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Low-Frequency Impurity-Pair Conductivity in Doped Semiconductors*

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A field-theoretical diagrammatic method is used to investigate the low-frequency ac impurity-pair conductivity for doped semiconductors, originally treated semiclassically by Pollak and Geballe. The result agrees with that of the above cited work. However, it is in disagreement with the recent work of Aldea. Discussions on the latter work are given.

I. INTRODUCTION

The low-frequency impurity-hopping conductivity of doped semiconductors at low temperatures was first investigated by Pollak and Geballe[1(a)] (PG) in samples of weakly compensated n-type silicon. The physical picture in this case is as follows: The introduction of a relatively small number of acceptors "robs" an equal number of donor atoms of their electrons (which are all condensed on donor sites at low temperatures); electron transfer can then occur between occupied and unoccupied donor sites. Owing to the electric fields arising from the (negatively) charged acceptor sites and the (equally numerous) ionized donor sites, local site electronic energies are in general noncoincident; a real energy-conserving charge transfer requires the simultaneous emission or absorption of one, or more, phonons.

In the original treatment by PG, attention was focused on the situation (prevalent for low compensation), wherein the principal contribution to the ac conductivity is provided by "back-and-forth" electron hopping between isolated donor pairs (each pair situated in the vicinity of an acceptor site). The two-site ac hopping conductivity was recently treated by Aldea[2] by means of the standard temperature-diagram technique; as will be shown below, his result disagrees with that of PG. However, as will also be shown below, his analysis is beset with serious errors. In what follows, we present what we believe to be a correct temperature-diagrammatic calculation of the ac conductivity. The result is in complete agreement with that of PG.

Following PG, we restrict our analysis to the indirect process, which prevails when the external frequency (ω) is much smaller than the energy difference ($\Delta\epsilon$) of the pair sites. At high frequency (i.e., $\hbar\omega \sim \Delta\epsilon$), the direct (resonant) process becomes dominant. To find the bulk conductivity, a complicated statistical averaging has to be performed on the pair conductivity[1(b)]: It is known[1(b)] that the indirect process leads mainly to an $\omega^{0.8}$ or ω^1 dependence of the bulk conductivity, whereas the direct process predicts an ω^2 dependence. Some systems show deviations in temperature, frequency dependence, and even the magnitude of the bulk conductivity at low frequency from the result predicted by the PG's pair-hopping mechanism. In these cases multiple hopping should be considered.[1(b)] A comprehensive discussion of the PG model as well as the frequency dependence of the conductivity is given in Ref. 1(b).

The Hamiltonian of the above-described system may be written as

$$H = H_0 + H_1 + H_{\text{ph}},$$

$$H_0 = \sum_n \epsilon_n^{(0)} a_n^\dagger a_n + \sum_{nm} J_{nm} a_n^\dagger a_m ,$$

$$H_1 = -\sum_{n\vec{q}} u_{\vec{q}}^{1/2} \hbar\omega_{\vec{q}} (e^{i\vec{q}\cdot\vec{r}_n} b_{\vec{q}} + e^{-i\vec{q}\cdot\vec{r}_n} b_{\vec{q}}^\dagger) a_n^\dagger a_n ,$$

$$H_{\text{ph}} = \sum_{\vec{q}} \hbar\omega_{\vec{q}} b_{\vec{q}}^\dagger b_{\vec{q}} ,$$

where $a_n^\dagger$ (a_n) creates (annihilates) an impurity state at site $\vec{r}_n$ with an energy $\epsilon_n^{(0)}$ and J_{nm}, $\omega_{\vec{q}}$, $b_{\vec{q}}^\dagger$ ($b_{\vec{q}}$) are, respectively, transfer integral, phonon frequency corresponding to the wave vector $\vec{q}$, and phonon creation (annihilation) operator. Finally $u_{\vec{q}}$ is given, respectively, for acoustic and optical modes:

$$u_{\vec{q}}^{\text{ac}} = \frac{g^2}{2MN(\hbar\omega_{\vec{q}})^3}\, q^2 , \quad u_{\vec{q}}^{\text{op}} = \frac{\gamma^2}{2MN(\hbar\omega_{\vec{q}})^3} ,$$

where N, M are number and mass of atoms and g, γ are coupling constants. Only the acoustic phonons will here be considered.

It is convenient to transform the above Hamiltonian to the so-called "small-polaron" representation. This is achieved by a canonical transformation (cf. e.g. Schnakenberg,[3] especially pp. 624–625). The result is

$$\tilde{H} = \tilde{H}_0 + \tilde{H}_1 + \tilde{H}_{\text{ph}},$$

$$\tilde{H}_0 = \sum_n (\epsilon_n^{(0)} - E_p) a_n^\dagger a_n + \sum_{nm} \tilde{J}_{nm} a_n^\dagger a_m ,$$

$$\tilde{J}_{nm} = J_{nm} \langle B_{mn} \rangle$$

$$\tilde{H}_1 = \sum_{nm} J_{nm} a_n^\dagger a_m (B_{mn} - \langle B_{mn} \rangle), \quad (1)$$

where $E_p = \sum_{\vec{q}} u_{\vec{q}} \hbar\omega_{\vec{q}}$ is the polaron binding energy and

$$B_{mn} = \exp\left\{ \sum_{\vec{q}} u_{\vec{q}}^{1/2} \left[(e^{-i\vec{q}\cdot\vec{r}_m} - e^{-i\vec{q}\cdot\vec{r}_n}) b_{\vec{q}}^\dagger - \text{H.c.} \right] \right\},$$

$$\langle B_{mn} \rangle = \exp\left\{ -2 \sum_{\vec{q}} u_{\vec{q}} \sin^2[\vec{q}\cdot(\vec{r}_m - \vec{r}_n)/2] \times \coth(\beta\hbar\omega_{\vec{q}}/2) \right\}. \quad (2)$$

II. AC CONDUCTIVITY

The ac-conductivity tensor is given by

$$\sigma_{xy}(\omega) = -i\omega n e^2 F_{xy}(\hbar\omega + i0), \quad (3)$$

where $F_{xy}(\hbar\omega + i0)$ is the analytic continuation of the correlation function,

$$F_{xy}(\hbar\omega_r) = \frac{1}{\beta}\int_0^\beta F_{xy}(u)\, e^{\hbar\omega_r u}\, du,$$

$$F_{xy}(u) \equiv \langle T p_x(u) p_y(0) \rangle, \quad (4)$$

where $\omega_r = 2\pi r i/\hbar\beta$ (r = integer), and the operators are in Heisenberg representation. The dipole moment operator is given by[4]

$$\vec{p} = \sum_n \vec{r}_n a_n^\dagger a_n .$$

In conformance with the remarks in the Introduction, we confine the treatment to the two-site problem involving transitions between a single pair (n, m). In addition, for low-frequency conduction ($\hbar\omega \ll \Delta\epsilon^{(0)} \equiv \epsilon_n^{(0)} - \epsilon_m^{(0)}$), one can neglect the contribution from the direct (or resonant) process ($\hbar\omega \simeq \Delta\epsilon^{(0)}$). Therefore we drop the resonant term of $\tilde{H}_0$ in (1) (i.e., the term proportional to $\tilde{J}_{nm}$).

