Polarons in Degenerate Semiconductors

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The second-order self-energies of an electron in a degenerate Fermi gas arising from polar coupling to longitudinal optic phonons and from both piezoelectric and deformation-potential coupling to (Debye) acoustic phonons are evaluated exactly and analytically. Numerical calculations of the resulting density of states for optical phonons exhibit logarithmic singularities at the Fermi energy μ and at $\mu+\omega_0$. Similar structure due to the electron's interaction with acoustical phonons is exhibited by the proper self-energy but is smoothed out in the density of states by the nonvanishing imaginary part of the self-energy. The singularities at the Fermi surface are removed by the random-phase-approximation screening of the electron-phonon interaction due to mobile charge carriers. These results indicate that several proposed explanations for low-bias conductance anomalies in tunnel diodes are inapplicable.

I. INTRODUCTION

TUNNELING experiments, originally introduced in semiconductors and given new impetus by the reported work on the tunnel diode by Esaki,[1] have been utilized extensively to study the bulk properties of other materials, notably superconductors. Despite their success in probing the modifications in the density of states of superconductors wrought by many-body effects, the analysis of tunneling experiments in semiconductors has been confined to independent-particle models of the tunneling process.[2] However, no satisfactory explanation, based on any models, has been proposed for the anomalously low conductance near zero bias in tunnel diodes, originally observed by Hall, Racette, and Ehrenreich,[3] and more recently studied by several other workers.[4,5]

The original interpretation[3] of these anomalies attributed them to the polar interaction between the electron and optical phonons. It was argued that, if α denotes the polar-interaction coupling constant and ω_0 the longitudinal optic (LO) phonon energy, then an electron or hole must give up the polaron binding energy $\Sigma_0=\alpha\omega_0$ before tunneling, and a correlation was noted between Σ_0 and the size of the anomaly. This argument is incorrect for several reasons. One reason is that the self-energy of an electron near the Fermi energy in a degenerate semiconductor is not $\alpha\omega_0$. This expression is only appropriate for a single electron in an insulator. For degenerate semiconductors, the electron's self-energy is altered by exclusion-principle effects, and also by the mobile charge screening of the electron-phonon interaction. In Sec. III we give the quantitative calculation of this effect using the dynamic dielectric function evaluated within the random-phase approximation. Secondly, the number of phonons is quantized, so that any energy change of a polarization cloud must be $n\omega_0$, where n is an integer. The argument that Σ_0 must be furnished by the external battery hinges on the assumption that the electron is suddenly removed from one side of the junction to the other. In calculations of the tunneling current based on the usual concepts of perturbation theory, the tunneling process is treated as an energy-conserving one for which questions concerning the rapidity of the transition cannot be precisely defined. Furthermore, such calculations[6] lead to the result that polaron effects cause a decreased current through the junction at all values of the bias and not low-bias anomalies. Therefore, we feel that the original interpretation of the experiments is unsatisfactory.

An alternative explanation of these anomalies is that, in analogy to the description of tunneling in superconductors, they are caused by structure in the density of states on one or both sides of the diode. Even in the absence of a collective initial or final state, if the tunneling probability is a constant, the tunneling differential conductance is proportional to a two-dimensional weighted projection of the joint density of states and thereby reflects structure exhibited by the single-particle density of states. Therefore, we have calculated some of the many-body properties of electrons and holes interacting with phonons in degenerate semiconductors. The self-energies of these quasiparticles interacting with phonons through the polar, piezoelectric, and deformation-potential interactions have been calculated analytically and exactly in second-order perturbation theory. Other authors,[7–9] noting that in metals this is a strong-coupling problem, have attempted to solve a Dyson's equation for the one-electron propagator. However, their models[10] or approximations render the calcu-

[1] L. Esaki, Phys. Rev. **109**, 603 (1957).
[2] See, e.g., R. T. Shuey, Phys. Rev. **137**, A1268 (1965).
[3] R. N. Hall, J. H. Racette, and H. Ehrenreich, Phys. Rev. Letters **4**, 456 (1960); R. N. Hall, in *Proceedings of the International Conference on Semiconductors, Prague, 1960* (Academic Press Inc., New York, 1961), p. 193.
[4] R. A. Logan and J. M. Rowell, Phys. Rev. Letters **13**, 404 (1964).
[5] R. M. Williams and J. Shewchun, Phys. Rev. Letters **14**, 824 (1965); *ibid.* **15**, 160 (1965).
[6] W. A. Harrison and C. B. Duke (unpublished).
[7] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinsky, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1963), Chaps. 2 and 3. This reference is hereafter referred to as AGD.
[8] S. Engelsberg and J. R. Schrieffer, Phys. Rev. **131**, 993 (1963).
[9] T. Holstein, Ann. Phys. (N. Y.) **29**, 410 (1964).
[10] The Engelsberg-Schrieffer and AGD approximations of a constant density of states used in evaluating the one-electron self-energies is in effect a model electron-phonon coupling.

lations equivalent to second order perturbation theory. An outline of this reduction is given in Sec. II of Holstein's paper.[9] Furthermore, as these authors have been primarily concerned with metals, they typically neglect dielectric screening and usually consider just one type of interaction. Their approximations[7–10] concerning the nature of the interaction and the constancy of the density of states may be adequate in metals where the Fermi energy is much larger than the phonon energies. They are not sufficiently accurate in lightly doped degenerate polar semiconductors. Our calculations yield structure in the proper self-energy which would be missed if the standard approximations were employed. Furthermore, we believe that the underlying physics of our model is more soundly based than in metals. In lightly doped degenerate semiconductors, in contrast to the situation in metals, the Debye model adequately describes the acoustical phonon spectrum for those phonons of importance in the self-energy calculations. As the polar and piezoelectric coupling constants are small in III-V compounds, we anticipate that the perturbation-theory results are applicable even in the absence of an explicit Migdal's theorem.[7]

We also investigate the influence of the screening of the electron-phonon vertex[11,12] on the structure in the density of states, and show that the screening eliminates logarithmic singularities predicted at the Fermi energy using the bare vertices.

Keldysh and Kopaev (KK) have advanced an explanation of the conductance anomalies based on logarithmic singularities in the density of states in the bulk semiconductors due to polar electron-phonon interactions.[13] That such singularities may arise in second-order perturbation theory for a system of degenerate fermions interacting via an appropriate vertex through an intermediate boson field is a well-known result.[14] However, as indicated above, we shall show in this paper that a consideration of the effects of the screening of the electron-phonon vertex in the random-phase approximation eliminates the Keldysh-Kopaev singularities.

Further studies by Logan and Rowell[4] of Si and Ge diodes indicate that the conductance anomalies are not confined to polar materials. Williams and Shewchun[5] have emphasized that a wide variety of "anomalies" can occur in the conductance. These anomalies seem quite sensitive to the structure of the particular diodes.[15] Similar phenomena have been observed by Wyatt[16] in Al oxide–Ta junctions. Kim[17] has proposed an explanation based on a magnetic scattering (spin-flip) mechanism suitable for metals. However, there are many possible mechanisms for the anomalies. Kim's explanation needs detailed calculations and comparison with data, and its relevance to semiconductors has not been established.

As the bulk-polaron effects in the density of states do not seem to be the cause of the observed conductance anomalies, we have considered other mechanisms in detail. One of these is the nonlinearities in the tunneling probabilities calculated in the independent-particle models.[18] Although several interesting effects are found, their energy scale is that of the Fermi energies involved, and they cannot account for the narrow zero-bias effects discussed herein.

In Sec. II of this paper we collect the results in the Matsubara formalism needed as a starting point for our calculations. In Secs. III and IV we study the effects of optical and acoustical phonons, respectively, on the density of states. We conclude in Sec. V with a brief summary of our results.

