf{\Sigma}(p)=[1-Z(p)]p_0\mathbf{I}+\chi(p)\tau_3+\varphi_1(p)\tau_1+\varphi_2(p)\tau_2, \tag{4}$$

where $\chi(p)$ is the exchange contribution to the Hartree-Fock energy, $\varphi(p)=Z(p)\Delta(p)$, and $\Delta(p)$ is the superconducting energy-gap function. The exact Green's function then has the form

$$\mathbf{G}(p)=\frac{e^{i\eta p_0\tau_3}}{Z(p)p_0\mathbf{I}-\tilde{\epsilon}(p)\tau_3-\varphi_1(p)\tau_1-\varphi_2(p)\tau_2+i\eta}, \tag{5}$$

where $\tilde{\epsilon}(p)=\epsilon(\mathbf{p})+\chi(p)$. Equation (5) may be written as

$$\mathbf{G}(p)=\frac{[Z(p)p_0\mathbf{I}+\tilde{\epsilon}(p)\tau_3+\varphi_1(p)\tau_1+\varphi_2(p)\tau_2]e^{i\eta p_0\tau_3}}{[Z(p)p_0]^2-\tilde{\epsilon}(p)^2-\varphi_1(p)^2-\varphi_2(p)^2+i\eta}. \tag{6}$$

We will next calculate the lowest-order dressed phonon and dressed Coulomb contributions to $\mathbf{\Sigma}(p)$. These are given by the diagram shown in Fig. 1, where double dashed lines indicate the total dressed interaction, including both Coulomb and phonon parts.

We then obtain

$$\mathbf{\Sigma}(p)=\frac{i\Omega}{\hbar^3(2\pi)^4}\int \tau_3 G(p')\tau_3 V(p-p')d^4p', \tag{7}$$

where $V(p-p')$ is the total interaction, and Ω is the crystal volume.

In many cases it is a good approximation to divide the total dressed interaction into a dressed Coulomb interaction and a sum over dressed phonon interactions. The most important case in which such a division is a good approximation is when the plasma frequency is large compared to phonon frequencies. Another important case is the case of only one phonon mode. The conditions for this separation are discussed in the Appendix. When such a separation is possible we have

$$V(p-p')=V_c(p-p')+\sum_\lambda\{\{\bar{g}_{\lambda(p-p')}\}\}^2 D_\lambda(p-p'). \tag{8}$$

Here $V_c(p-p')$ is the screened Coulomb interaction, $D_\lambda(p-p')$ is the exact phonon propagator, and

$$\{\{g_\lambda(p-p')\}\}^2=\bar{g}_\lambda(p-p')\bar{g}_\lambda(-p+p'),$$

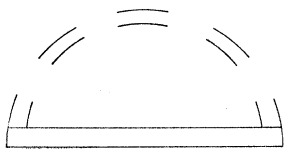

FIG. 1. Self-energy diagram used to compute $\Sigma(p)$. The double dashed lines indicate that the total dressed interaction (Coulomb and phonon) is used.

where $g_\lambda(p-p')$ is the screened electron-phonon coupling for phonon mode λ. The sum over λ is a sum over phonon modes allowed by symmetry, which we assume to be independent.

We note that in calculating the self-energy, we have included no "crossing diagrams," that is, we have set the vertex function Γ equal to one. For the case $\epsilon_F \gg \hbar\omega_{\rm ph}$ this is a good approximation even for strong coupling[17] in the interaction through the phonon field. Since the condition $\epsilon_F \gg \hbar\omega_{\rm p}$ is never valid, the neglect of "crossing diagrams" is never justified for the Coulomb interaction and this approximation corresponds to a calculation using $r_s \ll 1$, that is, weak coupling. When the condition $\epsilon_F \gg \hbar\omega_{\rm ph}$ is not satisfied, the phonon interaction calculated with no "crossing diagrams" is strictly valid only to lowest order in the electron phonon coupling, so that in this case our equations will be good only for the case of weak electron-phonon coupling. For completeness, the functions $Z(\epsilon,p_0)$ and $\chi(\epsilon,p_0)$ are retained in the case $\epsilon_F < \hbar\omega_{\rm ph}$, although they represent corrections to the gap equation of higher order in the electron-phonon coupling than is consistent with the condition $\Gamma=1$.

Substituting Eq. (6) into Eq. (7) we have

$$\mathbf{\Sigma}(p)=\frac{i\Omega}{\hbar^3(2\pi)^4}\int_{-\infty}^{\infty}dp_0'\int d\mathbf{p}' \times\frac{[Z(p')p_0'\mathbf{I}+\tilde{\epsilon}(p')\tau_3-\varphi(p')\tau_1]e^{i\eta p_0'\tau_3}}{[Z(p')p_0']^2-\tilde{\epsilon}(p')^2-\varphi(p')^2+i\eta}V(p-p'). \quad (9)$$

In writing Eq. (9) we have fixed the phase of $\varphi(p)$ by setting $\varphi_1(p)=\varphi(p)$ and $\varphi_2(p)=0$.

We next take $\epsilon^{i\eta p_0'\tau_3}=\mathbf{I}\cos\eta p_0'+i\tau_3\sin\eta p_0'$ and write the integral over $\mathbf{p}'$ as an integral over azimuthal angle, over wave vector $q=|\mathbf{p}-\mathbf{p}'|/\hbar$ and over $\epsilon(\mathbf{p})$:

$$\int d\mathbf{p}'\rightarrow\frac{2\pi\hbar^2 m_b}{|\mathbf{p}|}\int_{-\epsilon_F}^{\hbar\omega_{\rm cb}-\epsilon_F}d\epsilon(\mathbf{p}')\int_{q_1}^{q_2}qdq,$$

where $q_1=(1/\hbar)||\mathbf{p}|-|\mathbf{p}'||$, $q_2=(1/\hbar)||\mathbf{p}|+|\mathbf{p}'||$, and m_b is the "band mass." We call this the band mass because it would be the result of a band structure calculation that considered an electron moving in the potentials of the fixed ion screened by the electrons in the valence band only. This mass is also the experimental density-of-states effective mass in the absence of renormalization effects arising from phonons and from other electrons in the conduction band.

We also use rotational symmetry about the vector $\mathbf{p}$. This is an approximation for intravelley process since it assumes a spherical Fermi surface. It is also approximate for intervalley processes because it assumes $q_0 \gg k_F$ where q_0 is the wave vector difference between valleys. The energy $\hbar\omega_{\rm cb}$ is the width of the conduction band.

We will proceed to calculate all quantities assuming one minimum in the conduction band. The results will also apply directly to intervalley interactions between two equivalent minima since generalizations to many valleys are straightforward.[1] Equation (9) becomes

$$\mathbf{\Sigma}(\epsilon,p_0)=\frac{i\Omega m_b}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{-\epsilon_F}^{\hbar\omega_{\rm cb}-\epsilon_F}d\epsilon'\int_{[(2m_b)^{1/2}/\hbar]|(\epsilon+\epsilon_F)^{1/2}-(\epsilon'+\epsilon_F)^{1/2}|}^{[(2m_b)^{1/2}/\hbar]|(\epsilon+\epsilon_F)^{1/2}+(\epsilon'+\epsilon_F)^{1/2}|}qdq$$
$$\times\int_{-\infty}^{\infty}dp_0'(\{[Z(\epsilon',p_0')p_0'\cos\eta p_0'+i\tilde{\epsilon}(\epsilon',p_0')\sin\eta p_0']\mathbf{I}$$
$$+[\tilde{\epsilon}(\epsilon',p_0')\cos\eta p_0'+iZ(\epsilon',p_0')p_0'\sin\eta p_0']\tau_3-\varphi(\epsilon',p_0')\cos\eta p_0'\tau_1\}/$$
$$\{[Z(\epsilon',p_0')p_0']^2-\tilde{\epsilon}(\epsilon',p_0')^2-\varphi(\epsilon',p_0')^2+i\eta\})V(q,\,p_0-p_0'). \quad (10)$$

By equating coefficients of the linearly independent matrices $\mathbf{I}$, τ_1, and τ_3 in Eqs. (4) and (10), one can obtain three coupled equations for the quantities $Z(\epsilon,p_0)$, $\varphi(\epsilon,p_0)$, and $\chi(\epsilon,p_0)$. In Eq. (10) all primed quantities refer to the intermediate state in the self-energy calculation and are summed over.

We note that Z, χ, and φ all depend on both p_0 and ϵ. The p_0 dependence arises from retardation effects and enters through the dependence of the interaction $V(q,\,p_0-p_0')$ on p_0 and p_0'. An instantaneous interaction such as the unscreened Coulomb interaction has no p_0 or p_0' dependence. The interaction $V(q,\,p_0-p_0')$ is roughly constant as long as p_0 and p_0' are much less than the energy of the mode involved in the interaction, i.e., the phonon frequency for the phonon interaction, and the plasma frequency for the screened Coulomb interaction.

Since ϵ is the unrenormalized quasiparticle energy in the normal state, the dependence of Z, χ, and φ on ϵ arises from changes in the product of the interaction times the unrenormalized density of states. The density of states varies on a scale of the order of the Fermi energy ϵ_F.