III. EVALUATION OF CORRELATION FUNCTION AND CONDUCTIVITY TENSOR

For the evaluation of the correlation function one has to use the canonical ensemble rather than the grand-canonical ensemble characteristic of the standard temperature-diagram technique; in addition, one must project out the contributions from the *unphysical* states representing cases where none or both of the sites (n, m) are occupied.[5] This may be achieved by adding to the physical Hamiltonian (1) Abrikosov's[6] "projection" Hamiltonian $H_\lambda = \lambda \sum_n a_n^\dagger a_n$, multiplying the correlation function by a factor $e^{\beta\lambda}$ and then taking the limit $\beta\lambda \to \infty$. One thereby has for the correlation function of (4)

$$F_{xy}(u) = \lim_{\beta\lambda\to\infty} \frac{Z_p^0 Z_\lambda^0 e^{\beta\lambda}}{Z} \times \frac{\text{Tr}^*\{ e^{-\beta(\tilde{H}+H_\lambda)}\, T e^{u(\tilde{H}+H_\lambda)} p_x e^{-u(\tilde{H}+H_\lambda)} p_y \}}{Z_\lambda^0 Z_p^0}, \quad (5)$$

where Z, Z_p^0 are the canonical partition function of the total system and the unperturbed partition function for the phonon system, respectively. The symbol Tr* means that one sums over both physical and unphysical states. Z_λ^0 is the unperturbed canonical electronic partition function including the projection Hamiltonian (i.e., $Z_\lambda^0 = \text{Tr}^* e^{-\beta(\tilde{H}_0 + H_\lambda)}$). It can be readily seen that $\lim_{\lambda\beta\to\infty} Z_\lambda^0 = 1$.

The most important contribution to the correlation function arises from a series of "ladder" diagrams such as shown in Fig. 1.[7] The solid (broken) lines are full electron (multiphonon) propagators and the wiggly lines are external field lines.

At this point it is pertinent to state that, in the treatment of Aldea, only the first term in Fig. 1 was retained. However, it is well known[8] that all terms in the ladder series are equally important, because, as will be seen explicitly in Appendix B, each rung introduces a factor $J_{nm}^2 \langle B_{mn} \rangle^2/\hbar\omega$ or $J_{nm}^2 \langle B_{mn} \rangle^2/\Gamma_j$ ($j = m, n$), whichever is smaller[9] due to the overlapping resonances of the electron propagators. In view of the remarks of footnote 9 this is of zeroth order in the interaction strength. Therefore all of the terms in Fig. 1 should be considered. Physically, as will be seen later in Eq. (15), the series of ladders give rise to the scattering-in term in the transport equation.

For the multiphonon propagators we will use "bare" propagators given by the unperturbed thermodynamic average:

$$D_{mn}^{(0)}(u) = \langle T(B_{mn}(u) - \langle B_{mn} \rangle)(B_{nm} - \langle B_{nm} \rangle) \rangle_0$$
$$= \langle B_{mn} \rangle^2 \left\{ \exp\left[\sum_{\vec{q}} 4u_{\vec{q}} \sin^2[\vec{q}\cdot(\vec{r}_n - \vec{r}_m)/2][\coth(\beta\hbar\omega_{\vec{q}}/2)\cosh\hbar\omega_{\vec{q}}u - \sinh\hbar\omega_{\vec{q}}u] \right] - 1 \right\}, \quad (6)$$

which upon Fourier transformation and concomitant use of the weak-coupling approximation[10] reduces to

$$D^{(0)}(\omega_l) = \frac{1}{\beta}\int_0^\beta D^{(0)}(u)\, e^{u\omega_l} du = \frac{1}{\beta} \sum_{\vec{q}\pm} \frac{\gamma_{\vec{q}}}{\hbar\omega_{\vec{q}} \pm \omega_l},$$

$$\gamma_{\vec{q}} \equiv 4u_{\vec{q}} \langle B_{mn} \rangle^2 \sin^2 \vec{q}\cdot(\vec{r}_n - \vec{r}_m)/2, \quad (7)$$

where $\omega_l = 2\pi i l/\beta$ (l = integer) and subscripts are dropped from the phonon propagators due to symmetry with respect to interchange of site indices. The full electron propagators are given by

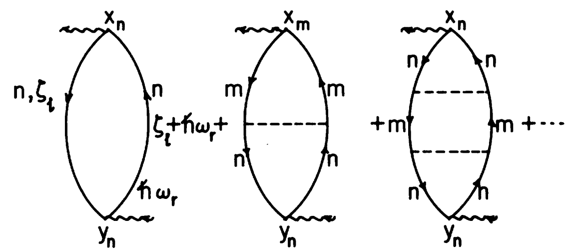

FIG. 1. Ladder diagram contribution to the correlation function.

$$\langle Ta_n^\dagger(u)\,a_n\rangle = \frac{1}{\beta}\sum_l \frac{e^{u\zeta_l}}{\zeta_l - E_{n\lambda}^{(0)} - G_n(\zeta_l)}\,,$$

where

$$\zeta_l = \frac{(2l+1)\pi i}{\beta} \qquad (l=\text{integer}),$$

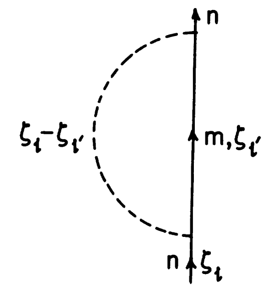

FIG. 2. Lowest-order electronic self-energy part.

$$E_{n\lambda}^{(0)} = \epsilon_n^{(0)} - E_p + \lambda. \tag{8}$$

The above thermodynamic average for the electron propagator includes the effect of the unphysical states as well as the projection Hamiltonian.

The main contribution to the self-energy part $G_n(\zeta_l)$ arises from the diagram shown in Fig. 2, and is given by

$$G_n(\zeta_l) = J_{nm}^2 \sum_{\vec q\pm}\gamma_{\vec q}\sum_{l'}\frac{1/\beta}{[\hbar\omega_{\vec q}\pm(\zeta_l-\zeta_{l'})][\zeta_{l'}-E_{m\lambda}^{(0)}-G_m(\zeta_{l'})]}\,;$$

the l' summation can be performed according to

$$\sum_{l'}\sum_{\pm}\frac{1}{\hbar\omega_{\vec q}\pm(\zeta_l-\zeta_{l'})}(\cdots\zeta_{l'}\cdots) = \sum_{\pm}\frac{\beta}{2\pi i}\int_{\Gamma\to\Gamma_0} d\zeta'\,\frac{[f^{(-)}(\zeta')+N(\pm\hbar\omega_{\vec q})]}{\hbar\omega_{\vec q}\pm(\zeta_l-\zeta')}(\cdots\zeta'\cdots), \tag{9}$$

where one defines

$$f^{(-)}(x) = \frac{1}{e^{\beta x}+1}\,,\qquad N(\pm x) = \frac{1}{e^{\pm\beta x}-1}\,.$$