II. FORMALISM

We calculate the density of states of a degenerate electron gas. One interest is in structure caused by interactions with phonons. The lowest order self-energy by perturbation theory is[7,11]

$$\Sigma(p,ip_n)=-T\sum_{\omega_n}\int\frac{d^3q}{(2\pi)^3}\frac{V(q)}{\epsilon^2(\mathbf{q},i\omega_n)}\times\mathfrak{D}(\mathbf{q},i\omega_n)\mathcal{G}^{(0)}(\mathbf{p}+\mathbf{q},\,i\omega_n+ip_n)\,. \quad (2.1)$$

Dielectric screening has been included in shielding the interaction. We use the random-phase-approximation dielectric function arising from electron-electron Coulomb interactions in a medium with a dielectric constant $\epsilon(\infty)$:

$$\epsilon(q,Z)=1+\frac{K_{\mathrm{FT}}^2}{2q^2}\left\{1+\frac{1}{8\epsilon_q^{3/2}\sqrt{\mu}}[4\epsilon_q\mu-(Z-\epsilon_q)^2]\ln\left(\frac{Z-\epsilon_q-2(\epsilon_q\mu)^{1/2}}{Z-\epsilon_q+2(\epsilon_q\mu)^{1/2}}\right)+\frac{1}{8\epsilon_q^{3/2}\sqrt{\mu}}[4\epsilon_q\mu-(Z+\epsilon_q)^2]\ln\left(\frac{Z+\epsilon_q+2(\epsilon_q\mu)^{1/2}}{Z+\epsilon_q-2(\epsilon_q\mu)^{1/2}}\right)\right\}. \quad (2.2)$$

The Fermi energy is denoted by μ, the kinetic energy by $\epsilon_q=q^2/2m$, and the Fermi-Thomas wave vector by $K_{\mathrm{FT}}^2=6\pi ne^2/\epsilon(\infty)\mu$. Equations (2.1) and (2.2) are well known to describe screening in the high-density limit.[11]

[11] A. Ron, Phys. Rev. **132**, 978 (1963).

[12] J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin, Inc., New York, 1964), Chap. 6.

[13] L. V. Keldysh and Yu. V. Kopaev, Fiz. Tverd. Tela **5**, 1411 (1963) [English transl.: Soviet Phys.—Solid State **5**, 1026 (1963)].

[14] In other contexts see, e.g., A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, England, 1953), p. 77; R. Balian and D. R. Fredkin, Phys. Rev. Letters **15**, 480 (1965) (He^3 atoms interacting through zeroth-sound bosons).

[15] J. Conley and J. J. Tiemann (private communication).

[16] A. F. G. Wyatt, Phys. Rev. Letters **13**, 401 (1964); L. Shen and J. M. Rowell, Bull. Am. Phys. Soc. **11**, 224 (1966).

[17] D. J. Kim, Phys. Letters **18**, 215 (1965).

[18] D. J. BenDaniel and C. B. Duke (to be published).

The criterion for the validity of this limit is that $r_S=(9\pi/4)^{1/3}(E_B/\mu)^{1/2}$ be small. For lightly doped n-type III-V semiconductors the shallow-donor binding energy is $E_B\sim 5$ meV and Fermi energies are $\mu\sim 100$ meV. Thus, $r_S\sim\frac{1}{2}$ and Eqs. (2.1) and (2.2) adequately describe the screening. However, for lightly doped p-type III-V semiconductors, $E_B\sim 25$ meV for the heavy-hole band whereas $\mu\sim 30$ meV. Thus $r_S\sim 3$, and the high-density limit is invalid. However, Eq. (2.2) is still valid in the long-wavelength region where the electronic potential energy induced by the phonon is much less than the Fermi energy.

In the random-phase approximation (RPA), the phonon propagator is also screened[11,12]:

$$\mathfrak{D}(q)^{-1}=\mathfrak{D}^{(0)}(q)^{-1}-[V(q)P_0(q)/\epsilon(q)]\,,$$
$$P_0(q)=[2T/(2\pi)^3]\sum_{\omega_n}\int d^3k\mathcal{G}_0(k+q)\mathcal{G}_0(k)\,. \tag{2.3}$$

For a lightly doped semiconductor it is possible to ignore the effects of the electron gas on the phonons, and (2.3) can be approximated by

$$\mathfrak{D}(q)\approx\mathfrak{D}^{(0)}(q)=-2\omega_q/(\omega_n^2+\omega_q^2)\,. \tag{2.4}$$

For acoustical phonons the electron-phonon interaction serves mainly to alter the speed of sound.[19] For optical phonons it makes the LO and TO (transverse optic) phonons nearly degenerate in the long-wavelength limit.[20]

After finding the self-energy, the retarded Green's function is found by making the analytical continuation $ip_n+\mu\rightarrow E+i\delta$, and the spectral function is

$$A(p,E)=-2\,\mathrm{Im}G_{\mathrm{ret}}(p,E)$$
$$=-2\Sigma_I/[(E-\epsilon_p-\Sigma_R)^2+\Sigma_I^2]\,. \tag{2.5}$$

The density of states is

$$\rho(E)=\frac{1}{(2\pi)^3\pi}\int d^3qA(q,E) \tag{2.6}$$

which, in the limit that $\Sigma_I\rightarrow 0$, becomes

$$\rho(E)=\frac{mp(E)/\pi^2\hbar^2}{\left[1+\left(\dfrac{\partial\Sigma_R(p,E)}{\partial\epsilon_p}\right)_{p(E)}\right]} \tag{2.7a}$$

$$E=\epsilon_p+\Sigma_R(p(E),E)\,. \tag{2.7b}$$

The limit $\Sigma_I\rightarrow 0$ occurs at the Fermi surface, but (2.7) is a generally useful approximation near the Fermi energy.

We proceed by doing the Matsubara sum in (2.1):

$$\Sigma(p,ip_n)=\int\frac{d^3q}{(2\pi)^3}V(q)\left\{\frac{N_q}{ip_n+\omega(q)-\epsilon_{p+q}+\mu}\,\mathrm{Re}[\epsilon^{-2}(q,\omega_q)]+\frac{N_q+1}{ip_n-\omega(q)-\epsilon_{p+q}+\mu}\,\mathrm{Re}[\epsilon^{-2}(q,-\omega_q)]\right.$$
$$-\frac{N_F(\mathbf{p}+\mathbf{q})}{\epsilon^2(q,ip_n-\epsilon_{p+q}+\mu)}\,\frac{2\omega(q)}{(ip_n-\epsilon_{p+q}+\mu)^2-\omega^2(q)}-\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\,\frac{1}{e^{\beta\omega}-1}\,\frac{2\omega(q)}{\omega^2-\omega^2(q)}$$
$$\left.\times\frac{1}{ip_n+\omega-\epsilon_{p+q}+\mu}\,\mathrm{Im}[\epsilon^{-2}(q,\omega+i\delta)]+S_{\mathrm{plasmon}}\right\}. \tag{2.8}$$

The contribution of the plasmon pole is indicated in the last term. The second from last term comes from the branch cuts of the dielectric function (2.2). Note that the frequency dependence of the dielectric function is different for the various terms. The phonon terms, which depend upon the thermal occupation probabilities N_q and N_q+1, have the phonon frequency governing the dielectric response. The term depending upon the electron occupation N_F has a frequency dependence governed by the difference of the electron's initial energy ($ip_n+\mu\rightarrow E$) and final energy ϵ_{p+q}. The dielectric medium responds with a frequency determined by the energy transferred by the electron to the various excitations of medium.