If the crystal has inversion symmetry, the functions $Z(\epsilon',p_0')$, $\chi(\epsilon',p_0')$, and $\varphi(\epsilon',p_0')$ are even in p_0'. Variation of these quantities with p_0' is expected to be appreciable over energies of the order of the phonon energies appearing in $D_\lambda(q,\,p_0-p_0')$. The variation of $Z(\epsilon',p_0')$,

[17] A. B. Migdal, Zh. Eksperim. i Teor. Fiz. 34, 1438 (1958) [English transl.: Soviet Phys.—JETP 7, 996 (1958)].

$\chi(\epsilon',p_0')$, and $\varphi(\epsilon',p_0')$ with ϵ' is expected to be appreciable over energies of the order of ϵ_F.

Therefore, when the condition $\hbar\omega_{\rm ph}\ll\epsilon_F$ does not hold, it is not permissible to approximate Eq. (10) by setting $\epsilon=\epsilon'=0$ in the limits of the integration over q and in $Z(\epsilon',p_0')$, $\chi(\epsilon',p_0')$, and $\varphi(\epsilon',p_0')$. This is the approximation commonly used for metals where the condition $\hbar\omega_{\rm ph}\ll\epsilon_F$ holds.[11]

It would, however, be quite difficult to solve Eq. (10) self-consistently over the entire ϵ,p_0 plane, and some approximation is necessary.

III. APPROXIMATION METHOD FOR $\epsilon_F\gtrsim\hbar\omega_{\rm ph}$

When the condition $\epsilon_F\gg\hbar\omega_{\rm ph}$ holds, the limits of the integral over q in Eq. (10) becomes independent of energy, and the integral of q times the interaction $V(q,\,p_0-p_0')$ may be performed. Also, when $\epsilon_F\gg\hbar\omega_{\rm ph}$ it is a good approximation to take φ, Z, and χ to be independent of ϵ'. The integral over ϵ', which in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$ may be taken to be between $-\infty$ and $+\infty$, may also be performed, leaving a single integral over p_0' in the equations for φ, Z, and χ. Because these equations are already in the literature,[6,11] and because our equations reduce to these in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$, we will not repeat them here.

We will consider the case $\epsilon_F\gtrsim\hbar\omega_{\rm ph}$. Our equations will be most appropriate when the screened electron-phonon coupling $\tilde{g}$ is nearly independent of wave vector q, and the phonon modes of interest have little dispersion over the range of integration over q. This is not an unusual circumstance, and should be the case for intervalley interactions in doped semiconductors, as well as for some metals. The equations derived in this section should be applicable to intervalley interactions in GeTe and SnTe, for example, where the Fermi energy is larger than phonon energies, but not orders of magnitude larger. However, for these materials the modification of T_c or of $\Delta(0)$ should be small.

It has been noted that the self-energy of an electron arising from the electron-phonon interaction in the normal state is independent of ϵ and depends only on p_0 when the electron-phonon coupling is independent of the wave vector and the electron is coupled to a phonon which has little dispersion.[18] This is also the case for a superconductor, because the integral over q then yields $\frac{1}{2}q^2$, which, when evaluated between the indicated limits yields $(4m_b/\hbar^2)[(\epsilon+\epsilon_F)(\epsilon'+\epsilon_F)]^{1/2}$. When the term outside the integral is considered, we see that the integral equations for Z, χ, and φ are independent of ϵ, and we may, therefore, take Z, χ, and φ to be independent of ϵ, as was done in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$.

We are, however, left with a density of states factor proportional to $(\epsilon'+\epsilon_F)^{1/2}$, which is approximated by $\sqrt{\epsilon_F}$ in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$, and the integral over ϵ' may be performed with no further approximations. After integration over q, Eq. (10) becomes

$$\mathbf{\Sigma}_{\rm ph}(p_0)=\frac{im_b^{3/2}\Omega}{(2)^{3/2}\pi^3\hbar^3}\int_{-\epsilon_F}^{\infty}d\epsilon'(\epsilon_F+\epsilon')^{1/2}\times\int_{-\infty}^{\infty}dp_0'\left(\frac{Z(p_0)p_0'\mathbf{I}-\varphi(p_0')\tau_1}{[Z(p_0')p_0']^2-(\epsilon+\chi)^2-\varphi(p_0')^2}\right)\times\{\{\tilde{g}_\lambda\}\}^2D(p_0-p_0'),\quad(11)$$

where we have taken the limit $\eta\to0$, because the functions $Z(p_0')$, $\chi(p_0')$, and $\varphi(p_0')$ are complex. It will be important to keep η finite when we consider the limit $\epsilon_F\ll\hbar\omega_{\rm ph}$. We have assumed that $\tilde{g}_\lambda$ is independent of p_0 and p_0', and that χ is a constant, as in the case $\epsilon_F\gg\hbar\omega_{\rm ph}$. As a result of the frequency dependence of the dielectric screening, this approximation is more serious in the case $\epsilon_F\gtrsim\hbar\omega_{\rm ph}$.

We will not explicitly calculate the Coulomb contribution to $\mathbf{\Sigma}$ when $\epsilon_F\gtrsim\hbar\omega_{\rm ph}$; the equations valid in the[11] limit $\epsilon_F\gg\hbar\omega_{\rm ph}$ are also valid here. We have also made the approximation that the width of the conduction band is large compared to the Fermi energy and phonon energies.

Equation (11) may be simplified by using the integration procedure of Eliashberg.[6] The phonon propagator D is written as a sum D^u+D^l, where D^u is analytic in the upper half-plane and D^l is analytic in the lower half-plane. We may then deform the contour of integration over D^u around the branch cut above the negative real axis, and deform the contour of integration over D^l around the branch cut below the positive real axis. We then use the relation

$$G_0(p,\,p_0+i\delta)=G_0^*(p,\,p_0-i\delta),\quad(12)$$

and the fact that φ, Z, and χ are even functions of p_0,

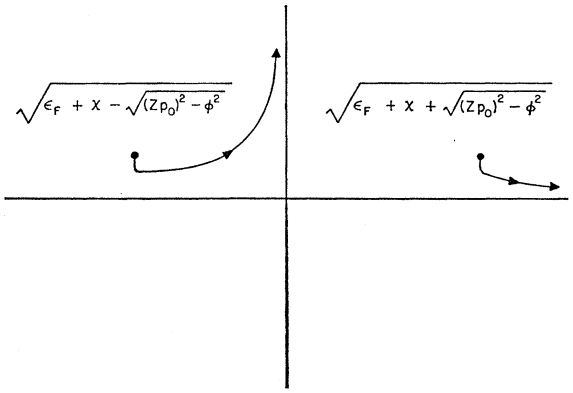

FIG. 2. Qualitative movement of the functions $\{\epsilon_F+\chi-[(Zp_0)^2-\varphi^2]^{1/2}\}^{1/2}$ and $\{\epsilon_F+\chi+[(Zp_0)^2-\varphi^2]^{1/2}\}^{1/2}$ in the complex plane. Arrows indicate direction of increasing p_0.

[18] S. Engelsberg and J. R. Schrieffer, Phys. Rev. **131**, 993 (1963).

to obtain

$$\Sigma_{\rm ph}(p_0)=\frac{\Omega m_b^{3/2}}{\sqrt{2}\pi^3\hbar^3}\int_{-\epsilon_F}^{\infty}d\epsilon'(\epsilon'+\epsilon_F)^{1/2}\int_0^{\infty}dp_0'\times{\rm Im}\left(\frac{Z(p_0')p_0'\mathbf{I}+\varphi(p_0')\tau_1}{[Z(p_0')p_0']^2-[\epsilon'-\chi(p_0')]^2-\varphi(p_0')^2}\right)\{\{\bar{g}_\lambda\}\}^2\times[D_\lambda{}^u(p_0+p_0')\pm D_\lambda{}^l(p_0-p_0')],\quad(13)$$

where the minus sign should be used with the $\mathbf{I}$ component, and the plus sign with the τ_1 component.

The integral over ϵ' may be evaluated by using the transformation $u=(\epsilon_F+\epsilon')^{1/2}$, and noting the resulting integral is even in u so that its value is $\frac{1}{2}$ the value of the integral from $-\infty$ to ∞. If we adopt the convention that the positive square root of a complex number lies in the upper half-plane, we obtain

$$\Sigma_{\rm ph}(p_0)=-\frac{\Omega N(0)}{\sqrt{\epsilon_F}}\int_0^{\infty}dp_0'\,{\rm Re}\left(\frac{Z(p_0')p_0'\mathbf{I}+\varphi(p_0')\tau_1}{\{\epsilon_F+\chi+[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}+\{\epsilon_F+\chi-[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}}\right)\times\{\{\bar{g}_\lambda\}\}^2[D_\lambda{}^u(p_0+p_0')\pm D_\lambda{}^l(p_0-p_0')],\quad(14)$$

where $N(0)=m_b k_F/2\pi^2\hbar^2$ is the unrenormalized density of states for electrons of a single-spin orientation.