The integration contour Γ is shown in Fig. 3. This can be deformed into Γ_0 using the fact that the residues at phonon poles vanish. The result of the integration is given by

$$\begin{aligned} G_n(\zeta_l) &= J_{nm}^2\sum_{\vec q\pm}\gamma_{\vec q}\,\frac{f^{(-)}(E_m^\lambda)+N(\pm\hbar\omega_{\vec q})}{\hbar\omega_{\vec q}\pm(\zeta_l-E_m^\lambda)} \\ &= J_{nm}^2\sum_{\vec q\pm}\frac{\gamma_{\vec q}N(\pm\hbar\omega_{\vec q})}{\hbar\omega_{\vec q}\pm(\zeta_l-E_m^\lambda)} \\ &\equiv G(\zeta_l-E_m^\lambda), \end{aligned} \tag{10}$$

where the second equality is due to the fact that $\beta\lambda\to\infty$. In (10), the renormalized energy E_m^λ is given by $E_m^\lambda - E_{m\lambda}^{(0)} - M_m(E_m^\lambda) = 0$, where the real part of the self-energy $M_m(\zeta)$ is defined by

$$G_\mu(E_\mu^\lambda \mp i0) \equiv M_\mu(E_\mu^\lambda) \pm i\Gamma_\mu(E_\mu^\lambda) \equiv M_\mu \pm i\Gamma_\mu \qquad (\mu = m, n). \tag{11}$$

Because the self-energy is a slowly varying function of energy at $\zeta = E_{\mu\lambda}^{(0)}$ [cf. Eq. (13)], one has $E_m^\lambda = E_{m\lambda}^{(0)} + M_m(E_{m\lambda}^{(0)})$,

Experimentally one has

$$\beta\hbar\omega \ll 1,\quad \beta\Gamma_\mu \ll 1. \tag{12}$$

In Appendix A we show, using the second condition of (12), that the derivative of the electron self-energy part is very small except for some weak divergences (inverse-square-root type) arising from the Van Hove singularities in the phonon density of states, i.e.,

$$\left|\frac{\partial}{\partial\zeta}G(\zeta\pm i0)\right| \ll 1. \tag{13a}$$

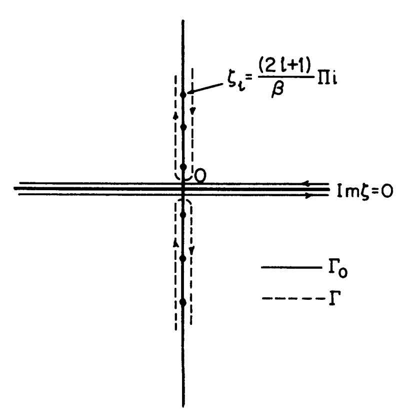

FIG. 3. Contours Γ and Γ_0 for the evaluation of the electronic self-energy part.

In particular,

$$\left|\frac{\partial}{\partial E_\mu^\lambda} G_\mu(E_\mu^\lambda \mp i0)\right| \ll 1. \tag{13b}$$

To evaluate the ladder series, it is convenient to define the external-field vertex parts (Λ) according to the diagrammatic relations shown in Fig. 4, and given by

$$\Lambda_{nn}(\zeta_l, \zeta_l+\hbar\omega_r)=y_n+\sum_{l'} \frac{J_{mn}^2 D^{(0)}(\zeta_l-\zeta_{l'})\,\Lambda_{mn}(\zeta_{l'}, \zeta_{l'}+\hbar\omega_r)}{[\zeta_{l'}-E_{m\lambda}^{(0)}-G_m(\zeta_{l'})][\zeta_{l'}+\hbar\omega_r-E_{m\lambda}^{(0)}-G_m(\zeta_{l'}+\hbar\omega_r)]}, \tag{14a}$$

$$\Lambda_{mn}(\zeta_l, \zeta_l+\hbar\omega_r)=\sum_{l'} \frac{J_{mn}^2 D^{(0)}(\zeta_{l'}-\zeta_l)\,\Lambda_{nn}(\zeta_{l'}, \zeta_{l'}+\hbar\omega_r)}{[\zeta_{l'}-E_{n\lambda}^{(0)}-G_n(\zeta_{l'})][\zeta_{l'}+\hbar\omega_r-E_{n\lambda}^{(0)}-G_n(\zeta_{l'}+\hbar\omega_r)]}. \tag{14b}$$

The l' summation can be performed according to (9). However, the integration contours Γ, Γ_0 are given in this case in Fig. 5. In Appendix B, Eqs. (14) are evaluated and the result analytically continued to the real axis is given by the coupled transport equations,

$$-i\omega\Phi_{mn}=y_n+\frac{2\Gamma_n}{\hbar}(\Phi_{mn}-\Phi_{nn}),$$
$$-i\omega\Phi_{mn}=\frac{2\Gamma_m}{\hbar}(\Phi_{nn}-\Phi_{mn}), \tag{15}$$

where one defines

$$\Phi_{\mu n}=\frac{i\hbar\Lambda_{\mu n}(E_\mu^\lambda-i0, E_\mu^\lambda+\hbar\omega+i0)}{\hbar\omega+2i\Gamma_\mu} \quad (\mu=m,n). \tag{16}$$

In the above derivation use has been made of (12) and (13). It is seen in (15) that the ladder series give rise to the scattering-in term.[11]

The correlation function is then given by the diagrammatic relation shown in Fig. 6, which can be written as[12]

$$F_{xy}(\hbar\omega_r)=\lim_{\beta\lambda\to\infty}\frac{Z_p^0 e^{\beta\lambda}}{Z}\sum_{mn}\frac{-1}{\beta}\sum_l\left\{\frac{x_n\Lambda_{nn}(\zeta_l, \zeta_l+\hbar\omega_r)}{[\zeta_l-E_{n\lambda}^{(0)}-G_n(\zeta_l)][\zeta_l+\hbar\omega_r-E_{n\lambda}^{(0)}-G_n(\zeta_l+\hbar\omega_r)]}\right.$$
$$\left.+\frac{x_m\Lambda_{mn}(\zeta_l, \zeta_l+\hbar\omega_r)}{[\zeta_l-E_{m\lambda}^{(0)}-G_m(\zeta_l)][\zeta_l+\hbar\omega_r-E_{m\lambda}^{(0)}-G_m(\zeta_l+\hbar\omega_r)]}\right\}. \tag{17}$$