The term containing N_F in (2.8) is the one most likely to cause structure near the Fermi energy. The other terms have reference to the Fermi energy only indirectly through the dielectric function. The integral around the branch cuts in (2.8) is examined in the Appendix, and it is shown not to be singular at the Fermi energy. The wave-vector integration of the phonon terms also involves integrals around branch cuts. These branch-cut contributions have also been examined and do not lead to singularities. The plasmon pole is like a high-frequency unscreened phonon, which contributes nothing peculiar to the density of states

[19] A. R. Hutson and D. L. White, J. Appl. Phys. 33, 40 (1962).

[20] R. A. Cowley and G. Dolling, Phys. Rev. Letters 14, 549 (1965); W. Cochran, R. A. Cowley, G. Dolling, and M. M. Elcombe (to be published). We have made calculations of the phonon propagator using the full RPA $P_0(q)$. For PbTe our results reproduce the dispersion relation given in Fig. 2 of the above reference. The dynamic limit used by KK is valid only for wave vectors q such that $\hbar qv_F/\omega_0<1$ which for Cowley and Dolling's PbTe samples requires $q<10^5$ cm^{-1}. In such materials Eq. (2.4) is valid if the LO and TO energies are nearly degenerate.

near the Fermi energy. Thus, the main structure arises from the $N_F(p+q)$ term, which we designate Σ_F:

$$\Sigma_F(p,Z)=-\int\frac{d^3kN_F(k)}{(2\pi)^3}\frac{V(\mathbf{p}-\mathbf{k})}{\epsilon(\mathbf{p}-\mathbf{k},Z-\epsilon_k)^2}\times\frac{2\omega(\mathbf{p}-\mathbf{k})}{(Z-\epsilon_k)^2-\omega(\mathbf{p}-\mathbf{k})^2}. \quad (2.9)$$

Changing the angular variable to $x=(\mathbf{p}-\mathbf{k})^2$ gives

$$\Sigma_F(p,Z)=-\frac{1}{2(2\pi)^2p}\times\int_0^{kF}k\,dk\int_{(p-k)^2}^{(p+k)^2}dx\frac{V(x)}{\epsilon^2(x,Z-\epsilon_k)}\times\frac{2\omega(x)}{(Z-\epsilon_k)^2-\omega^2(x)}. \quad (2.10)$$

To find the quasiparticle density of states, we take the derivative of the real part of $\Sigma_F(p,E)$ with respect to ϵ_p:

$$\frac{\partial}{\partial\epsilon_p}\Sigma_F(p,Z)=-\sum_F(p,Z)/2\epsilon_p-\frac{1}{4\pi^2\epsilon_p}\int_{-p_F}^{p_F}kdk\frac{(p+k)V(p+k)}{\epsilon(p+k,Z-\epsilon_k)^2}\times\frac{\omega(p+k)}{(Z-\epsilon_k)^2-\omega(p+k)^2}. \quad (2.11)$$

We obtain the retarded function by letting $Z\rightarrow E+i\delta$.

The integral in (2.11) cannot be done exactly because of the complicated functional form of ϵ. However, our interest is primarily in logarithmic singularities of (2.11), which come from poles in the integrand. Were $\epsilon(p+k,E-\epsilon_k)$ a meromorphic function, then a logarithmic singularity caused by a pole at $k=k_i$ would be screened by

$$\epsilon(p+k_i,E-\epsilon_{k_i}). \quad (2.12)$$

Although ϵ is not a meromorphic function, it can be approximated by one in the vicinity of the poles of interest, and the form (2.12) can still be employed. This approximation allows us to evaluate the effect of screening on the various singularities which occur in the density of states.

III. OPTICAL PHONONS: POLAR COUPLING

The density of states near the Fermi energy $|E-\mu|\ll\omega_0$, was evaluated by Keldysh and Kopaev[13] (KK) for polar coupling to optical phonons. They neglected the dielectric screening of the electron-phonon vertex. Their result, which had a sign error, predicted logarithmic singularities in the density of states at the Fermi surface. However, it is shown below that these logarithmic singularities at the Fermi surface disappear entirely when screening is included in a realistic approximation. These singularities are caused by long-wavelength phonons which *are* screened out by the plasma. Note that the frequency dependence of the dielectric function in (2.11) depends upon $E-\epsilon_k$ (after integration, upon $E-\epsilon_p$) and not upon ω_0. The function $\epsilon(q,\omega_0)$ does *not* screen out long-wavelength phonons.

For optical phonons, polar interaction,

$$\omega(q)=\omega_0, \quad (3.1a)$$

$$V(q)=[4\pi\alpha\omega_0^{3/2}/(2m)^{1/2}q^2]. \quad (3.1b)$$

If screening is neglected, the self-energy integral (2.8) may be done analytically. The part depending upon N_F is expressed in terms of Euler's dilogarithm function:[21]

$$L_2(x)=-\int_0^x\ln(1-t)dt/t. \quad (3.2)$$

This function is well behaved at $x=1$, but it has a logarithmic singularity in the derivative at $x=1$.

The relevant self-energy is

$$\Sigma_F(p,Z)=\frac{-\alpha}{2\pi}\frac{\omega_0^{3/2}}{\epsilon_p^{1/2}}\left\{\ln\left|\frac{p+k_F}{p-k_F}\right|\ln\left[\frac{\mu-Z-\omega_0}{\epsilon_p-Z-\omega_0}\frac{\epsilon_p-Z+\omega_0}{\mu-Z+\omega_0}\right]+L_2\left(\frac{p-p_F}{p+y-}\right)-L_2\left(\frac{p+p_F}{p+y-}\right)\right.$$
$$\left.+L_2\left(\frac{p-p_F}{p-y-}\right)-L_2\left(\frac{p+p_F}{p-y-}\right)-L_2\left(\frac{p-p_F}{p+y+}\right)+L_2\left(\frac{p+p_F}{p+y+}\right)-L_2\left(\frac{p-p_F}{p-y+}\right)+L_2\left(\frac{p+p_F}{p-y+}\right)\right\}, \quad (3.3)$$

where

$$y\pm=[2m(Z\pm\omega_0)]^{1/2}. \quad (3.4)$$

The approximate result given by KK had just the first term of the above and with an incorrect sign.[22] The dilogarithm functions do cause structure, but not at the Fermi energy. This structure is a discontinuity in $\mathrm{Re}\Sigma_F(p,E)$ at $E=\epsilon_p\pm\omega_0$ for $p<p_F$. The self-energy from the phonon term has an equal and opposite discontinuity at $E=\epsilon_p+\omega_0$ for all p. So the total real unscreened self-energy has a discontinuity at $E=\epsilon_p-\omega_0$ for $p<p_F$ and at $E=\epsilon_p+\omega_0$ for $p>p_F$. There is also a logarithmic singularity in $\mathrm{Re}\Sigma_F(p,E)$ at $E=\mu\pm\omega_0$. None of this structure is eliminated when screening is

[21] *Higher Transcendental Functions*, edited by A. Erdilyi (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, p. 31.

[22] The first term of (3.3) appears with the same sign as the same term in (1.10) of Ref. 13. However, we have defined Σ_F with the opposite sign, so the two results differ.

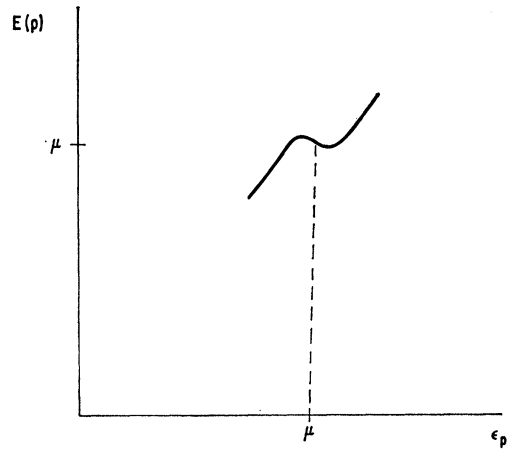

FIG. 1. A schematic representation of the dispersion relation for a polaron when screening is neglected. The extrema near the Fermi energy are exaggerated in the figure. Dielectric screening in the random-phase approximation eliminates this instability.

included, since none of it depends upon long-wavelength phonons. Finally, we note that the parameter for the perturbation theory expansion for energies near the Fermi energy is $\alpha(\omega_0/\mu)^{1/2}$ rather than just α.