If we require ${\rm Im}\{(Zp_0')^2-\varphi^2\}>0$, then ${\rm Re}(\{\epsilon_F+\chi-[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2})<0$. Figure 2 shows the movement of $\{\epsilon_F+\chi+[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}$ and $\{\epsilon_F+\chi-[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}$ in the complex plane as a function of p_0' using the condition ${\rm Im}[(Zp_0')^2-\varphi^2]>0$. Since χ is much smaller than ϵ_F when $\hbar\omega_{\rm ph}\lesssim\epsilon_F$, we may set $\chi=0$ in Eq. (14) with little error.

To obtain the equation for $\Sigma_{\rm ph}(p_0)$ in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$, we may expand the square roots in Eq. (14) for small $[(Zp_0')^2-\varphi^2]^{1/2}$. Noting that ${\rm Re}\{\epsilon_F+\chi-[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}<0$, we obtain

$$\Sigma_{\rm ph}(p_0)=-\Omega N(0)\int_0^{\infty}dp_0'\,{\rm Re}\left\{\frac{Zp_0'\mathbf{I}+\varphi\tau_1}{[(Zp_0')^2-\varphi^2]^{1/2}}\right\}\{\{\bar{g}_\lambda\}\}^2[D_\lambda{}^u(p_0+p_0')\pm D_\lambda{}^l(p_0-p_0')]\quad(15)$$

plus terms of order $(p_0'/\epsilon_F)^2$, which are roughly of order $(\hbar\omega_{\rm ph}/\epsilon_F)^2$. Equation (15) is the usual equation obtained in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$.[11]

Equation (14) differs from Eq. (15) because of a different effective density of states, and the integral over the imaginary part of the Green's function evaluated to obtain Eq. (14) is, except for the τ_3 component, similar to the integral necessary to obtain the tunneling density of states, which is proportional to the derivative of the runneling current with respect to the applied voltage. This difference may be observable in a normal-superconductor tunneling experiment, where a plot of the second derivative of the current with respect to the voltage as a function of voltage could give structure near $[\epsilon_F{}^2+\Delta(\epsilon_F)^2]^{1/2}$. As a result of the large imaginary part introduced into $\Delta(p_0)$ and $Z(p_0)$ when $p_0\geq\hbar\omega_{\rm ph}$ (and real phonons can be emitted), the structure discussed above may not be observable unless $\hbar\omega_{\rm ph}>\epsilon_F$.

The generalization of Eq. (14) to finite temperature is straightforward, and can be accomplished using the same methods used in the limit $\epsilon_F\gg\hbar\omega_{\rm ph}$,[15] since only the integral over ϵ was changed, and this integral is the same in the zero-temperature and finite temperature developments. We obtain

$$\Sigma_{\rm ph}(p_0)=\frac{\Omega N(0)}{\sqrt{\epsilon_F}}\int_0^{\infty}dp_0'\,{\rm Re}\left\{\frac{Zp_0'\mathbf{I}-\varphi\tau_1}{\{\epsilon_F+\chi+[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}+\{\epsilon_F+\chi-[(Zp_0')^2-\varphi^2]^{1/2}\}^{1/2}}\right\}\times\int_0^{\infty}d\nu\sum_\lambda B_\lambda(q,\nu)|\bar{g}_\lambda|^2\left[\frac{1}{p_0-p_0'-\nu+i\delta}\frac{1}{1+e^{-\beta p_0'}}+\frac{1}{p_0-p_0'+\nu+i\delta}\frac{1}{1+e^{+\beta p_0'}}\right]+\frac{i\pi\Omega N(0)}{\sqrt{\epsilon_F}}\int_0^{\infty}d\nu\sum_\lambda\sum_{s=0}^{1}\frac{p_{0s}Z(p_{0s})\mathbf{I}-\varphi(p_{0s})\tau_1}{\{\epsilon_F+\chi+[(Zp_{0s})^2-\varphi^2]^{1/2}\}^{1/2}+\{\epsilon_F+\chi-[(Zp_{0s})^2-\varphi^2]^{1/2}\}^{1/2}}|\bar{g}_\lambda|^2\frac{B_\lambda(q,\nu)}{1-e^{\beta\nu}},\quad(16)$$

where $p_{0s}=p_0+(-1)^s\nu+i\delta$. Equation (16) is a generalization of Eq. (2.20a) of Ref. (15) for the case $\hbar\omega_{\rm ph}\lesssim\epsilon_F$, and $B_\lambda(q,\nu)$ is defined in that reference.

IV. APPROXIMATION METHOD FOR $\epsilon_F\lesssim\hbar\omega_{\rm ph}$

When the Fermi energy is much less than important phonon energies, and when the Fermi energy is of the same order of magnitude as the phonon energies and the screened electron-phonon coupling $\bar{g}(k)$ has a strong k dependence, we cannot approximate the functions $Z(\epsilon,p_0)$, $\chi(\epsilon,p_0)$, and $\varphi(\epsilon,p_0)$ by functions of p_0 alone. For sufficiently small Fermi energy, the ϵ dependence of these functions will be more important than the p_0 dependence. The results derived in this section should

apply to doped $SrTiO_3$, where the Fermi energy is much less than important phonon frequencies.

In the evaluation of the integrals over p_0' and ϵ' in Eq. (10), knowledge of $Z(\epsilon',p_0')$, $\chi(\epsilon',p_0')$, and $\varphi(\epsilon',p_0')$ is most important when the remainder of the integrand is large. This occurs when $p_0'=\pm E(\epsilon',p_0')$, where

$$E(\epsilon',p_0')=\{[\epsilon+\chi(\epsilon',p_0')]^2+\varphi(\epsilon',p_0')^2\}^{1/2}/Z(\epsilon',p_0').$$

We will therefore approximate $Z(\epsilon',p_0')$ by $Z(\epsilon')=Z(\epsilon',\, p_0'=\pm E')$, $\chi(\epsilon',p_0')$ by $\chi(\epsilon')=\chi(\epsilon',\, p_0'=\pm E')$, and $\varphi(\epsilon',p_0')$ by $\varphi(\epsilon')=\varphi(\epsilon',\, p_0'=\pm E')$, in order to calculate $Z(\epsilon,p_0)$, $\chi(\epsilon,p_0)$, and $\varphi(\epsilon,p_0)$ from Eq. (10).

Because we evaluate Z, χ, and φ on the branch cut of $G(\epsilon',p_0')$, Eq. (12) indicates that Z, χ, and φ must be real. We must therefore keep η in Eq. (10) finite until the p_0' integration has been completed. The functions $Z(\epsilon,p_0)$, $\chi(\epsilon,p_0)$, and $\varphi(\epsilon,p_0)$ calculated using this approximation for $Z(\epsilon',p_0')$, $\chi(\epsilon',p_0')$, and $\varphi(\epsilon',p_0')$ will depend on p_0 and are complex. The important variation in p_0 and the imaginary part of these functions is important for $p_0\gtrsim\hbar\omega_{\rm ph}$, and these values of p_0 are of little importance when $\epsilon_F\lesssim\hbar\omega_{\rm ph}$. An iterative solution to these equations may be obtained by evaluating the functions Z, χ, and φ at $p_0=\pm E$ and inserting into the integral equation.

This method of solving the integral equation should be compared with the alternate procedure of assuming a nonretarded interaction, that is, assuming $V(q,\, p_0-p_0')$ to be independent of p_0 and p_0'. The assumption of a nonretarded interaction is also best when $\hbar\omega_{\rm ph}\gg\epsilon_F$, and leads to a real energy gap. The best nonretarded approximation to $V(q,\, p_0-p_0')$ is not determined by this method however. It is logical to evaluate $V(q,\, p_0-p_0')$ at $p_0=\pm E$ and $p_0'=\pm E'$, but the interaction depends on the choice of plus or minus signs. If both plus signs or both minus signs are taken, an interaction of the Bardeen-Pines form results. If instead, both p_0 and p_0' are taken to be zero, the phonon contribution to $V(q,\, p_0-p_0')$ has infinite range leading to an infinite transition temperature. We will avoid the ambiguity in the choice of a nonretarded interaction by making no approximations on $V(q,\, p_0-p_0')$, only approximating φ, χ, and Z inside the integral.

We will now consider the integral over p_0' in Eq. (10) where φ, Z, and χ are independent of p_0'. For very large p_0' the total interaction $V(q,\, p_0-p_0')$ must approach the bare Coulomb interaction $V_c{}^B(q)$. Also, the denominator of the Green's function is proportional to $(p_0')^2$ as $p_0'\to\infty$. For the terms in the numerator that are constant as $p_0'\to\infty$, we may close either in the upper or lower half-plane. For these terms we may then take the limit of $\eta\to 0$ before integration.

To integrate the terms in the numerator linear in p_0', we must keep η finite until after integration. It is convenient in this case to divide the interaction into two parts:

$$V(q,\, p_0-p_0')=V^s(q,\, p_0-p_0')+V_c{}^B(q), \qquad (17)$$

and

$$V_c{}^B(q)=4\pi e^2/\Omega q^2\kappa_\infty, \qquad (18)$$

where $V^s(q,\, p_0-p_0')\to 0$ as $p_0'\to\infty$. In all integrals over $V^s(q,\, p_0-p_0')$ we may take $\eta=0$, and integrals over $V_c{}^B(q)$ are easily evaluated.