The evaluation of (17) is given in Appendix C. The result based on the assumption of (12) and (13) and analytically continued to the real axis is given by

$$F_{xy}(\hbar\omega+i0)=\frac{Z_p^0}{Z}\sum_{mn}\{x_n\beta e^{-\beta(\epsilon_n-E_p)}(i\hbar\omega\Phi_{nn}+y_n)+ix_m\beta\hbar\omega\Phi_{mn}e^{-\beta(\epsilon_m-E_p)}\}$$
$$=\frac{Z_p^0 e^{-\beta[(\epsilon_n+\epsilon_m)/2-E_p]}(x_m-x_n)(y_m-y_n)\Gamma}{Z\,2kT\cosh\beta\Delta E/2}\,\frac{1}{-i\hbar\omega+\Gamma}, \quad \Gamma=2(\Gamma_m+\Gamma_n), \quad \Delta E=\epsilon_n-\epsilon_m \tag{18}$$

where, as noted before, E_p is the polaron binding energy (negligible in the weak-coupling regime), and ϵ_μ is the renormalized electronic energy given by $E_\mu^\lambda=\epsilon_\mu-E_p+\lambda$ [cf. Eq. (8)]. One notes that the above result is independent of the choice of the origin of the coordinate. Using[13] $Z/Z_p^0=e^{-\beta(\epsilon_m-E_p)}+e^{-\beta(\epsilon_n-E_p)}$ $(\equiv Z_e)$ and inserting (18) into (3), one obtains finally

$$\sigma_{yy}(\omega)=\frac{ne^2|\vec{r}_n-\vec{r}_m|^2\cos^2\theta\,\Gamma}{4\hbar kT\cos^2\beta\Delta E/2}\,\frac{(\hbar\omega)^2-i\hbar\omega\Gamma}{(\hbar\omega)^2+\Gamma^2}, \tag{19}$$

where θ is the angle between the direction of (n, m) and the external field. One notes that (19) coinicides identically[14] with the expression derived by Pollak and Geballe[1(a)] in a semiclassical way (cf. Ref. 1, left-hand column of p. 1750).

As already mentioned, the approximation of Ref. 2 corresponds to retaining only the first diagram on the right-hand side of Fig. 4(a), discarding the rest of the diagrams with rungs in Fig. 4 (see the diagonal term in Eq. 6 of Ref. 2). Algebraically, this means setting $\Lambda_{nn}=y_n$ and $\Lambda_{mn}=0$ in (14). The correlation function is then given by

$$F_{xy}(\hbar\omega_r)=\lim_{\beta\lambda\to\infty}\frac{e^{\beta\lambda}}{Z_e}\sum_n\frac{-1}{\beta}\sum_l\frac{x_n y_n}{[\zeta_l-E_{n\lambda}^{(0)}-G_n(\zeta_l)][\zeta_l+\hbar\omega_r-E_{n\lambda}^{(0)}-G_n(\zeta_l+\hbar\omega_r)]},$$

which upon summing on ζ_l and analytically continuing to the real axis yields

$$F_{xy}(\hbar\omega+i0)=\lim_{\beta\lambda\to\infty}\frac{e^{\beta\lambda}}{Z_e}\sum_n\frac{x_ny_n\,(\partial f^{(-)}(E_n^\lambda)/\partial E_n^\lambda)\hbar\omega}{\hbar\omega+2i\Gamma_n}\;.$$

Hence

$$\mathrm{Re}\sigma_{yy}(\omega)=-\frac{ne^2}{\hbar}\sum_n y_n^2\lim_{\beta\lambda\to\infty}\frac{e^{\beta\lambda}(\partial f^{(-)}(E_n^\lambda)/\partial E_n^\lambda)}{Z_e}\;\frac{2\Gamma_n(\hbar\omega)^2}{(\hbar\omega)^2+(2\Gamma_n)^2}\;. \tag{20}$$

Choosing the coordinate origin such that $\vec{r}_n+\vec{r}_m=0$ and defining $\vec{r}=\vec{r}_n-\vec{r}_m$, one finds

$$\mathrm{Re}\sigma_{yy}(\omega)=\frac{ne^2}{\hbar}\sum_n\frac{r^2\cos^2\theta}{4}\left[\lim_{\beta\lambda\to\infty}\frac{e^{\beta\lambda}}{Z_e}\left(\frac{-\partial f^{(-)}(E_n^\lambda)}{\partial E_n^\lambda}\right)\right]\frac{2\Gamma_n(\hbar\omega)^2}{(\hbar\omega)^2+(2\Gamma_n)^2}\;.$$

The above result is equivalent[15] to the "indirect" absorption term in Eq. 11 of Ref. 2 apart from the factor in the bracket, which, if one does not project out the unphysical states, would be replaced by $-\partial f^{(-)}(\epsilon_n)/\partial\epsilon_n$. The cosine factor was incorrectly omitted. We note that (20) is not even invariant under the translation of the origin of the coordinate.

ACKNOWLEDGMENTS

We wish to thank S. E. Barnes and J. Zitkova-Wilcox for very helpful discussions on Abrikosov's projection method.

APPENDIX A

In this appendix we study some properties of the electronic self-energy part. This is given by (10), which may be written as

$$G(\zeta-i\eta 0)=\sum_{\vec{q}\pm}\frac{\pm\gamma_{\vec{q}}J_{mn}^2N(\pm\hbar\omega_{\vec{q}})}{\zeta-i\eta 0\pm\hbar\omega_{\vec{q}}}\qquad(\eta=\pm 1). \tag{A1}$$

After taking the angular average and using the Debye approximation,[16] $\gamma_{\vec{q}}$ is a function of frequency, i.e., $\gamma_{\vec{q}}\equiv\gamma(\hbar\omega_{\vec{q}})$. Introducing the phonon density of states $n(\hbar\omega_{\vec{q}})$, (A1) is rewritten as

$$G(\zeta-i\eta 0)=\int_0^\infty dx\,n(x)\gamma(x)\times J_{nm}^2\left\{\frac{N(x)}{\zeta-i\eta 0+x}\quad\frac{N(-x)}{\zeta-i\eta 0-x}\right\}. \tag{A2}$$

Defining

$$G(\zeta-i\eta 0)=M(\zeta)+i\eta\Gamma(\zeta), \tag{A3}$$

one obtains

$$\Gamma(\zeta)=-\pi J_{mn}^2n(\zeta)\gamma(\zeta)N(-\zeta),\qquad \zeta>0\quad\text{(phonon emission)}$$

$$\Gamma(\zeta)=\pi J_{mn}^2n(-\zeta)\gamma(-\zeta)N(-\zeta),\qquad \zeta<0\quad\text{(phonon absorption)} \tag{A4}$$

and the Kronig–Kramer's relation

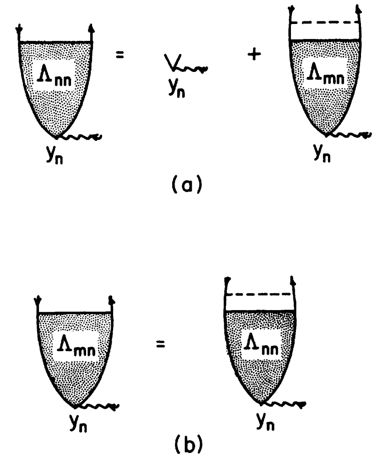

FIG. 4. Diagrammatic equations for external-field vertices.

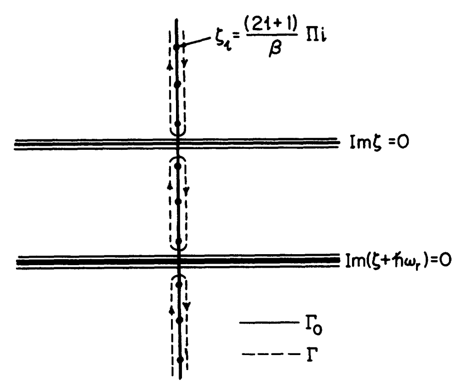

FIG. 5. Contours Γ and Γ_0 for the evaluation of the external-field vertex.