Using the unscreened self-energy (3.3) would predict an instability in the electron gas near the Fermi energy. This interesting phenomenon is eliminated when dielectric screening is included in the random phase approximation. The instability is demonstrated by solving the quasiparticle dispersion relation

$$E(p)=\epsilon_p+\Sigma(p,E(p))\,. \tag{3.5}$$

This is evaluated approximately by setting $E(p)=\epsilon_p$ in the self-energy, and retaining only the important terms near $\epsilon_p\approx\mu$ in (3.3)

$$E(p)\approx\epsilon_p-\frac{\alpha}{\pi}(\omega_0/\mu)^{1/2}(\epsilon_p-\mu)\ln|2p_F/(p-p_F)|\,. \tag{3.6}$$

The right-hand side of (3.6) is plotted schematically in Fig. 1, which shows that $E(p)$ has a maximum and a minimum near the Fermi energy. The position of the extremum $E_{\rm ext}$ is easily found by setting $\partial E(p)/\partial\epsilon_p$ to zero

$$E_{\rm ext}=\mu\{1\pm\exp[-1-(\pi/\alpha)(\mu/\omega_0)^{1/2}]\}\,. \tag{3.7}$$

An electron gas with this dispersion relation is unstable because electrons above the Fermi sphere have less energy than those above. The sign error of KK caused them to miss this instability, which only occurs with the correct sign of the self-energy.

To find the density of states from (2.7a) we need the derivative

$$\frac{\partial\,\mathrm{Re}\,\Sigma_F}{\partial\epsilon_p}=\frac{1}{2}\frac{\Sigma_F}{\epsilon_p}\frac{\alpha}{2\pi}\frac{\omega_0^{3/2}}{\epsilon_p}\times\left\{\frac{-2\omega_0\sqrt{\epsilon_p}}{\omega_0^2-(E-\epsilon_p)^2}\ln\left|\frac{p-p_F}{p+p_F}\right|+\frac{(E+\omega_0)^{1/2}}{\omega_0+E-\epsilon_p}\ln\left|\frac{p_F-y_+}{p_F+y_+}\right|+\frac{(E-\omega_0)^{1/2}}{\omega_0-E+\epsilon_p}\ln\left|\frac{p_F-y_-}{p_F+y_-}\right|\right\}\,. \tag{3.8}$$

The quasiparticle density of states is quite good for optical phonons, since the imaginary part of the total

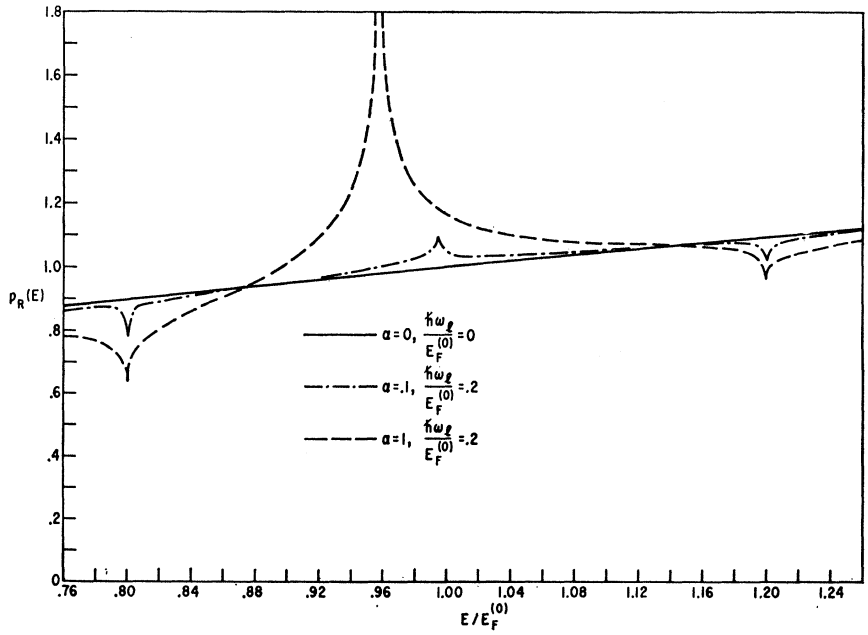

FIG. 2. The reduced electronic density of states $\rho_R=\pi^2\hbar p/mp_F$ calculated using the unshielded polar interaction between the electrons and longitudinal optical phonons. The introduction of screening eliminates the singularity at $E=\mu$ but not those at $E=\mu\pm\omega_0$. The coupling constants and phonon frequencies are indicated in the figure.

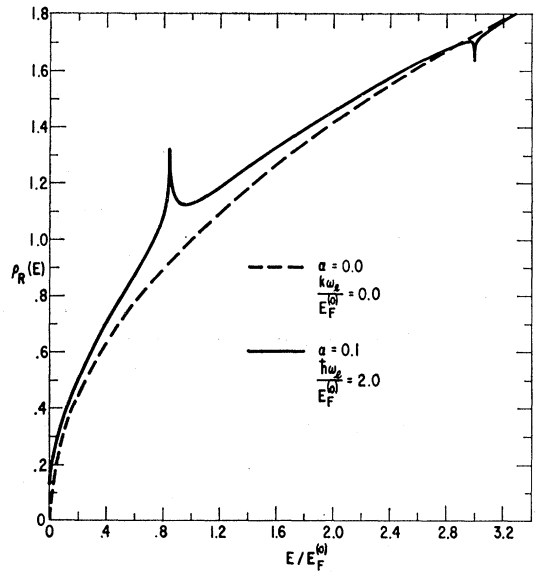

FIG. 3. The reduced electronic density of states $\rho_R=\pi^2\hbar\rho/mp_F$ calculated using the unshielded polar interaction between the electrons and longitudinal optical phonons. The introduction of screening eliminates the singularity at $E=\mu$ but not those at $E=\mu\pm\omega_0$. The coupling constants and phonon frequencies are indicated in the figure.

unscreened Σ vanishes for $|E-\mu|\leq\omega_0$. Screening changes this result by including contributions from phonon-induced electron-hole pair production, which are usually small. Near the Fermi surface, $E=\epsilon_p\approx\mu$, and the density of states is dominated by the singular term

$$\partial\,\mathrm{Re}\Sigma_F/\partial\epsilon_p\approx +(\alpha/\pi)(\omega_0/\mu)^{1/2}\ln|(p-p_F)/(p+p_F)|\,. \quad (3.9)$$

This is the same result as derived by KK[13] except for their sign error.