The term in Eq. (10) proportional to **I** gives

$$Z(\epsilon,p_0)=1+\int_{-\epsilon_F}^{\hbar\omega_{\rm cb}-\epsilon_F}\frac{d\epsilon'}{Z(\epsilon')}K_Z(\epsilon,\epsilon',p_0), \qquad (19)$$

where

$$K_Z(\epsilon,\epsilon',p_0)=-\frac{i\Omega m_b}{p_0(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\times\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}qdq\int_{-\infty}^{\infty}dp_0'\frac{p_0'}{(p_0')^2-E(\epsilon')^2+i\eta}\times V^s(q,\, p_0-p_0'), \qquad (20)$$

$$A(\epsilon,\epsilon')=(2m_b)^{1/2}/\hbar\,|\,(\epsilon+\epsilon_F)^{1/2}-(\epsilon'+\epsilon_F)^{1/2}\,|\,,$$

and

$$B(\epsilon,\epsilon')=(2m_b)^{1/2}/\hbar\,|\,(\epsilon+\epsilon_F)^{1/2}+(\epsilon'+\epsilon_F)^{1/2}\,|\,.$$

We see that instantaneous interactions do not contribute to $Z(\epsilon,p_0)$, and their effects are completely accounted for in the normal state by $\chi(\epsilon,p_0)$. This indicates that as the ratio $\hbar\omega_{\rm ph}/\epsilon_F$ increases, the relative importance of χ increases.

The term in Eq. (10) proportional to τ_3 gives

$$\chi(\epsilon,p_0)=\chi_B(\epsilon)+\int_{-\epsilon_F}^{\hbar\omega_{\rm cb}-\epsilon_F}\frac{d\epsilon'}{Z(\epsilon')}K_\chi(\epsilon,\epsilon',p_0)\times\frac{\tilde\epsilon(\epsilon')}{Z(\epsilon')E(\epsilon')}, \qquad (21)$$

where $\chi_B(\epsilon')$ is the contribution of the bare Coulomb interaction to $\chi(\epsilon,p_0)$.

$$\chi_B(\epsilon)=-\frac{e^2m_b}{\pi\hbar\kappa_\infty[2m_b(\epsilon+\epsilon_F)]^{1/2}}\times\int_{-\epsilon_F}^{\hbar\omega_{\rm cb}-\epsilon_F}\frac{d\epsilon'}{Z(\epsilon')}\left[1-\frac{\tilde\epsilon(\epsilon')}{Z(\epsilon')E(\epsilon')}\right]\times\ln\left|\frac{(\epsilon+\epsilon_F)^{1/2}+(\epsilon'+\epsilon_F)^{1/2}}{(\epsilon+\epsilon_F)^{1/2}-(\epsilon'+\epsilon_F)^{1/2}}\right| \qquad (22)$$

and

$$K_\chi(\epsilon,\epsilon',p_0)=\frac{i\Omega m_b}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\times\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}qdq\int_{-\infty}^{\infty}dp_0'\frac{E(\epsilon')}{(p_0')^2-E(\epsilon')^2+i\eta}\times V^s(q,\, p_0-p_0'). \qquad (23)$$

From the τ_1 component of Eq. (10) we obtain

$$\Delta(\epsilon,p_0)=-\frac{1}{Z(\epsilon,p_0)}\int_{-\epsilon_F}^{\hbar\omega_{cb}-\epsilon_F}\frac{d\epsilon'}{Z(\epsilon')}\frac{\Delta(\epsilon')}{E(\epsilon')}K_\Delta(\epsilon,\epsilon',p_0), \quad (24)$$

where

$$K_\Delta(\epsilon,\epsilon',p_0)=\frac{i\Omega m_b}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\times\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}qdq\int_{-\infty}^{\infty}dp_0'\frac{E(\epsilon')}{(p_0')^2-E(\epsilon')^2+i\eta}\times V(q,p_0-p_0'). \quad (25)$$

If $V(q,p_0-p_0')$ is taken to be independent of p_0 and p_0', the integral over p_0' in Eq. (25) may be accomplished, leading to a kernel $K_\Delta(\epsilon,\epsilon')$ of the form given in Ref. (1). The correct form of the nonretarded interaction $V(q)$ is not obtained, however.

To obtain the superconducting energy gap, we must solve Eqs. (19), (21), and (24) simultaneously for Z, χ, and Δ. When $\Delta\ll\epsilon_F$, as is usually the case, we may approximate Eqs. (20) and (23) by taking $\Delta=0$ inside the integrals. The kernels K_Z and K_χ then become independent of Δ, and $Z(\epsilon,p_0)$ and $\chi(\epsilon,p_0)$ can be determined independent of Δ. Equation (23) is then a single integral equation for $\Delta(\epsilon,p_0)$.

When $\Delta\ll\epsilon_F$ the term $\{1-[\tilde{\epsilon}(\epsilon')/Z(\epsilon')E(\epsilon')]\}$ in Eq. (22) for χ_B becomes $[1-\mathrm{sgn}(\tilde{\epsilon}(\epsilon'))]$ and Eq. (22) becomes

$$\chi_B(\epsilon)\cong-\frac{2e^2m_b}{\pi\hbar\kappa_\infty[2m_b(\epsilon+\epsilon_F)]^{1/2}}\times\int_{-\epsilon_F}^{\epsilon_m}\frac{d\epsilon'}{Z(\epsilon')}\ln\left|\frac{(\epsilon+\epsilon_F)^{1/2}+(\epsilon'+\epsilon_F)^{1/2}}{(\epsilon+\epsilon_F)^{1/2}-(\epsilon'+\epsilon_F)^{1/2}}\right|, \quad (26)$$

where ϵ_m is the solution to the equation $\epsilon'+\chi(\epsilon')=0$. In the weak-coupling limit, $\chi(\epsilon_F)\ll\epsilon_F$ and $\epsilon_m\approx0$, and χ_B becomes the Hartree-Fock energy of the electron gas.

$$\chi_B(\epsilon')\approx\chi_B{}^0(\epsilon')=-\frac{e^2}{2\pi\kappa_\infty}\left(2k_F+\frac{k_F^2-k^2}{k}\ln\left|\frac{k+k_F}{k-k_F}\right|\right). \quad (27)$$

If the total interaction is weak, we may approximate Z and χ by their weak-coupling limit, obtained by taking $Z(\epsilon')=1$ and $\chi(\epsilon')=0$ in the equations for K_Z, K_χ, $Z(\epsilon,p_0)$, and $\chi(\epsilon,p_0)$. If the total interaction is very weak, we may set $Z(\epsilon')=1$ and $\chi(\epsilon')=0$ in the equations for $\Delta(\epsilon,p_0)$ and Eqs. (24) and (25).

We will next simplify the kernels $K_\chi(\epsilon,\epsilon',p_0)$, $K_\Delta(\epsilon,\epsilon',p_0)$, and $K_Z(\epsilon,\epsilon',p_0)$. We will consider two methods for this simplification, one of which will be more accurate than the other. Which method is more accurate will depend on which normal state properties are known to a higher degree of accuracy.

The first method is to expand the total interaction $V(q,p_0-p_0')$ in a spectral weight function and then perform the p_0' integration in the equations for the kernels. This will be appropriate when the total interaction, or equivalently, the total dielectric function including phonon contributions is known.

The second method is to divide the interactions into screened Coulomb and screened phonon parts. This method is useful when the total dielectric function is not known but the phonon spectral weight function is known or can be approximated.

A. Kernels Using Total Interaction

We will begin by considering the kernels when the total dielectric function is known. We then have

$$V(q,p_0-p_0')=4\pi e^2/\Omega q^2\kappa_T(q,p_0-p_0'), \quad (28)$$

where

$$\kappa_T(q,p_0-p_0')=\kappa_{ph}(q,p_0-p_0')+\kappa_e(q,p_0-p_0')-\kappa_\infty(q) \quad (29)$$

is the total dielectric function. The function $\kappa_{ph}(q,p_0-p_0')$ is the dielectric function of the crystal with no electrons in the conduction band, and it may be measured in the undoped crystal; $\kappa_{ph}(q,p_0-p_0')$ arises from the motion of the ions and the polarizability of the ion cores, which include electrons in the valence band. The electronic function $\kappa_e(q,p_0-p_0')$ is the dielectric function of the crystal when the ions are rigid, that is, the dielectric function arising from electrons in the conduction band plus those in the valence band, while $\kappa_\infty(q)$ is the dielectric function of electrons in the valence band only. The approximations involved in Eqs. (28) and (29) are discussed in the Appendix.