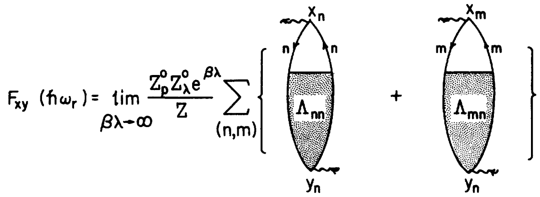

FIG. 6. Diagrammatic expression for the correlation function.

$$M(\zeta)=\frac{1}{\pi}\,\mathcal{P}\int_{-\infty}^{\infty}\frac{\Gamma(x)}{\zeta-x}\,dx\,. \tag{A5}$$

To estimate the magnitude of the derivative of the self-energy, one assumes $n(x)=C_1x^2$, $\gamma(x)=C_2/x$ (C_1, C_2 = constant) in conformance with the Debye spectrum and in view of the definition of $u_{\vec q}^{ac}$ given in the text just prior to Eq. (1). Then in view of (12) and assuming $|\beta\Delta E|$ not too large,

$$\left|\frac{\partial\Gamma(\zeta)}{\partial\zeta}\right|=\beta\Gamma_m\,\frac{e^{\beta\Delta E}-1}{\beta\Delta E}\left|\frac{\partial}{\partial y}\,\frac{y}{e^y-1}\right|\sim\beta\Gamma_m\ll 1$$

$$\text{(for all } y), \tag{A6}$$

$$\left|\frac{\partial^2\Gamma(\zeta)}{\partial\zeta^2}\right|=\beta^2\Gamma_m\,\frac{e^{\beta\Delta E}-1}{\beta\Delta E}\left|\frac{\partial^2}{\partial y^2}\,\frac{y}{e^y-1}\right|\sim\beta^2\Gamma_m\ll\beta,$$

where $y=-\beta\zeta$, $\Delta E=E_n^\lambda-E_m^\lambda$. In particular

$$\left|\frac{\partial\Gamma(E_m^\lambda-E_n^\lambda)}{\partial E_m^\lambda}\right|=\left|\frac{\partial\Gamma(E_m^\lambda-E_n^\lambda)}{\partial E_n^\lambda}\right|\ll 1, \tag{A7a}$$

$$\left|\frac{\partial^2\Gamma(E_m^\lambda-E_n^\lambda)}{\partial E_m^{\lambda 2}}\right|=\left|\frac{\partial^2\Gamma(E_m^\lambda-E_n^\lambda)}{\partial E_n^{\lambda 2}}\right|\ll\beta. \tag{A7b}$$

The derivative of real part is given by

$$\frac{\partial M(\zeta)}{\partial\zeta}=-\frac{1}{\pi}\,\mathcal{P}\int_{-\infty}^{\infty}\frac{[d\Gamma(x)/dx]}{\zeta-x}\,dx \tag{A8}$$

$$=\beta\Gamma_m\,\frac{e^{\beta\Delta E}-1}{\beta\Delta E}\,\frac{1}{\pi}$$

$$\times\,\mathcal{P}\int_{-\infty}^{\infty}\left[\frac{d}{dx}\left(\frac{xS(|x|)}{e^{-\beta x}-1}\right)\Big/(\zeta-x)\right]dx, \tag{A9}$$

where $S(x)$ is artificially introduced to insure that the phonon density of states vanishes beyond a certain upper limit. Therefore $S(x)\sim 1$ for $x\lesssim x_D$ (Debye energy) and $S(x)$ decays to zero above $x\sim x_D$. The integral is expected to be of order unity. Therefore if $\beta\Delta E$ is not too large,

$$\left|\frac{\partial M(\zeta)}{\partial\zeta}\right|\sim\beta\Gamma_m\ll 1. \tag{A10}$$

In particular

$$\left|\frac{\partial M(E_m^\lambda-E_n^\lambda)}{\partial E_m^\lambda}\right|=\left|\frac{\partial M(E_m^\lambda-E_n^\lambda)}{\partial E_n^\lambda}\right|\ll 1. \tag{A11a}$$

Furthermore

$$\left|\frac{\partial^2 M(E_m^\lambda-E_n^\lambda)}{\partial E_m^{\lambda 2}}\right|=\left|\frac{\partial^2 M(E_m^\lambda-E_n^\lambda)}{\partial E_n^{\lambda 2}}\right|\ll\beta. \tag{A11b}$$

The above estimation of the derivative of the self-energy is not correct at some points of ζ where one actually has weak divergence. These arise from the Van Hove singularities in the general form of the phonon density of states $n(x)$ which is given, for example, near a typical singularity $x\equiv x_0$, by

$$n(x)=n_1+C_3(x-x_0)^{1/2}\quad(n_1, C_3=\text{constant}). \tag{A12}$$

Hence from (A4) and (A8),

$$\frac{\partial\Gamma(x)}{\partial x}\propto\frac{1}{(x-x_0)^{1/2}}\,,\quad\frac{\partial M(x)}{\partial x}\propto\frac{1}{(x_0-x)^{1/2}}\,, \tag{A13}$$

which diverges at $x=x_0$. However, usually $x_0\gg\Delta E$ and (A7), (A11) are always valid.

APPENDIX B

In this appendix a derivation of (15) is given. As already explained in the text, one can replace the l' summations in (14) by integrations, introducing a contour Γ and then deforming it into Γ_0 as shown in Fig. 5. Here one assumes that $\Lambda(\zeta, \zeta+\hbar\omega_r)$ is continuous over the whole complex plane, with exception of two cuts $\mathrm{Im}\,\zeta=0$, $\mathrm{Im}(\zeta+h\omega_r)=0$, as can be proved *a posteriori*. By using (7) and by analytically continuing to the real axis, one thus obtains for (14)[17]

$$\Lambda_{\mu n}(\zeta-i0,\zeta+\hbar\omega+i0)=y_n\,\delta_{\mu n}+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\sum_{\vec q\pm}\pm\gamma_{\vec q}J_{nm}^2\left\{\frac{f^{(-)}(\zeta')+N(\pm\hbar\omega_{\vec q})}{\zeta-i0-\zeta'\pm\hbar\omega_{\vec q}}-\frac{f^{(-)}(\zeta'+\hbar\omega)+N(\pm\hbar\omega_{\vec q})}{\zeta+i0-\zeta'\pm\hbar\omega_{\vec q}}\right\}$$

$$\times\frac{\Lambda_{\bar\mu n}(\zeta'-i0,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'-i0)]\,[\zeta'+\hbar\omega-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+\hbar\omega+i0)]}+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\sum_{\vec q\pm}\pm\gamma_{\vec q}J_{nm}^2$$

$$\times\left\{\frac{[f^{(-)}(\zeta'+\hbar\omega)+N(\pm\hbar\omega_{\vec q})]\,\Lambda_{\bar\mu n}(\zeta'-i0,\zeta'+\hbar\omega-i0)}{[\zeta+i0-\zeta'\pm\hbar\omega_{\vec q}]\,[\zeta'-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'-i0)]\,[\zeta'+\hbar\omega-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+\hbar\omega-i0)]}\right.$$