In order to appreciate the type of effects which may occur, we have numerically evaluated the density of states using the unscreened self-energies. This includes Σ_F in (3.3) and the self-energy from the phonon pole, both taken at zero temperature. In Fig. 2 is shown a "reduced" density of states $\rho_R=(\pi^2\hbar^2/mp_F)\rho$ for $\omega_0=0.2\,\mu$ and $\alpha=1.0$ and $\alpha=0.1$. In the quasiparticle "window" $|E-\mu|<\omega_0$, the density of states is obtained from (2.7a), while in the regions where $\mathrm{Im}\Sigma\neq0$ the results are found by numerical integration. The central peak is caused by the term in (3.9), and is eliminated (or very smoothed over) when screening is included. The peaks at $E=\mu\pm\omega_0$ remain when screening is included although their sign and magnitude depend on the value of r_s. Figure 3 shows a similar calculation for $\alpha=0.1$ and $\omega_0=2.0\,\mu$. The central peak does not occur at the unperturbeed Fermi energy because $\mathrm{Re}\Sigma$ is nonzero in this region. A self-consistent calculation, which accounted for the renormalization of the Fermi energy, would place this peak at the Fermi energy.[23]

We now show that the singular term (3.9) in the density of states at the Fermi surface is screened out. That is, the singular term (3.9) is eliminated when screening is included. We use (2.11) and (2.12) to show that the result (3.9) is screened by a dielectric function

$$\frac{\partial\,\mathrm{Re}\Sigma_F}{\partial\epsilon_p}(p,E)=(\alpha/\pi)(\omega_0/\mu)^{1/2}1/\epsilon(0,E-\epsilon_p)^2 \times\ln|(p-p_F)/(p+p_F)|\,. \quad (3.10)$$

The function $\epsilon(0,E-\epsilon_p)$ diverges as $E\to\epsilon_p$, which means that the above term vanishes on the mass shell. Thus screening does eliminate this logarithmic singularity in the density of states at the Fermi surface. This also eliminates the instability which depends upon this logarithmic singularity.

The other singular terms in (3.8) at $E=\mu+\omega_0$ remain when screening is included. The magnitude and sign of the coefficient of these logarithmic terms depends upon the screening parameters. The polaron self-energy and density of states were evaluated analytically using Fermi-Thomas screening. The results for $\alpha=1$ and $\omega_0=0.2\,\mu$ are shown in Fig. 4. Various values of r_s are indicated in the figure. The $r_s=0$ limit corresponds to Fig. 2. The peak in the density of states at the Fermi energy vanishes at r_s greater than 10^{-3}. The peaks at $E=\mu\pm\omega_0$ remain but diminish in intensity as r_s is increased. The coefficient of the peak at $E=\mu-\omega_0$ appears to change sign as r_s is increased. However, the peaks at $E=\mu\pm\omega_0$ have additional structure which cannot be shown on the scale of Fig. 3. We conclude that the nature of these singularities at $E=\mu\pm\omega_0$ can vary among different electronic systems, since they depend upon both the screening parameters and the ratio ω_0/μ.

IV. ACOUSTICAL PHONONS: PIEZOELECTRIC AND DEFORMATION-POTENTIAL INTERACTIONS

The polaron self-energies and density of states are now evaluated for acoustical-phonon interactions. We will show that, as in the preceding optical-phonon case, there are logarithmic singularities near the Fermi surface from the piezoelectric interaction which are screened out by the dielectric function. There are also logarithmic singularities at $E=\mu\pm2p_FC_s$ which are broadened by the imaginary parts of the self-energy. The latter results apply to both the piezoelectric and deformation-potential interactions. The deformation-potential coupling is the strongest interaction in most cases.

Since for electrons with $p<p_F$ the phonons have wave vectors $q<2p_F$, and p_F is not large in a semiconductor, it is possible to use the Debye model for acoustic

[23] C. B. Duke, Phys. Rev. 136, B59 (1964).

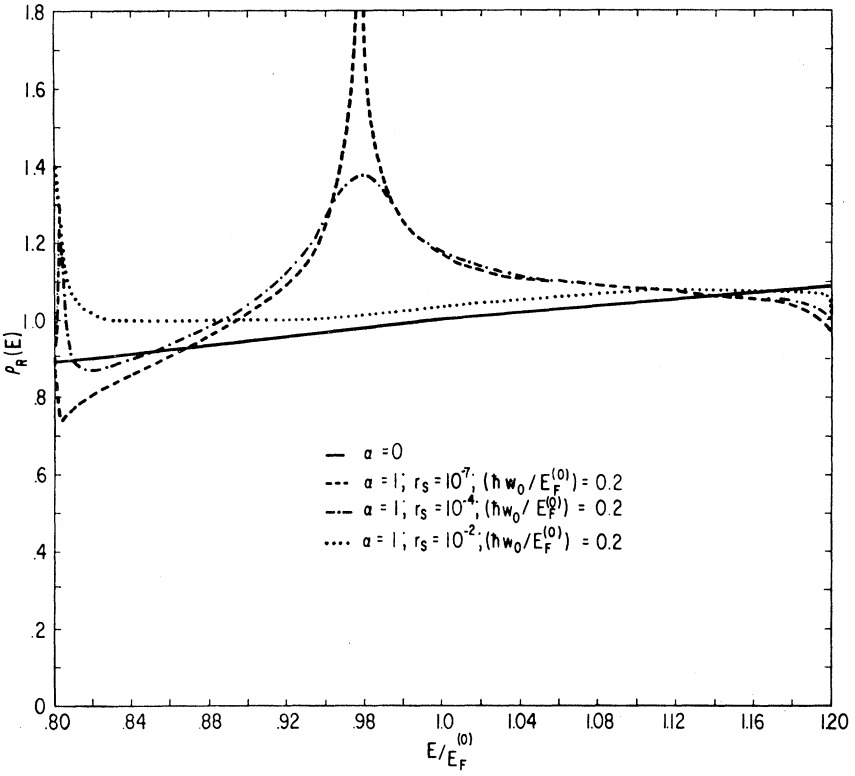

FIG. 4. The reduced electronic density of states $\rho_R=\pi^2\hbar\rho/mp_F$ calculated using the polar interaction between electrons and longitudinal optical phonons. The dielectric screening of the plasma was included in the Fermi-Thomas approximation. Different values of the standard density parameter r_s are indicated in the figure. For increasing values of r_s, the coefficient of the logarithmic singularity at $E=\mu-\omega_0$ changes sign. For values of $r_s\gtrsim 0.1$, the logarithmic singularities at $E=\mu\pm\omega_0$ are not discernible on the present scale of the figure.

phonons, $\omega(q)=C_sq$. The two vertex interactions are

$$\textit{piezoelectric interaction}\quad V(q)=2\pi g\hbar^2C_s^2/|q|\,, \tag{4.1a}$$

$$\textit{deformation potential}\quad V(q)=D_0^2\hbar|q|/2\rho C_s\,. \tag{4.1b}$$

The dimensionless piezoelectric constant g equals the electromechanical coupling constant times $e^2/\hbar C_s\epsilon_0$, and we use an isotropic form for the interaction.[24] The deformation-potential constant is D_0, and ρ is the density of the semiconductor.

When screening is neglected, the self-energy (2.1) can be evaluated exactly. These results are of interest and are presented below. The deformation potential self-energy has been estimated by Holstein,[9] but we present the exact result as Eq. (4.9).

Without screening, the result for the piezoelectric interaction is

$$\Sigma_F(p,Z)=(g/2\pi)(\epsilon_s/\epsilon_p)^{1/2}\sum_{i,\,j=1}^{2}(-)^{i+j}f_+(i,j)\times f_-(i,j)\ln[f_+(i,j)/f_-(i,j)]\,, \tag{4.2}$$

$$f\pm(i,j)=[Z+(-)^iC_sp+\epsilon_s]^{1/2}+(-)^j\sqrt{\epsilon_s}\pm\sqrt{\mu}\,, \tag{4.3}$$

$$\epsilon_s=mC_s^2/2\,.$$

The real and imaginary parts can be found by letting $Z\to E+i\delta$. For $E=\epsilon_p$, the functions f_- vanish at

$$E=\mu,\quad i\neq j;\qquad E=(\sqrt{\mu}\pm 2\sqrt{\epsilon_s})^2\approx\mu\pm 2C_sp_F,\quad i=j. \tag{4.4}$$

[24] C. B. Duke and G. D. Mahan, Phys. Rev. **139**, A1965 (1965).