The function $\kappa_\infty/\kappa_T(q,p_0-p_0')$ may be expanded in terms of a spectral weight function,

$$\frac{\kappa_\infty}{\kappa_T(q,p_0-p_0')}=1+\int_0^\infty F(q,\omega)\left(\frac{1}{p_0-p_0'-\omega+i\delta}-\frac{1}{p_0-p_0'+\omega-i\delta}\right)d\omega, \quad (30)$$

where $F(q,\omega)$ is given by

$$F(q,\omega)=-(1/\pi)\,\mathrm{Im}\left[\frac{\kappa_\infty}{\kappa_T(q,\omega)}\right], \quad (31)$$

since we only need $F(q,\omega)$ for $\omega>0$. We note that a special case of Eq. (30) is

$$\frac{\kappa_\infty}{\kappa_T(q,0)}=1-\int_0^\infty\frac{F(q,\omega)}{\omega}2d\omega \quad (32)$$

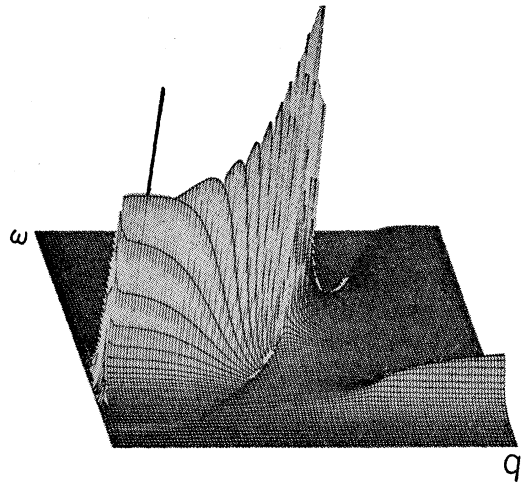

FIG. 3. Spectral weight function $F(q,\omega)$ for a degenerate polar material having one optically-active phonon mode. Parameters used were $\kappa_0=20$, $\kappa_\infty=5$, $m_b=2.5m_e$, $\nu=3$, $\omega_\lambda=0.1$ eV, electron concentration $n=10^{20}$ cm^{-3}, transverse optic phonon frequency $\omega_t=0.05$ eV, damping $\gamma=0.03$ eV. The plasma frequency $\hbar\omega_p=(4\pi ne^2/m_b\kappa_\infty)^{1/2}=0.105$ eV. Only intravalley interactions are shown. Note that using these parameters for small wave vector q the high-frequency branch of the coupled phonon plasmon modes is important, while for large q the phonon mode screened by single-particle excitations is important. All modes are damped in the region $\hbar(q^2-2qk_F)<2m_b\omega<\hbar(q^2+2qk_F)$. The maximum of q shown is $5.127k_F$, $k_F=0.996\times10^7$ cm^{-1}. The maximum value of ω shown is 0.4149 eV. The viewing angles are 60° from the perpendicular to the plane and 255° from the q axis.

and we may rewrite Eq. (30) as

$$\frac{\kappa_\infty}{\kappa_T(q,\,p_0-p_0')}=\frac{\kappa_\infty}{\kappa_T(q,0)}+\int_0^\infty F(q,\omega)\left(\frac{1}{p_0-p_0'-\omega+i\delta}-\frac{1}{p_0-p_0'+\omega-i\delta}+\frac{2}{\omega}\right)d\omega. \quad (33)$$

We also note from Eqs. (17), (28), and (30) that

$$V^S(q,\,p_0-p_0')=V_c^B(q)\int_0^\infty F(q,\omega)\left(\frac{1}{p_0-p_0'-\omega+i\delta}-\frac{1}{p_0-p_0'+\omega-i\delta}\right)d\omega. \quad (34)$$

Equation (34) may be used in Eqs. (20) and (23) to simplify K_Z, K_χ, and K_Δ. After performing the p_0' integration, we obtain

$$K_Z=-\frac{\Omega m_b\pi}{p_0(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dq\,qV_c^B(q)\times\int_0^\infty d\omega\,F(q,\omega)\left(\frac{1}{p_0-E(\epsilon')-\omega+i\eta}+\frac{1}{p_0+E(\epsilon')+\omega-i\eta}\right), \quad (35)$$

$$K_\chi=\frac{\Omega m_b\pi}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dq\,qV_c^B(q)\times\int_0^\infty d\omega\,F(q,\omega)\left(\frac{1}{p_0-E(\epsilon')-\omega+i\eta}-\frac{1}{p_0+E(\epsilon')+\omega-i\eta}\right), \quad (36)$$

and

$$K_\Delta=\frac{\Omega m_b\pi}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dq\,qV_c^B(q)\times\left\{1+\int_0^\infty d\omega\,F(q,\omega)\left(\frac{1}{p_0-E(\epsilon')-\omega+i\eta}-\frac{1}{p_0+E(\epsilon')+\omega-i\eta}\right)\right\}. \quad (37)$$

Or we may use Eq. (33) to obtain

$$K_\Delta=\frac{\Omega m_b\pi}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dq\,qV_c^B(q)\times\left[\frac{\kappa_\infty}{\kappa_T(q,0)}+\int_0^\infty d\omega\,F(q,\omega)\left(\frac{1}{p_0-E(\epsilon')-\omega+i\eta}-\frac{1}{p_0+E(\epsilon')+\omega-i\eta}+\frac{2}{\omega}\right)\right]. \quad (38)$$

Equation (38) is included not only because it may provide a more accurate method for calculating K_Δ, but also because the integral over $F(q,\omega)$ gives an estimate of the importance of the frequency dependence of the interaction.

We have obtained equations for Δ, Z, and χ in terms of a spectral weight function $F(q,\omega)$ which is obtained directly from the total dielectric function $\kappa_T(q,\omega)$. If the phonon contribution to the total dielectric constant can be measured in the absence of carriers, $\kappa_T(q,\omega)$ can be obtained by adding to this the electronic polarizability calculated in the random-phase approximation, which is equivalent to the self-consistent-field approach.[19] If, in addition, the electronic wave functions are taken to be plane waves, the polarizability has the form given by Lindhard.[20] An example of a case in which $\kappa_{ph}(0,\omega)$ has been measured is $SrTiO_3$.[21]

A study of $F(q,\omega)$ is informative, because it reveals the frequency and strength of the coupled phonon and plasma modes with which the electron interacts as a function of wave vector (see Fig. 3).

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B. Kernels Using Coulomb Interaction Plus Phonon Interaction

For cases in which the total dielectric function is not known, but for which the electron-phonon coupling can be estimated, we must divide the interaction into a Coulomb interaction and a phonon interaction. We must, however, keep these interactions on the same footing since the condition $\omega_p \gg \omega_{ph}$ does not hold.

We therefore divide the total interaction into Coulomb and phonon parts, using Eq. (8). The corresponding kernels K_Z, K_χ, and K_Δ may also be divided into Coulomb and phonon parts. We note that the Coulomb contribution to the kernel is easily obtained from previous results for the total kernels using the total interaction, if we replace $F(q,\omega)$, as defined in Eq. (31), by

$$F_c(q,\omega) = -(1/\pi)\,\mathrm{Im}[\kappa_\infty/\kappa_e(q,\omega)] \tag{39}$$

and replace $\kappa_T(q,\omega)$ by $\kappa_e(q,\omega)$ everywhere. Equation (33) is then especially interesting because it separates the electronic screening into the appropriate screening for the case $\omega_{ph} \ll \omega_p$ and a correction term arising from the frequency dependence of the screening. The Coulomb contribution to the kernels $K_Z{}^c$, $K_\chi{}^c$, and $K_\Delta{}^c$ are then given by Eqs. (35)–(38) when the replacement of F by F_c and κ_T by κ_c is made. χ_B, which is caused by Coulomb effects, is left unchanged.

Having obtained the Coulomb contributions to the kernels, we will next obtain the phonon contributions. For the phonon contributions we see that in order to perform the p_0' integrations we must expand both the phonon propagator $D_\lambda(q, p_0 - p_0')$ and the screened interaction $\{\{\bar{g}_\lambda(q, p_0 - p_0')\}\}^2$ in terms of spectral weight functions. Even after the p_0' integration has been done, we will still have three integrals to perform to obtain the kernels. We will find, however, that in many cases we may approximate the phonon spectral weight function in order to reduce the number of integrals to two.

We expand the phonon propagator as

$$D_\lambda(q, p_0 - p_0') = \int_0^\infty B_\lambda(q,\omega)\left(\frac{1}{p_0 - p_0' - \omega + i\delta} - \frac{1}{p_0 - p_0' + \omega - i\delta}\right) \tag{40}$$

and

$$B_\lambda(q,\omega) = -(1/\pi)\,\mathrm{Im}D_\lambda(q,\omega)\,\mathrm{sgn}\omega. \tag{41}$$

The screened phonon coupling is

$$\{\{\bar{g}_\lambda(q, p_0 - p_0')\}\}^2 = \frac{g_\lambda(q) g_\lambda(-q)}{[\kappa_e(q, p_0 - p_0')/\kappa_\infty]\{\kappa_e[-q, -(p_0 - p_0')]/\kappa_\infty\}}. \tag{42}$$

Since we have inversion symmetry, $g(q)g(-q) = |g_\lambda(q)|^2$ and $\kappa_e(q, p_0 - p_0') = \kappa_e[-q, -(p_0 - p_0')]$. We use the spectral weight function for $\kappa_\infty{}^2/\kappa_e(q,q_0)^2$, i.e.,

$$\frac{\kappa_\infty{}^2}{\kappa_e(q,q_0)^2} = 1 + \int_0^\infty F_c'(q,\omega)\left(\frac{1}{q_0 - \omega + i\delta} - \frac{1}{q_0 + \omega - i\delta}\right)d\omega, \tag{43}$$

or we may write

$$\frac{\kappa_\infty{}^2}{\kappa_e(q,q_0)^2} = \frac{\kappa_\infty{}^2}{\kappa_e(q,0)^2} + \int_0^\infty F_c'(q,\omega)\left(\frac{1}{q_0 - \omega + i\delta} - \frac{1}{q_0 + \omega - i\delta} + \frac{2}{\omega}\right), \tag{44}$$

where

$$\mathrm{Im}[\kappa_\infty{}^2/\kappa_e(q,q_0)^2] = -\pi F_c'(q,q_0)\,\mathrm{sgn}q_0. \tag{45}$$