$$\left.-\frac{[f^{(-)}(\zeta')+N(\pm\hbar\omega_{\vec q})]\,\Lambda_{\bar\mu n}(\zeta'+i0,\zeta'+\hbar\omega+i0)}{[\zeta'-i0-\zeta'\pm\hbar\omega_{\vec q}]\,[\zeta'-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+i0)]\,[\zeta'+\hbar\omega-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+\hbar\omega+i0)]}\right\}, \tag{B1a}$$

$$\Lambda_{\mu n}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)=y_n\,\delta_{\mu n}+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\sum_{\vec q\pm}\pm\gamma_{\vec q}J_{nm}^2$$
$$\times\frac{[f^{(-)}(\zeta')-f^{(-)}(\zeta'+\hbar\omega)]\,\Lambda_{\bar\mu n}(\zeta'-i0,\,\zeta'+\hbar\omega+i0)}{[\zeta+i\eta 0-\zeta'\pm\hbar\omega_{\vec q}][\zeta'-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'-i0)][\zeta'+\hbar\omega-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+\hbar\omega+i0)]}$$
$$+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\sum_{\vec q\pm}\frac{\pm\gamma_{\vec q}J_{mn}^2}{\zeta+i\eta 0-\zeta'\pm\hbar\omega_{\vec q}}\left\{\frac{[f^{(-)}(\zeta'+\hbar\omega)+N(\pm\hbar\omega_{\vec q})]\,\Lambda_{\bar\mu n}(\zeta'-i0,\,\zeta'+\hbar\omega-i0)}{[\zeta'-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'-i0)][\zeta'+\hbar\omega-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+\hbar\omega-i0)]}\right.$$
$$\left.-\frac{[f^{(-)}(\zeta')+N(\pm\hbar\omega_{\vec q})]\,\Lambda_{\bar\mu n}(\zeta'+i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+i0)][\zeta'+\hbar\omega-E_{\bar\mu\lambda}^{(0)}-G_{\bar\mu}(\zeta'+\hbar\omega+i0)]}\right\},\quad\text{(B1b)}$$

where $(\mu,\bar\mu)=(n,m)$ or (m,n), $\eta=\pm 1$. In the above derivation use has been made of the relation $f^{(-)}(\zeta'+\hbar\omega_r)=f^{(-)}(\zeta')$. Noting that the dominant contribution to the integrals in the above equations arises from near the resonances (i.e., $\zeta'\sim\lambda$) one can drop the Fermi factors. Therefore one obtains, using Eqs. (10) and (A3),

$$\Lambda_{nn}(\zeta-i0,\,\zeta+\hbar\omega+i0)=y_n+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\,\frac{2i\Gamma(\zeta-\zeta')\,\Lambda_{mn}(\zeta'-i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{m\lambda}^{(0)}-G_m(\zeta'-i0)][\zeta'+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta'+\hbar\omega+i0)]}$$
$$+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\left\{\frac{G(\zeta-\zeta'+i0)\,\Lambda_{mn}(\zeta'-i0,\,\zeta'+\hbar\omega-i0)}{[\zeta'-E_{m\lambda}^{(0)}-G_m(\zeta'-i0)][\zeta'+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta'+\hbar\omega-i0)]}\right.$$
$$\left.-\frac{G(\zeta-\zeta'-i0)\,\Lambda_{mn}(\zeta'+i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{m\lambda}^{(0)}-G_m(\zeta'+i0)][\zeta'+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta'+\hbar\omega+i0)]}\right\},\quad\text{(B2a)}$$

$$\Lambda_{mn}(\zeta-i0,\,\zeta+\hbar\omega+i0)=\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\,\frac{2i\Gamma(\zeta-\zeta')\,\Lambda_{nn}(\zeta'-i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'-i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega+i0)]}$$
$$+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\left\{\frac{G(\zeta-\zeta'+i0)\,\Lambda_{nn}(\zeta'-i0,\,\zeta'+\hbar\omega-i0)}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'-i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega-i0)]}\right.$$
$$\left.-\frac{G(\zeta-\zeta'-i0)\,\Lambda_{nn}(\zeta'+i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'+i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega+i0)]}\right\},\quad\text{(B2b)}$$

$$\Lambda_{nn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)=y_n+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\,G(\zeta-\zeta'+i\eta 0)\left\{\frac{\Lambda_{mn}(\zeta'-i0,\,\zeta'+\hbar\omega-i0)}{[\zeta'-E_{m\lambda}^{(0)}-G_m(\zeta'-i0)][\zeta'+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta'+\hbar\omega-i0)]}\right.$$
$$\left.-\frac{\Lambda_{mn}(\zeta'+i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{m\lambda}^{(0)}-G_m(\zeta'+i0)][\zeta'+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta'+\hbar\omega+i0)]}\right\},\quad\text{(B2c)}$$

$$\Lambda_{mn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)=\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\,G(\zeta-\zeta'+i\eta 0)\left\{\frac{\Lambda_{nn}(\zeta'-i0,\,\zeta'+\hbar\omega-i0)}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'-i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega-i0)]}\right.$$
$$\left.-\frac{\Lambda_{nn}(\zeta'+i0,\,\zeta'+\hbar\omega+i0)}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'+i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega+i0)]}\right\}.\quad\text{(B2d)}$$

First of all, to solve (B2c) and (B2d) one uses an iteration method. Namely, one assumes that the second term of (B2c) is very small and sets $\Lambda_{nn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)=y_n$ in (B2d). Then one substitutes the obtained value of $\Lambda_{mn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)$ into (B2c), etc. It will be shown that the series converges rapidly. Thus

$$y_n^{-1}\Lambda_{mn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)=\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}\,G(\zeta-\zeta'+i\eta 0)$$
$$\times\left\{\frac{1}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'-i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega-i0)]}-(-i0\to i0)\right\}.$$

For the quantity in the curly bracket, one introduces the identity

$$\frac{1}{[\zeta'-E_{n\lambda}^{(0)}-G_n(\zeta'\mp i0)][\zeta'+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta'+\hbar\omega\mp i0)]}$$

$$= \frac{1}{\hbar\omega}\left\{\frac{1}{\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' \mp i0)} - \frac{1}{\zeta' + \hbar\omega - E_{n\lambda}^{(0)} - G_n(\zeta' + \hbar\omega \mp i0)}\right\}$$

$$- \frac{(1/\hbar\omega)[G_n(\zeta' + \hbar\omega \mp i0) - G_n(\zeta' \mp i0)]}{[\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' \mp i0)][\zeta' + \hbar\omega - E_{n\lambda}^{(0)} - G_n(\zeta' + \hbar\omega \mp i0)]} . \quad \text{(B4)}$$

One then approximates, using (10),

$$\frac{1}{\hbar\omega}[G_n(\zeta' + \hbar\omega \mp i0) - G_n(\zeta' \mp i0)] = \frac{\partial}{\partial \zeta'} G(\zeta' - E_m^\lambda \mp i0). \quad \text{(B5)}$$