The self-energy is well behaved because of the $f\ln(f)$ form for $f\to 0$. However, the density of states can have structure. The main contribution near the Fermi energy in the quasiparticle approximation is[25]

$$\frac{\partial\,\mathrm{Re}\Sigma_F}{\partial\epsilon_p}\simeq\frac{g}{2\pi}\left(\frac{\epsilon_s}{\epsilon_p}\right)\times\ln\left[\left|\frac{E-\mu+C_s(p-p_F)}{E-\mu+C_s(p+p_F)}\right|\left|\frac{E-\mu-C_s(p+p_F)}{E-\mu-C_s(p-p_F)}\right|\right]. \tag{4.5}$$

This has four logarithmic singularities. However, the two singularities at $E=\mu\pm C_s(p-p_F)$ cancel at $p=p_F$. It will be shown below that these two singularities, which are caused by long-wavelength phonons, are screened out when the dielectric function is included. The other two singular points, at $E=\mu\pm C_s(p+p_F)$, remain even when screening is included. There is not, however, an actual logarithmic singularity at these points because the imaginary part of the self-energy is finite here. At $E_0=\mu\pm 2C_sp_F$, the imaginary part of the self-energy is

$$\mathrm{Im}\Sigma(p,E_0)\simeq-2g\epsilon_s\,, \tag{4.6}$$

which is generally larger than $\mathrm{Re}\Sigma$ at this point.

The contribution to the self-energy from the phonon poles in (2.8) has also been evaluated at zero temperature. The q integral for this term must be cut off at the

[25] There are additional logarithmic terms whose coefficients are smaller by C_s/v_F.

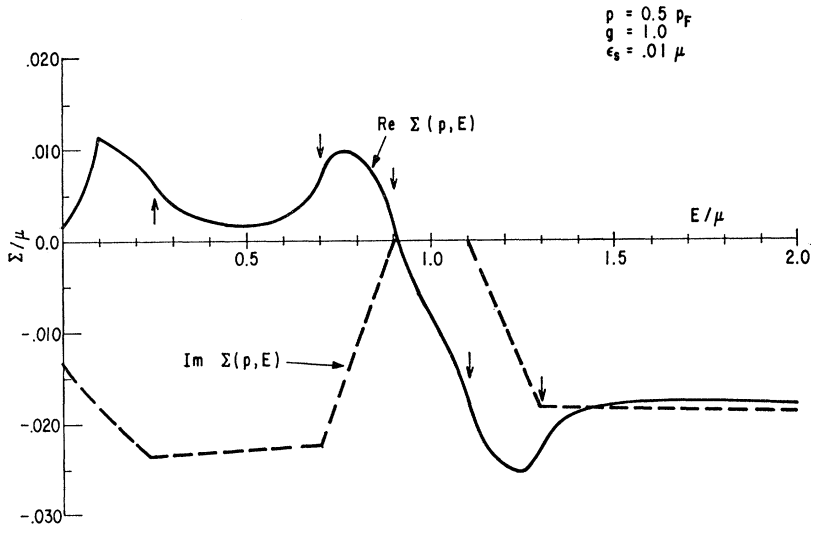

FIG. 5. The real and imaginary parts of the electron's self-energy $\Sigma_{ph}+\Sigma_F$, (4.7) and (4.2), for unscreened, piezoelectric, acoustical-phonon interactions. The parameters are $\epsilon_s=0.01\ \mu$, $p=0.5\ p_F$, and $T=0$. The down arrows (↓) point to the Kohn-type anomalies when the f_- functions vanish in (4.2). The up arrow (↑) is where h vanishes in (4.7), which occurs at $E=\epsilon_p$. The imaginary part of Σ vanishes approximately for $|E-\mu|<C_s|p-p_F|$.

Debye wave vector q_D. However, the important terms depending upon q_D either change Σ by a constant, or else change the effective mass. We can omit such terms and use the measured effective mass and band minimum. The remaining terms in Σ from the phonon poles are

$$\Sigma_{\rm ph}=-(g\epsilon_s/\pi\sqrt{\epsilon_p})\sum_{i,\,j=1}^{2} h(i,j)\ln h(i,j)\,,$$
$$h(i,j)=\sqrt{\epsilon_p}+(-)^i\sqrt{\epsilon_s}+(-)^j[Z+(-)^iC_sp+\epsilon_s]^{1/2}. \tag{4.7}$$

The terms depending upon the phonon thermal occupation N_q should be unimportant at low temperatures. The magnitude of N_q depends upon the average magnitude of $\hbar\omega_q/kT$. For the degenerate case, $\langle q\rangle\simeq\langle p\rangle\approx p_F$, and $\langle\hbar C_sq/kT\rangle\approx(\epsilon_s\mu)^{1/2}/kT\gg1$. This is quite different from the nondegenerate case, since here $\langle q\rangle\approx\langle p\rangle\approx(2mkT)^{1/2}$ and $\langle\hbar\omega_q/kT\rangle\approx(\epsilon_s/kT)^{1/2}\ll1$.

Sample numerical calculations were also performed on the spectral densities and density of states for degenerate electrons with piezoelectric interactions. Figure 5 shows the real and imaginary part of the total unscreened self-energy $\Sigma_F+\Sigma_{\rm ph}$, calculated for $\epsilon_s=0.01\mu$, $p=0.5p_F$, $g=1$, and zero temperature. The places where the four f functions vanish are marked by arrows (↓), and a Kohn-type anomaly is evident. The h functions vanish at $E=\epsilon_p$, which is also marked (↑). Although the real part of Σ shows much structure, the most interesting result is that for a fixed value of p the imaginary part of the self-energy vanishes for value of E near the Fermi energy. This quasiparticle window extends approximately from $\mu-C_s|p-p_F|$ to $\mu+C_s|p-p_F|$; it vanishes at $p=p_F$ and scales with C_s. If one plots $\mathrm{Im}\Sigma(p,E)$ as a function of p for a fixed E, then $\mathrm{Im}\Sigma$ is nonzero in the region around p_F from $p=p_F-|E-\mu|/C_s$ to $p=p_F+|E-\mu|/C_s$. The imaginary part of Σ has a similar window for deformation potential scattering. This structure was not reported in previous discussions[7–9] of electron–acoustical-phonon interactions, which demonstrates the desirability of avoiding unnecessary approximations.

Numerical integrations have been performed to obtain the density of states $\rho(\epsilon)$ for $\epsilon_s/\mu=0.1$ and 0.001 and $g=1$. No structure appears at $E=\mu\pm2p_FC_s$, and the singularity in $\partial\Sigma/\partial\epsilon_p$ is undoubtedly smoothed out by the large value $\mathrm{Im}\Sigma$. The structure at $E=\mu$ is not discernible on an energy scale of $\Delta E=10^{-3}\mu$. As $g=1$, $\epsilon_s/\mu=0.001$ is a strong-coupling situation for the valence band electrons, we conclude that the piezoelectric interaction with acoustic phonons is not an important source of structure in the electronic density of states.

We introduce screening by using (2.11) and (2.12). For acoustical phonons, the frequency dependence of the dielectric function can be ignored since $v_F\gg C_s$. This gives

$$\frac{\partial}{\partial\epsilon_p}\mathrm{Re}\,\Sigma_F\simeq\frac{g}{2\pi}\left(\frac{\epsilon_s}{\epsilon_p}\right)\frac{1}{\epsilon^2(2p_F,0)}\times\log\left|\frac{E-\mu-C_s(p+p_F)}{E-\mu+C_s(p+p_F)}\right|. \tag{4.8}$$

The terms at $E=\mu\pm2C_sp_F$ are screened by a dielectric function $\epsilon(2p_F,0)$, showing that $q\approx2p_F$ phonons are principally involved in causing this term. The singularities at $E=\mu$ have as an effective dielectric function $\epsilon(0,0)\to\infty$, so these singularities are screened out. The singularities at the Fermi surface are caused by long-wavelength phonons, which are screened by the degenerate electron gas. Were it not for the damping (4.6), this logarithmic term would also lead to instabilities in the excitation spectrum near $E=\mu+2C_sp_F$.