Using Eqs. (40) and (43), we obtain

$$K_\chi(\epsilon,\epsilon',p_0)_{ph} = K_\Delta(\epsilon,\epsilon',p_0)_{ph} = \frac{i\Omega m_b}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')} dqq \sum_\lambda \int_0^\infty d\omega' B_\lambda(q,\omega')$$
$$\times \int_{-\infty}^{\infty} dp_0'\left(\frac{E(\epsilon')}{p_0'^2 - E(\epsilon')^2 + i\eta}\right)\left(\frac{1}{p_0 - p_0' - \omega' + i\delta} - \frac{1}{p_0 - p_0' + \omega' - i\delta}\right)|g_\lambda(q)|^2\left[\left(\frac{\kappa_\infty}{\kappa_e(q,0)}\right)^2 + \int_0^\infty F_c'(q,\omega)\left(\frac{1}{p_0 - p_0' - \omega + i\delta} - \frac{1}{p_0 - p_0' + \omega - i\delta} + \frac{2}{\omega}\right)d\omega\right]. \tag{46}$$

We may again evaluate the p_0' integral by closing either above or below. Since poles now arise from the phonon propagator as well as from the Green's function and the screening, the integrals are slightly more tedious than in

the Coulomb case, but they are straightforward. We obtain

$$K_\chi(\epsilon,\epsilon',p_0)_{\rm ph}=K_\Delta(\epsilon,\epsilon',p_0)_{\rm ph}=\frac{\Omega m_b\pi}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dqq\sum_\lambda|g_\lambda(q)|^2\int_0^\infty d\omega' B_\lambda(q,\omega')$$
$$\times\left\{\frac{\left[\left(\frac{\kappa_\infty}{\kappa_e(q,0)}\right)^2+\int_0^\infty F_c'(q,\omega)\frac{2\omega'[p_0-E(\epsilon')]}{\omega(\omega+\omega')[p_0-E(\epsilon')-\omega+i\eta']}d\omega\right]}{[p_0-E(\epsilon')-\omega'+i\eta]}\right.$$
$$\left.-\frac{\left[\left(\frac{\kappa_\infty}{\kappa_e(q,0)}\right)^2+\int_0^\infty F_c'(q,\omega)\frac{2\omega'[p_0+E(\epsilon')]}{\omega(\omega+\omega')[p_0+E(\epsilon')+\omega-i\eta']}d\omega\right]}{[p_0+E(\epsilon')+\omega'-i\eta]}\right\}. \quad (47)$$

The form of Eq. (47) is quite interesting. As mentioned previously, the integrals over $F_c'(q,\omega)$ give the frequency dependence of the screening, and for the case of the low-electron-density systems considered here ($\epsilon_F<\hbar\omega_{\rm ph}$), represent a large modification of the first term $(\kappa_\infty/\kappa_e(q,0)^2$ which is the dominant term in the high-electron-density system. We see also, however, that the Eliashberg form for the kernel still appears in the denominator of the two terms. In addition, ω' (which for sharp modes becomes the phonon frequency) appears in the integrand of the integral over ω, so that the frequency of the phonon modes determines the importance of the inclusion of the frequency dependence of the dielectric function. We see that as ω' approaches zero, the high-density limit is reached.

We may write Eq. (47) in a more symmetric form by including the zero frequency screening in the integral over ω. We then have

$$K_\chi(\epsilon,\epsilon',p_0)_{\rm ph}=K_\Delta(\epsilon,\epsilon',p_0)_{\rm ph}=\frac{\Omega m_b\pi}{(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dqq\sum_\lambda|g_\lambda(q)|^2\int_0^\infty d\omega' B_\lambda(q,\omega')$$
$$\times\frac{\left\{1+\int_0^\infty d\omega F_c'(q,\omega)\left[\frac{2[p_0-E(\epsilon')-\omega-\omega']}{(\omega+\omega')[p_0-E(\epsilon')-\omega+i\eta']}\right]\right\}}{[p_0-E(\epsilon')-\omega'+i\eta]}-\frac{\left\{1+\int_0^\infty d\omega F_c'(q,\omega)\left[\frac{2[p_0+E(\epsilon')+\omega+\omega']}{(\omega+\omega')[p_0+E(\epsilon')+\omega-i\eta']}\right]\right\}}{[p_0+E(\epsilon')+\omega'-i\eta]}. \quad (48)$$

We note that if screening is neglected, and the weak-coupling limit is used ($Z=1$, $\chi=0$), and the Coulomb interaction is omitted, the gap equation obtained from Eqs. (48) and (24) is equivalent to that obtained by Liu,[22] when $\Delta(\epsilon,p_0)$ is evaluated at $p_0=\pm E(\epsilon)$.

The phonon contribution to $K_Z(\epsilon,\epsilon',p_0)$ may be calculated in the same way:

$$K_Z(\epsilon,\epsilon',p_0)_{\rm ph}=-\frac{i\Omega m_b}{p_0(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dqq\sum_\lambda|g_\lambda(q)|^2$$
$$\times\int_0^\infty d\omega' B_\lambda(q,\omega')\int_{-\infty}^\infty dp_0'\left(\frac{p_0'}{(p_0')^2-E(\epsilon')^2+i\eta}\right)\left(\frac{1}{p_0-p_0'-\omega'+i\delta}-\frac{1}{p_0-p_0'+\omega'-i\delta}\right)$$
$$\times\left[\left(\frac{\kappa_\infty}{\kappa_e(q,\omega)}\right)^2+\int_0^\infty F_c'(q,\omega)\left(\frac{1}{p_0-p_0'-\omega+i\delta}-\frac{1}{p_0-p_0'+\omega-i\delta}+\frac{2}{\omega}\right)d\omega\right]. \quad (49)$$

After integration over p_0' one obtains

$$K_Z(\epsilon,\epsilon',p_0)_{\rm ph}=-\frac{\Omega m_b\pi}{p_0(2\pi)^3\hbar[2m_b(\epsilon+\epsilon_F)]^{1/2}}\int_{A(\epsilon,\epsilon')}^{B(\epsilon,\epsilon')}dqq\sum_\lambda|g_\lambda|^2\int_0^\infty d\omega' B_\lambda(q,\omega')$$
$$\times\left\{\frac{\left[\left(\frac{\kappa_\infty}{\kappa_e(q,0)}\right)^2+\int_0^\infty F_c'(q,\omega)\frac{2\omega'[p_0-E(\epsilon')]}{\omega(\omega+\omega')[p_0-E(\epsilon')-\omega+i\eta]}d\omega\right]}{[p_0-E(\epsilon')-\omega'+i\eta]}\right.$$
$$\left.+\frac{\left[\left(\frac{\kappa_\infty}{\kappa_e(q,0)}\right)^2+\int_0^\infty F_c'(q,\omega)\frac{2\omega'[p_0+E(\epsilon')]}{\omega(\omega+\omega')[p_0+E(\epsilon')+\omega-i\eta]}d\omega\right]}{[p_0+E(\epsilon')+\omega-i\eta]}\right\}. \quad (50)$$

[22] S. H. Liu, Phys. Rev. **125**, 1244 (1962).

Again $K_Z(\epsilon,\epsilon',p_0)$ is not singular as p_0 approaches zero since the two terms in the integral approach zero as p_0 approaches zero so that the complete term is finite as p_0 approaches zero.

We also note the similarity between Eqs. (50) and (47). Just as in the high-electron-density case, the only difference is the sign of one of the two terms in the phonon kernel. The modifications of the screening are the same for all kernels.

When $\epsilon_F \ll \hbar\omega_{\rm ph}$ and $\epsilon_F \ll \hbar\omega_p$, all equations derived in this section may be evaluated at $p_0=\pm E(\epsilon)$, leading to a nonretarded gap equation. The correct nonretarded "interaction" has therefore been obtained. See Eqs. (37) and (48).

For a many-valley semiconductor (see Ref. 1) all integrals over wave vector q are separated into different regions of momentum space: the large-wave-vector intervalley processes and the smaller-wave-vector intravalley processes. The procedures for obtaining the intervalley and intervalley parts outlined earlier[1] for the case of the modified Bardeen-Cooper-Schrieffer equation hold also in the present case.

In particular, all equations derived in this section hold for a many-valley degenerate semiconductor if the following modifications are made. First, all kernels are the sum of intervalley and intravalley contributions. The intravalley contributions have the form derived above if it is understood that $k_F=(3\pi^2 n/\nu)^{1/3}$ when n is the total carrier concentration and ν is the number of valleys. For the intervalley contribution, an over-all factor of $(\nu-1)$ multiplies all kernels. Also, the bare Coulomb interaction is given by

$$V_c{}^B(q)^{er}=4\pi e^2/\Omega q_0{}^2\kappa_\infty{}^{er}, \tag{51}$$

where q_0 is the wave-vector separation between valleys.