In Appendix A it is shown that the above quantity [right-hand side of (B5)] is very small (compared to unity) except for some weak divergences (inverse-square-root type) arising from the Van Hove singularities in the phonon density of states. Actually for the case when $\hbar\omega \sim G_n$, the left-hand side is always smaller than unity and we are overestimating this value near the divergences by the above approximation. This kind of divergence appears throughout the calculation. However, we will demonstrate in the following that the contribution (ΔI) from said type of divergence is negligibly small; the total contribution (defined as I) from the last term of (B4) to (B3) is given by

$$I = \int_{-\infty}^{\infty} \frac{d\zeta'}{2\pi i} G(\zeta - \zeta' + i\eta 0) \frac{\partial G(\zeta' \mp i0 - E_m^\lambda)/\partial \zeta'}{[\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' \mp i0)][\zeta' + \hbar\omega - E_{n\lambda}^{(0)} - G_n(\zeta' + \hbar\omega \mp i0)]} . \quad \text{(B6)}$$

As shown in Appendix A, one has, in the vicinity of the divergence,

$$\frac{\partial}{\partial \zeta'} G(\zeta' - E_m^\lambda - i\eta 0) \propto \frac{1}{(E_m^\lambda - \zeta' + x_0)^{1/2}}, \quad \Delta E \ll x_0 \leq x_D \quad (x_D \hbar^{-1} = \text{Debye frequency}). \quad \text{(B7)}$$

Since the quantity multiplying $\partial G(\zeta' - E_m^\lambda \mp i0)/\partial \zeta'$ has no singularity over a sufficiently large range (of order $\Delta E \equiv E_n^\lambda - E_m^\lambda$) near the divergence, one estimates

$$|\Delta I| \sim \left|\frac{G_1(G_2 - G_3)}{x_0^2}\right| \ll 1, \quad \text{(B8)}$$

where G_1, G_2, G_3 are values of the self-energy at intermediate, upper limit, lower limit of the integration range. Therefore in view of (A6) and (A10) one can neglect (B6) or the last term of (B4).

To calculate the contribution from the first term of (B4), one changes $\zeta' + \hbar\omega \to \zeta'$ for the second term in the curly bracket, obtaining

$$y_n^{-1}\Lambda_{mn}(\zeta + i\eta 0, \zeta + \hbar\omega + i\eta 0) = \int_{-\infty}^{\infty} \frac{d\zeta'}{2\pi i} \frac{1}{\hbar\omega} [G(\zeta - \zeta' + i\eta 0) - G(\zeta - \hbar\omega - \zeta' + i\eta 0)]$$

$$\times \left\{\frac{1}{\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' - i0)} - \frac{1}{\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' + i0)}\right\}$$

$$= -\frac{\partial}{\partial \zeta} \int_{-\infty}^{\infty} \frac{d\zeta'}{2\pi i} G(\zeta - \zeta' + i\eta 0) \frac{2i\Gamma_n(\zeta')}{[\zeta' - E_{n\lambda}^{(0)} - M_n(\zeta')]^2 + \Gamma_n(\zeta')^2} .$$

Approximating

$$\frac{1}{\pi} \frac{\Gamma_n(\zeta')}{[\zeta' - E_{n\lambda}^{(0)} - M(\zeta')]^2 + \Gamma_n(\zeta')^2} \simeq \delta(\zeta' - E_n^\lambda), \quad \text{(B9)}$$

one obtains

$$y_n^{-1}\Lambda_{mn}(\zeta + i\eta 0, \zeta + \hbar\omega + i\eta 0) = -\frac{\partial}{\partial \zeta} G(\zeta - E_n^\lambda + i\eta 0) = \frac{\partial}{\partial E_n^\lambda} G(\zeta - E_n^\lambda + i\eta 0). \quad \text{(B10)}$$

It is to be noted that the approximations leading from (B3) to (B10) are equivalent to the replacement[18]

$$\frac{1}{[\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' \mp i0)][\zeta' + \hbar\omega - E_{n\lambda}^{(0)} - G_n(\zeta' + \hbar\omega \mp i0)]} \to -\frac{\partial}{\partial \zeta'} \frac{1}{\zeta' - E_{n\lambda}^{(0)} - G_n(\zeta' \mp i0)}$$

$$= \frac{\partial}{\partial \zeta'}\left\{\pm \pi i \delta(\zeta' - E_n^\lambda) + \mathcal{P} \frac{1}{\zeta' - E_n^\lambda}\right\}. \quad \text{(B11)}$$

Turning, now, to the evaluation of (B2c), one has from (B10) and (B11)

$$y_n^{-1}\Lambda_{nn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)=1+\int_{-\infty}^{\infty}\frac{d\zeta'}{2\pi i}G(\zeta-\zeta'+i\eta 0)\left\{-\frac{\partial}{\partial E_n^\lambda}M(\zeta'-E_n^\lambda)\frac{\partial}{\partial\zeta'}\delta(\zeta'-E_m^\lambda)2\pi i+2i\frac{\partial}{\partial E_n^\lambda}\Gamma(\zeta'-E_n^\lambda)\frac{\partial}{\partial\zeta'}\mathcal{P}\frac{1}{\zeta'-E_m^\lambda}\right\}$$

$$=1+\frac{1}{\partial E_m^\lambda}G(\zeta-E_m^\lambda+i\eta 0)\frac{\partial}{\partial E_n^\lambda}M(E_m^\lambda-E_m^\lambda)-G(\zeta-E_m^\lambda+i\eta 0)\frac{\partial^2}{\partial E_n^{\lambda 2}}M(E_m^\lambda-E_n^\lambda)+\left(\frac{\partial}{\partial E_n^\lambda}\frac{\partial}{\partial\zeta}+\frac{\partial^2}{\partial E_n^{\lambda 2}}\right)\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{1}{\zeta'-E_m^\lambda}G(\zeta-\zeta'+i\eta 0)\Gamma(\zeta'-E_n^\lambda)d\zeta'. \quad \text{(B12)}$$

To estimate roughly the order of magnitude of the last term, one assigns a typical value to $G(\zeta'-\zeta-i\eta 0)\sim G(E_m^\lambda-\zeta-i\eta 0)$ and then takes this factor out of the integral:

$$\sim\left(\frac{\partial}{\partial E_n^\lambda}\frac{\partial}{\partial\zeta}+\frac{\partial^2}{\partial E_n^{\lambda 2}}\right)\left\{G(\zeta-E_m^\lambda+i\eta 0)\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\Gamma(\zeta'-E_n^\lambda)}{\zeta'-E_m^\lambda}d\zeta'\right\}=-\left(\frac{\partial}{\partial E_n^\lambda}\frac{\partial}{\partial\zeta}+\frac{\partial^2}{\partial E_n^{\lambda 2}}\right)\{G(\zeta-E_m^\lambda+i\eta 0)M(E_m^\lambda-E_n^\lambda)\}. \quad \text{(B13)}$$

Therefore this term is approximately of the same order of magnitude as the second and third terms, and can be discarded (as being of the same order). Using (12) and (A11b) one further neglects the third term of (B12), obtaining

$$y_n^{-1}\Lambda_{nn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)-1\sim\frac{\partial}{\partial E_n^\lambda}M(E_m^\lambda-E_n^\lambda)\frac{\partial}{\partial E_m^\lambda}G(\zeta-E_m^\lambda+i\eta 0). \quad \text{(B14)}$$