The electron self-energy for deformation potential coupling is (for N_0 denoting the atomic density of the

impurity atoms)

$$\Sigma_F(p,Z)=\frac{D_0^2N_0}{4\rho C_s^2\mu}\Big\{\mu-Z-20\epsilon_s+\frac{1}{16\epsilon_s(\mu\epsilon_p)^{1/2}}\times\sum_{i,j=1}^{2}(-)^{i+j}[(f_+f_--(E-\mu))^3+(E-\mu)^3]\ln[f_+/f_-]\Big\}. \quad (4.9)$$

There is no singularity in the unscreened density of states at $E=\mu$ since setting $f_-=0$ and $E=\mu$ causes $\partial\Sigma_F/\partial\epsilon_p$ to vanish identically. The terms at

$$E=\mu\pm 2C_sp_F$$

are

$$\frac{\partial\,\mathrm{Re}\Sigma_F}{\partial\epsilon_p}=\frac{D_0^2m^2}{2\pi^2\rho C_s\hbar^3}\ln\left|\frac{E-\mu-C_s(p+p_F)}{E-\mu+C_s(p+p_F)}\right|. \quad (4.10)$$

These are not really singular because of the finite imaginary part of Σ at this energy. It is interesting to note that the prefactor of this term is independent of the electronic density. Screening just adds a $\epsilon(2p_F,0)^{-2}$ factor to this result, as it did for the piezoelectric case (4.7). Thus, for deformation-potential interactions with acoustic phonons there are no singularities in the density of states at the Fermi surface.

V. SUMMARY AND CONCLUSIONS

In this paper we have obtained two new analytical results. For the unscreened electron-phonon vertices we evaluate analytically the second order self-energy associated with an electron in a degenerate Fermi gas interacting with LO phonons via polar coupling and with (Debye) acoustical phonons via piezoelectric and deformation potential coupling. From these self-energies we calculate the electronic density of states. For optical phonons the calculation was performed numerically and sample results given in Figs. 2, 3, and 4. The unscreened interaction led to logarithmic singularities at the energies μ and $\mu\pm\omega_0$. For acoustical phonons we both performed numerical calculations and investigated analytically the possibility of singularities in the electronic density of states. This investigation was carried out by use of the quasiparticle approximation in which singularities in the density of states are associated with singularities in $\partial\Sigma/\partial p$. We found that singularities in $\partial\Sigma/\partial p$ occur at the energies $\mu\pm 2C_sp_F$ for both piezoelectric and deformation-potential coupling. At these energies the quasiparticle approximation is not rigorously valid because $\mathrm{Im}\Sigma$ is nonzero, which tends to smooth out the structure. Numerical calculations for piezoelectric interactions did not reveal singularities at $E=\mu\pm 2C_sp_F$. Piezoelectric coupling causes two canceling singularities at $E=\mu$ whereas deformation-potential coupling does not yield any structure at $E=\mu$.

The singularity in the density of states at $E=\mu$ induced by optical phonons is an old result deduced by KK[13] (except for a sign error). Our second major result is the demonstration that, contrary to the claim of KK, the dielectric screening associated with the degenerate electron (hole) plasma eliminates this singularity. Although the remark of KK that the screening does not severely modify the phonon propagator (it renormalizes the optical-phonon frequency) is invalid in PbTe,[20] the primary effect which they failed to consider was the alteration in the electron-phonon vertex wrought by the screening.

The primary conclusion to be drawn from our results is that neither the original[3] nor the KK[13] explanations for the conductance anomalies in tunnel diodes are quantitatively applicable. We feel that these anomalies are not due to bulk-polaron effects.

ACKNOWLEDGMENTS

We are indebted to D. G. Scalapino and T. M. Wu for communicating to us their independently calculated results on the sign error in KK, its interpretation as indicating an instability at $E=\mu$, and the fact that RPA screening removes the instability at $E=\mu$. We also thank S. Engelsberg, who has done similar calculations using the polar and piezoelectric interactions, for a helpful comparison of results. The effects of the polar interaction were also considered by A. Suna and J. R. Schrieffer.

APPENDIX: BRANCH-CUT INTEGRAL

The Matsubara sum of the polaron self-energy was evaluated by means of a contour integral. One term in the result (2.8) came from the integral around the branch cuts of the RPA dielectric function. We now examine this term in detail to show that it does not contribute a singularity in the density of states at the Fermi surface. This analysis differs from that of Quinn and Ferrell,[26–28] who have considered similar cut integrals in the theory of Coulomb interactions in Fermi systems. They used time-ordered functions, in contrast to our retarded functions, which changes the path of the contour around the cut. Secondly, they were interested in deriving systematic corrections to the correlation energy, whereas we merely wish to reduce the integrals to a form which demonstrates that nothing peculiar occurs in this term at $E=\mu$ and $p=p_F$.

The integral is

$$\Sigma_c(p)=-\int\frac{d^3qd\omega}{(2\pi)^4}\frac{2\omega(q)V(q)}{e^{\beta\omega}-1}\frac{1}{\omega^2-\omega(q)^2}\times\frac{1}{ip_n+\omega-\epsilon_{p+q}+\mu}\frac{-4\epsilon_R\epsilon_I}{|\epsilon^2|^2}. \quad (A1)$$

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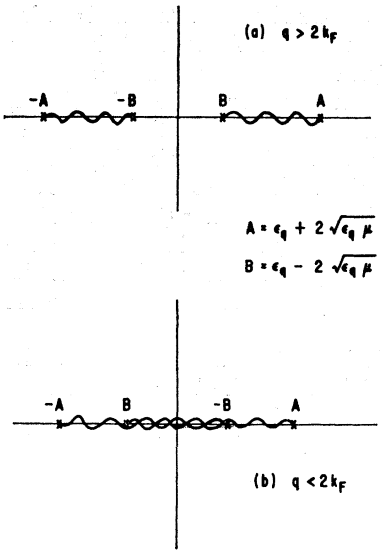

FIG. 6. The cuts of the RPA dielectric function $\epsilon(q,\omega)$ in ω space. The four logarithmic branch points can be connected by two branch cuts. These cuts are distinct for $q>2k_F$, but they overlap for $q<2k_F$. At the point $\omega=0$ $\epsilon(q,\omega)$ is analytic because $\epsilon_I(q,0)=0$ for all values of q.

The integral is only taken along the real ω axis where the imaginary part of ϵ is nonzero. Only the zero-temperature case is considered, which restricts ω to the negative real axis because of the $(\exp\beta\omega-1)^{-1}$ factor.