For practical calculations we will want to express the electron-phonon coupling for intravalley processes in terms of the polaron coupling α_λ, and express the electron-phonon coupling for intervalley processes in terms of the deformation potential ξ. For intravalley modes we have

$$|g_\lambda(q)|^2=[4\pi(\hbar\omega_\lambda)^2/\Omega q^2(2m^*\omega_\lambda/\hbar)^{1/2}]\alpha_\lambda, \tag{52}$$

where ω_λ is the bare phonon frequency of the λth mode.

For intervalley modes, the deformation potential ξ as defined in Ref. 1 can also be obtained in terms of $g_\lambda(q)$, where λ refers to the intervalley phonon mode. In the notation of Ref. 1, the electron-phonon coupling was expressed in terms of the matrix element M_q. We have

$$|M_q|^2=|g_{er}(q)|^2 \tag{53}$$

and

$$\xi^2=\frac{2MN\hbar\omega_{er}}{\alpha\hbar^2q_0{}^2}|g_{er}(q)|^2. \tag{54}$$

Here, α is the degeneracy of the phonon mode and ω_{er} is the frequency of the intervalley mode. The phonon spectrum for intervalley modes is well approximated by an Einstein spectrum, and $B_\lambda(q,\omega)^{er}\approx\delta(\omega-\omega_\lambda)$. We also note that the contribution of intervalley interactions to χ_B are obtained using Eq. (51) rather than Eq. (18) for $V_c{}^B(q)$ so that Eq. (22) must be modified for intervalley contributions to χ_B. It can then be seen that the intervalley contribution to χ_B is a constant independent of wave vector or energy:

$$\chi_B{}^{er}=-(\nu-1)4e^2k_F{}^3/3\pi\kappa_\infty{}^{er}q_0{}^2. \tag{55}$$

$\chi_B{}^{er}$ will be much less than $\chi_B{}^{ra}$ since $k_F \ll q_0$.

It is instructive to consider the phonon contributions to $\chi(\epsilon,p_0)$ and $Z(\epsilon,p_0)$ in the low-density limit $\epsilon_F\to 0$. We consider a normal material $[\Delta(\epsilon,p_0)=0]$ in the weak-coupling limit $\alpha_\lambda \ll 1$. We consider only intravalley coupling to longitudinal optic phonons and neglect Coulomb interactions between electrons, and therefore screening. Using Eqs. (48) and (21) with $B_\lambda(q,\omega')=\delta(\omega'-\omega_\lambda)$, $\hbar\omega_{ob}\to\infty$, and $F_c'(q,\omega)=0$, we obtain

$$\chi(\epsilon,p_0)=-\tfrac{1}{2}\alpha_\lambda\hbar\omega_\lambda\left(\frac{\hbar\omega_\lambda}{\epsilon}\right)^{1/2}\left\{\pi-\tan^{-1}\left[\left(\frac{\hbar\omega_\lambda+p_0}{\epsilon}\right)^{1/2}\right]-\tan^{-1}\left[\left(\frac{\hbar\omega_\lambda-p_0}{\epsilon}\right)^{1/2}\right]\right\}, \tag{56}$$

when $p_0<\hbar\omega_\lambda$. Also, using Eqs. (50) and (19), we obtain

$$Z(\epsilon,p_0)=1+\frac{\alpha_\lambda\hbar\omega_\lambda}{2p_0}\left(\frac{\hbar\omega_\lambda}{\epsilon}\right)^{1/2}\left\{\tan^{-1}\left[\left(\frac{\hbar\omega_\lambda+p_0}{\epsilon}\right)^{1/2}\right]-\tan^{-1}\left[\left(\frac{\hbar\omega_\lambda-p_0}{\epsilon}\right)^{1/2}\right]\right\}, \tag{57}$$

when $p_0<\hbar\omega_\lambda$. The renormalized quasiparticle energy $E_N=(\epsilon+\chi)/Z$ can then be obtained from Eqs. (56) and (57).

If we expand Eq. (56) for small ϵ and p_0 and keep only linear terms, we obtain[32]

$$\chi(\epsilon)\approx-\alpha_\lambda\hbar\omega_\lambda+\tfrac{1}{3}\alpha_\lambda\epsilon. \tag{58}$$

Expanding Eq. (57) we obtain

$$Z(\epsilon)\approx 1+\tfrac{1}{2}\alpha_\lambda-\tfrac{1}{2}\alpha_\lambda(\epsilon/\hbar\omega_\lambda) \tag{59}$$

and keeping only linear terms in α_λ we obtain[23]

$$E_N-\epsilon\approx-\alpha_\lambda\hbar\omega_\lambda-\tfrac{1}{6}\alpha_\lambda\epsilon, \tag{60}$$

which is the usual weak-coupling polaron result obtained by consideration of a single electron interacting with longitudinal optic phonons to first order in perturbation theory. Equation (60) yields

$$1/m^*\approx(1/m_b)(1-\tfrac{1}{6}\alpha_\lambda), \tag{61}$$

where m^* is the renormalized effective mass.

We can now compare the relative contributions of $\chi(\epsilon)$ and $Z(\epsilon)$ to the renormalization of the mass. From

[23] Note that $\alpha_\lambda\omega_\lambda{}^{-1.5}$ and $\alpha_\lambda\to 0$ as $\omega_\lambda\to\infty$, so that $z(\epsilon)=1$ for instantaneous interactions ($\omega_\lambda\to\infty$). Also, $x(\epsilon)\to 0$, because we have taken $\epsilon_F=0$.

Eqs. (58) and (59) we see that $\chi(\epsilon)$ has contributed a term $+\frac{1}{3}\alpha_\lambda$ and $Z(\epsilon)$ has contributed a term $-\frac{1}{2}\alpha_\lambda$. The contributions from χ and Z therefore tend to cancel, and in the low-density limit the cancellation is two-thirds complete. The partial cancellation of effects from χ and Z occurs for all values of the Fermi energy, but as the Fermi energy increases the relative contribution from χ becomes less important.

We also note that no linear terms in p_0 appear in Eqs. (58) and (59) since χ and Z are even in p_0. This result confirms our original approximation, that for $\epsilon_F<\hbar\omega_{\rm ph}$ the variation of χ, Z, and Δ with ϵ is more important than their variation with p_0.

APPENDIX

The electron-electron interaction in a degenerate polar material with any number of optically active phonon modes may be calculated using a random-phase approximation, that is, excluding vertex corrections. We will show that this interaction is exactly the same as that obtained by dividing the bare Coulomb interaction by one plus the sum of polarizabilities from electrons in the valence band plus those in the conduction band plus the polarizability of the lattice.

We will find that the total electron-electron interaction may be separated into an electron-electron interaction plus an electron-electron interaction through the phonon field for a system having only one optically active phonon mode. The interaction through the phonon field is different from the interaction given in a recent paper[24] and we therefore believe the interaction given in Ref. 23 to be incorrect.

For a material with more than one optically active phonon mode, the presence of electrons in the conduction band couples the modes so that the total interaction cannot be separated into an electron-electron interaction plus a sum of independent interactions through the separate phonon branches.

We will consider all frequencies involved, bare phonon frequencies ω_λ, and plasma frequencies ω_p, to be much less than the band gap between the valence band and the conduction band. Therefore, the polarizability of the electrons in the valence band is included in the bare electron–electron interaction $V_c{}^B(q)$ given in Eq. (18) and in the bare electron–phonon coupling $g_\lambda(q)$ and in the bare phonon frequency $\omega_\lambda(q)$. The bare phonon propagator

$$D_{\lambda_0}=2\omega_\lambda/(\omega^2-\omega_\lambda{}^2) \tag{A1}$$

is the propagator of phonons in the system with no electrons in the conduction band. The bare frequencies ω_λ are then measured in the undoped crystal.

We will consider the set of all diagrams connecting electron propagators which have no crossed diagrams and no modifications of the electronic polarizability. If there is one longitudinal phonon mode to which the electron may couple, we have the set of diagrams shown in Fig. 4. These diagrams are equivalent to the diagrams included in the Dyson equation shown in Fig. 5, used by Pines.[25]

For two phonon modes interacting with the electrons in the conduction band, we have the Dyson equation shown in Fig. 6. The generalization to more phonon modes is straightforward.

By defining

$$V_T{}^B=V_c{}^B+\sum_\lambda g_\lambda{}^2 D_{\lambda_0}, \tag{A2}$$

we obtain from the Dyson equation of Fig. 5

$$V=V_T{}^B/(1+PV_T{}^B), \tag{A3}$$

where P is the polarizability of electrons in the conduc-

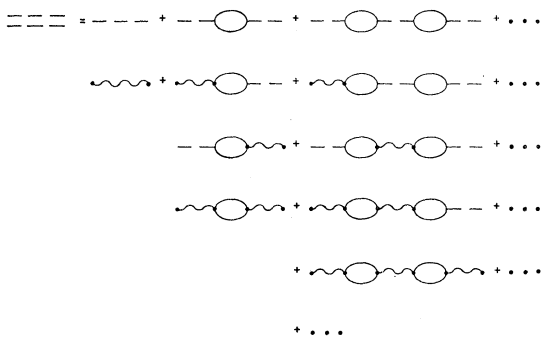

FIG. 4. Diagrams included in the random-phase approximation when only one phonon mode interacts with electrons.