The branch cuts of $\epsilon(q,\omega)$ are shown in Fig. 6. The two cuts are distinct for $q>2k_F$, but they overlap for $q<2k_F$. For $\omega<0$, the dielectric function for the single-cut region is

$$\epsilon_I{}^{(1)}=-\frac{\pi k^2{}_{FT}k_F{}^3}{16q^5\mu^2}[4\epsilon_q\mu-(\omega+\epsilon_q)^2]. \tag{A2}$$

For the region where the cuts overlap it is

$$\epsilon_I{}^{(2)}=-\frac{\pi k^2{}_{FT}k_F{}^3}{16q^5\mu^2}[-4\omega\epsilon_q]. \tag{A3}$$

The regions of integration where $\epsilon_I{}^{(1)}$ and $\epsilon_I{}^{(2)}$ are appropriate are

$$\Sigma_c=\int_0^{2k_F}dq\left\{\int_{-A}^{B}d\omega\ \epsilon^{(1)}+\int_B^0 d\omega\epsilon^{(2)}\right\}$$
$$-\int_{2k_F}^{\infty}dq\int_{-A}^{-B}d\omega\epsilon^{(1)}, \tag{A4}$$

where

$$A=\epsilon_q+2(\epsilon_q\mu)^{1/2}$$
$$B=\epsilon_q-2(\epsilon_q\mu)^{1/2}.$$

It is convenient to change the variables of integration to

$$x=q/p_F,\ y=(\omega+\epsilon_q)/2(\epsilon_q\mu)^{1/2}.$$

When we exchange the order of integration, the two $\epsilon^{(1)}$ terms in (A4) immediately combine. This gives

$$\Sigma_c=C_0\int_{-1}^{1}dy(1-y^2)$$
$$\times\int_{y+1}^{\infty}\frac{dx\,\omega(x)V(x)\epsilon_R(x,y)}{[(2y-x)^2-a(x)]x^3|\epsilon^{(1)}(x,y)^2|^2}g(p,x,y)$$
$$+C_0\left[\int_{-1}^{0}dy\int_0^{y+1}dx+\int_0^1 dy\int_{2y}^{y+1}dx\right]$$
$$\times\frac{(2y-x)\omega(x)V(x)}{[(2y-x)^2-a(x)]x^2}\frac{\epsilon_R}{|\epsilon^{(2)}(x,y)^2|^2}g(p,x,y), \tag{A5}$$

where

$$g(p,x,y)=2\mu x\int_{-1}^{1}\frac{d\nu}{ip_n-\epsilon_p+\mu+2\mu x(y-z-\eta\nu)}, \tag{A6}$$
$$\eta=p/p_F,$$
$$C_0=\frac{k_{FT}{}^2k_F}{4\pi^2\mu^2},$$

and

$$a(x)=(\omega_0/\mu x)^2 \quad \text{optical phonons},$$
$$=4\epsilon_s/\mu \quad \text{acoustical phonons}.$$

The integral in (A6) can be done to give

$$g(p,x,y)=-\frac{1}{\eta}\ln\frac{ip_n-\epsilon_p+\mu+2\mu x(y-x+\eta)}{ip_n-\epsilon_p+\mu+2\mu x(y-x-\eta)}. \tag{A7}$$

Our interest is in the density of states, for which we need $\partial\,\mathrm{Re}\Sigma_c/\partial\epsilon_p$, which means $\partial\,\mathrm{Re}g/\partial\epsilon_p$. The derivation of the η^{-1} term is of no interest. We take the derivative of the logarithm, and then go to the mass shell $(ip_n\to\epsilon_p-\mu)$

$$\left.\frac{\partial\,\mathrm{Re}g}{\partial\epsilon_p}\right|_{ip_n}\simeq\frac{2}{\epsilon_p x}\left[-2+\frac{y}{y-x-\eta}+\frac{y}{y-x+\eta}\right]. \tag{A8}$$

The -2 term cannot lead to structure at $\eta=1$ and will be dropped. We pursue the remaining terms by changing variables again

$$z=x-y,\ dz=dx$$

and also exchanging the order of the y and z integrations. This finally gives

$$\frac{\partial\,\mathrm{Re}\Sigma_c}{\partial\epsilon_p}\simeq-\frac{2C_0}{\epsilon_p}\int_0^{\infty}dzf(z)\left[\frac{1}{z+\eta}+\frac{1}{z-\eta}\right], \tag{A9}$$

where

$$f(z)=\int_{-\lambda}^{\lambda}dy\,y\frac{(\lambda^2-y^2)}{(z+y)^4}\frac{\omega(z+y)V(z+y)}{(y-z)^2-a(y+z)^2}\frac{\epsilon_R(y,z)}{|\epsilon^2|^2}, \tag{A10}$$
$$\lambda=1 \quad \text{for} \quad z>1$$
$$\lambda=z \quad \text{for} \quad 0<z<1.$$

In terms of the new variables, the real and imaginary

parts of the dielectric function are

$$\epsilon_R(y,z)=1+\frac{k_{FT}^2}{2k_F^2}\frac{1}{(z+y)^2}\times\left[1+\frac{1}{2(z+y)}(1-y^2)\ln\left|\frac{1-y}{1+y}\right|-\frac{1}{2(z+y)}(1-z^2)\ln\left|\frac{1+z}{1-z}\right|\right], \quad \text{(A11)}$$

$$\epsilon_I(y,z)=\frac{\pi k_{FT}^2}{4k_F^2(z+y)^3}(\lambda^2-y^2)\,. \quad \text{(A12)}$$

A singularity at the Fermi surface will occur if $f(z)$ is discontinuous at $z=1$. From its definition it is easy to see that $f(z)$ is continuous at $z=1$, so that (A9) has no logarithmic singularity at $\eta=1$. This cut integral does not contribute any singular behavior to the density of states at the Fermi surface.

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Infrared Lattice Vibrations in $GaAs_yP_{1-y}$ Alloys

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The infrared lattice-vibration spectra of mixed crystals of $GaAs_yP_{1-y}$ have been measured by reflection techniques. These crystals exhibit two distinct reststrahlen bands whose strengths and frequencies depend on y and which show considerable fine structure. A harmonic model has been developed to account for the significant features of these spectra. The main features of the model are (1) the inclusion of a clustering effect or nonrandom distribution of anions on a microscopic scale, (2) the existence of 5 distinct molecular complexes which leads to 2 groups of 4 closely spaced optical phonon modes, and (3) effective ionic charges that have both local and nonlocal parts. The model provides the frequencies and strengths of the optical phonon modes which with suitably chosen damping constants yield a good fit to the reflectivity spectrum over the entire range of solid solutions.

INTRODUCTION

MIXED crystals (or alloys) of $GaAs_yP_{1-y}$ can be grown over the entire composition range $y=0$ to 1. These alloys are interesting for several reasons, one being their electronic band structure. GaAs is a direct gap material while GaP has an indirect gap. For the alloy, as y is increased, the band structure near the gap appears to change continuously, the central $k=0$ conduction-band minimum falling relative to the other valleys until near $y=0.6$ the $k=0$ minimum becomes the lowest valley changing the material from indirect to direct gap and drastically affecting the threshold for laser action and the luminescence properties.

Whereas it is known that the alloys have the same crystal structure as the parent crystals GaP and GaAs (i.e., zinc-blende), the distribution of the constituent ions over the sublattices is not known. One usually assumes that the structure consists of a Ga fcc sublattice and an interpenetrating fcc sublattice over which the As and P ions are randomly distributed. It has been suggested, however,[1] that there may be a tendency for like-negative ions to cluster around positive ions. Such clustering, which tends to make small regions GaAs rich or GaP rich, should have some characteristic effect on the optical-phonon modes since they depend strongly on nearest-neighbor force constants.

We intend to show in this paper that a detailed analysis of the infrared reflectivity spectrum of $GaAs_yP_{1-y}$ supports the assumption of short-range clustering. A harmonic-oscillator model of the lattice dynamics of the alloy is developed including a short-range order parameter which accounts quantitatively for the significant features of the reflectivity spectrum. The characterization of the lattice modes serves as a useful basis for other work. It will be shown that the composition y of an unknown sample can be determined from the infrared spectrum. Also, additional infrared effects such as free-carrier susceptiblity can be properly evaluated only by first taking account of the pure lattice modes.

The extra degree of freedom provided by the composition y allows us to probe other features of the lattice dynamics of III-V compounds. Brodsky and Burstein have suggested[2] that the usual assumption of a localized, effective ionic charge on each ion, while probably correct for such ionic crystals as the alkali halides, cannot be properly applied to the III-V compounds. The reason they advance is that the valency electrons of the ions in these compounds have extended wave functions and that, thus, the effective ionic charges of the ions should

* Work performed in partial fulfillment of requirements for the Ph. D. degree, New York University.

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