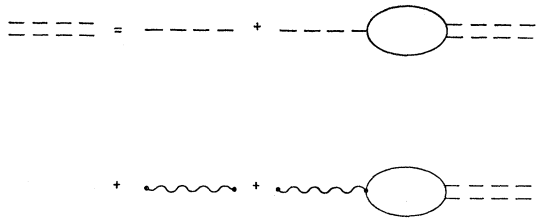

FIG. 5. Dyson equation for random-phase approximation when only one phonon mode interacts with electrons.

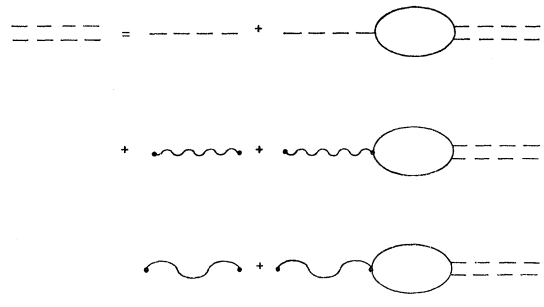

FIG. 6. Dyson equation when two phonon modes interact with electrons. The longer-wavelength wiggle indicates a longer-wavelength phonon.

[24] J. Appel, Phys. Rev. Letters **17**, 1045 (1966).

[25] D. Pines, *The Many-Body Problem* (W. A. Benjamin, Inc., New York, 1962), p. 86.

tion band. We will now show that this equation is the same as that obtained by dividing the bare Coulomb interaction by the total dielectric function.

In the rigid lattice $g_\lambda=0$ and the Coulomb interaction is

$$V_c=V_c^B/(1+PV_c^B)=V_c^B/[\kappa_e(q,\omega)/\kappa_\infty(q)]. \quad \text{(A4)}$$

When no electrons are in the conduction band the interaction is

$$V_{ph}=V_c^B+\sum_\lambda g_\lambda^2 D_{\lambda_0}=\frac{V_c^B}{[\kappa_{ph}(q,\omega)/\kappa_\infty(q)]}, \quad \text{(A5)}$$

where $\kappa_{ph}(q,\omega)$ is the dielectric function of the crystal with no electrons in the conduction band. We therefore have

$$\kappa_e(q,\omega)/\kappa_\infty(q)=1+PV_c^B \quad \text{(A6)}$$

and

$$\kappa_{ph}(q,\omega)/\kappa_\infty=V_c^B/(V_c^B+\sum_\lambda g_\lambda^2 D_{\lambda_0}). \quad \text{(A7)}$$

Using Eq. (A2) in Eq. (A3) we obtain

$$V=(V_c^B+\sum_\lambda g^2 D_{\lambda_0})/(1+PV_c^B+P\sum_\lambda g_\lambda^2 D_{\lambda_0}) \quad \text{(A8)}$$

or

$$V=V_c^B/(1+PV_c^B+[V_c^B/(V_c^B+\sum_\lambda g_\lambda^2 D_{\lambda_0})]-1) \quad \text{(A9)}$$

and

$$V=V_c^B/\{[\kappa_e(q,\omega)/\kappa_\infty]+[\kappa_{ph}(q,\omega)/\kappa_\infty]-1\}. \quad \text{(A10)}$$

And we see that the total interaction may be obtained by dividing the bare Coulomb interaction by the total dielectric constant.

We may separate Eq. (A8) into two terms:

$$V=\frac{V_c^B(q)}{[\kappa_e(q,\omega)/\kappa_\infty(q)]}+\sum_\lambda \frac{\bar{g}_\lambda^2 D_{\lambda_0}}{1+\{1-[\kappa_\infty(q)/\kappa_e(q,\omega)]\}\sum_{\lambda'}(g_{\lambda'}^2 D_{\lambda' 0}/V_c^B)} \quad \text{(A11)}$$

or

$$V=\frac{V_c^B(q)}{[\kappa_e(q,\omega)/\kappa_\infty(q)]}+\sum_\lambda \frac{\bar{g}_\lambda^2 2\omega_\lambda}{\omega^2-\omega_\lambda^2+(\omega^2-\omega_\lambda^2)[1-(\kappa_\infty/\kappa_e)]\sum_{\lambda'}(g_{\lambda'}^2/V_c^B)[2\omega_{\lambda'}/(\omega^2-\omega_{\lambda'}^2)]}, \quad \text{(A12)}$$

where $\bar{g}_\lambda=g_\lambda/(\kappa_e/\kappa_\infty)$. The renormalized phonon frequency is

$$\tilde{\omega}_\lambda^2=\omega_\lambda^2-(\omega^2-\omega_\lambda^2)\left(1-\frac{\kappa_\infty}{\kappa_e(q,\omega)}\right)\sum_{\lambda'}\frac{\bar{g}_{\lambda'}^2}{V_c^B}\frac{2\omega_{\lambda'}}{(\omega^2-\omega_{\lambda'}^2)}, \quad \text{(A13)}$$

and, in general, the frequency of a given renormalized phonon mode depends on all other phonon modes and their coupling to the electrons. When the bare phonon frequencies are widely separated, or when the plasma frequency is very large, the modes are approximately independent.

When the electron interacts with only one longitudinal optic phonon, one obtains

$$\tilde{\omega}_\lambda^2=\omega_\lambda^2-(2\omega_\lambda g_\lambda^2/V_c^B)[1-\kappa_\infty/\kappa_e(q,\omega)]. \quad \text{(A14)}$$

Also, for a system with one optic mode, we have

$$g_\lambda^2=\tfrac{1}{2}V_c^B(q)\kappa_\infty(1/\kappa_\infty-1/\kappa_0)\omega_\lambda, \quad \text{(A15)}$$

where κ_0 is the zero-frequency phonon dielectric function so that

$$V=\frac{V_c^B}{[\kappa_e(q,\omega)/\kappa_\infty(q)]}+\frac{[(1/\kappa_\infty)-(1/\kappa_0)]V_c^B(q)\kappa_\infty\omega_\lambda^2}{[\kappa_e(q,\omega)/\kappa_\infty(q)]^2[\omega^2-\tilde{\omega}_\lambda(q,\omega)^2]} \quad \text{(A16)}$$

and

$$\tilde{\omega}_\lambda(q,\omega)^2=\omega_\lambda^2[\kappa_\infty/\kappa_0+\kappa_\infty/\kappa_e(q,\omega)-\kappa_\infty^2/\kappa_0\kappa_e(q,\omega)]. \quad \text{(A17)}$$

Because of the frequency dependence of $\tilde{\omega}_\lambda(q,\omega)$, the longitudinal modes of the system occur at frequencies that satisfy the equation

$$\tilde{\omega}_\lambda(q,\omega)^2=\omega^2. \quad \text{(A18)}$$

For small q, there will be two solutions corresponding to the coupled phonons and plasmons. For large q there will be only one solution corresponding to phonons screened by single-particle excitations. These modes can be seen in Fig. 3.

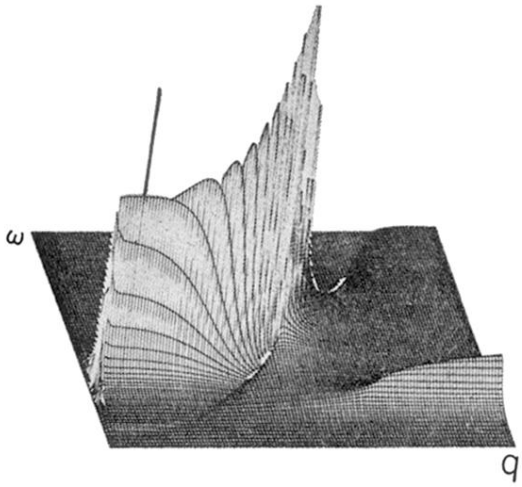

FIG. 3. Spectral weight function $F(q,\omega)$ for a degenerate polar material having one optically-active phonon mode. Parameters used were $\kappa_0=20$, $\kappa_\infty=5$, $m_b=2.5m_e$, $\nu=3$, $\omega_\lambda=0.1$ eV, electron concentration $n=10^{20}$ cm^{-3}, transverse optic phonon frequency $\omega_t=0.05$ eV, damping $\gamma=0.03$ eV. The plasma frequency $\hbar\omega_p=(4\pi ne^2/m_b\kappa_\infty)^{1/2}=0.105$ eV. Only intravalley interactions are shown. Note that using these parameters for small wave vector q the high-frequency branch of the coupled phonon plasmon modes is important, while for large q the phonon mode screened by single-particle excitations is important. All modes are damped in the region $\hbar(q^2-2qk_F)<2m_b\omega<\hbar(q^2+2qk_F)$. The maximum of q shown is $5.127k_F$, $k_F=0.996\times10^7$ cm^{-1}. The maximum value of ω shown is 0.4149 eV. The viewing angles are 60° from the perpendicular to the plane and 255° from the q axis.