The right-hand side of (B14) should not be taken literally; it represents only the order of magnitude of the terms in question. Terms generated by one more iteration are smaller by a factor of $\partial G(E_n^\lambda-E_m^\lambda\pm i0)/\partial E_n^\lambda$. One also notes that in view of (A6) and (A10) the right-hand side of (B10) and (B14) are small except for some weak divergences already discussed in Appendix A. However, as demonstrated, these divergences are quenched by the large denominators of the electronic propagators (which become off resonant at these divergences), and are therefore not significant for the purpose of intergrations. In summary, the solutions of (B2c) and (B2d) are (to order of magnitude Γ/kT or better)

$$\begin{aligned} y_n^{-1}\Lambda_{mn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)&=0,\\ y_n^{-1}\Lambda_{nn}(\zeta+i\eta 0,\,\zeta+\hbar\omega+i\eta 0)&=1. \end{aligned} \quad \text{(B15)}$$

We are now to evaluate (B2a) and (B2b). In view of (B15) and our previous discussions leading to (B15), we can drop the second integral of (B2a) and (B2b). To evaluate the remaining integrals in (B2a) and (B2b) one approximates in accordance with (B10):

$$\frac{1}{[\zeta'-E_{\mu\lambda}^{(0)}-G_\mu(\zeta'-i0)][\zeta'+\hbar\omega-E_{\mu\lambda}^{(0)}-G_\mu(\zeta'+\hbar\omega+i0)]}$$

$$=\frac{1}{\hbar\omega-G_\mu(\zeta'+\hbar\omega+i0)+G_\mu(\zeta'-i0)}\left\{\frac{1}{\zeta'-E_{\mu\lambda}^{(0)}-G_\mu(\zeta'-i0)}-\frac{1}{\zeta'+\hbar\omega-E_{\mu\lambda}^{(0)}-G_\mu(\zeta'+\hbar\omega+i0)}\right\}$$

$$\simeq\frac{2\pi i\delta(\zeta'-E_\mu^\lambda)}{\hbar\omega+G_\mu(E_\mu^\lambda-i0)-G_\mu(E_\mu^\lambda+\hbar\omega+i0)}\simeq\frac{2\pi i\delta(\zeta'-E_\mu^\lambda)}{\hbar\omega+2i\Gamma_\mu}, \quad \text{(B16)}$$

where the last approximation is due to (A6) and (A10). Therefore one finds

$$\begin{aligned} \Lambda_{nn}(\zeta-i0,\,\zeta+\hbar\omega+i0)&=y_n+\frac{2\Gamma(\zeta-E_m^\lambda)}{\hbar}\Phi_{mn},\\ \Lambda_{mn}(\zeta-i0,\,\zeta+\hbar\omega+i0)&=\frac{2\Gamma(\zeta-E_n^\lambda)}{\hbar}\Phi_{nn}, \end{aligned} \quad \text{(B17)}$$

where Φ_{mn} and Φ_{nn} are defined by relation (16). Eliminating the Λ's on the left-hand side of (B17), one has [with $\Gamma_n\equiv\Gamma(E_n^\lambda-E_m^\lambda)$, $\Gamma_m=\Gamma(E_m^\lambda-E_n^\lambda)$]

$$\left(-i\omega+\frac{2\Gamma_n}{\hbar}\right)\Phi_{nn}=y_n+\frac{2\Gamma_n}{\hbar}\Phi_{mn}, \quad \text{(B18b)}$$

$$\left(-i\omega+\frac{2\Gamma_m}{\hbar}\right)\Phi_{mn}=\frac{2\Gamma_m}{\hbar}\Phi_{nn}, \quad \text{(B18b)}$$

which are obviously equivalent to (15).

APPENDIX C

In this Appendix (17) is evaluated. One performs the l summation by replacing

$$\sum_l (\cdots) \to \frac{\beta}{2\pi i}\int_\Gamma d\zeta\, f^{(-)}(\zeta)(\cdots)$$

and then deforming the contour Γ into Γ_0 as shown in Fig. 5. The one obtains

$$F_{xy}(\hbar\omega+i0) = -\lim_{\beta\lambda\to\infty}\frac{Z_p^0 e^{\beta\lambda}}{Z}\sum_{mn}\Bigg\{x_n\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi i}\Bigg[\frac{[f^{(-)}(\zeta)-f^{(-)}(\zeta+\hbar\omega)]\Lambda_{nn}(\zeta-i0,\zeta+\hbar\omega+i0)}{[\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)][\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)]}$$

$$+\frac{f^{(-)}(\zeta+\hbar\omega)\Lambda_{nn}(\zeta-i0,\zeta+\hbar\omega-i0)}{[\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)][\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega-i0)]}-\frac{f^{(-)}(\zeta)\Lambda_{nn}(\zeta+i0,\zeta+\hbar\omega+i0)}{[\zeta-E_{n\lambda}^{(0)}-G_n(\zeta+i0)][\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)]}\Bigg]$$

$$+x_m\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi i}\Bigg[\frac{[f^{(-)}(\zeta)-f^{(-)}(\zeta+\hbar\omega)]\Lambda_{mn}(\zeta-i0,\zeta+\hbar\omega+i0)}{[\zeta-E_{m\lambda}^{(0)}-G_m(\zeta-i0)][\zeta+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta+\hbar\omega+i0)]}$$

$$+\frac{f^{(-)}(\zeta+\hbar\omega)\Lambda_{mn}(\zeta-i0,\zeta+\hbar\omega-i0)}{[\zeta-E_{m\lambda}^{(0)}-G_m(\zeta-i0)][\zeta+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta+\hbar\omega-i0)]}-\frac{f^{(-)}(\zeta)\Lambda_{mn}(\zeta+i0,\zeta+\hbar\omega+i0)}{[\zeta-E_{m\lambda}^{(0)}-G_m(\zeta+i0)][\zeta+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta+\hbar\omega+i0)]}\Bigg]\Bigg\}. \tag{C1}$$

Using (B15) one simplifies (C1) as

$$F_{xy}(\hbar\omega+i0) = -\lim_{\beta\lambda\to\infty}\frac{Z_p^0 e^{\beta\lambda}}{Z}\sum_{mn}\Bigg\{x_n\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi i}\Bigg[\frac{[f^{(-)}(\zeta)-f^{(-)}(\zeta+\hbar\omega)]\Lambda_{mn}(\zeta-i0,\zeta+\hbar\omega+i0)}{[\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)][\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)]}$$

$$+y_n f^{(-)}(\zeta)\Bigg(\frac{1}{[\zeta-\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta-\hbar\omega-i0)][\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)]}$$

$$-\frac{1}{[\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)][\zeta-E_{\lambda n}^{(0)}-G_n(\zeta+i0)]}\Bigg)\Bigg]$$

$$+x_m\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi i}\frac{[f^{(-)}(\zeta)-f^{(-)}(\zeta+\hbar\omega)]\Lambda_{mn}(\zeta-i0,\zeta+\hbar\omega+i0)}{[\zeta-E_{m\lambda}^{(0)}-G_m(\zeta-i0)][\zeta+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta+\hbar\omega+i0)]}\Bigg\}. \tag{C2}$$

The most important contribution arises from the resonances. Although the contribution from $\zeta \ll \lambda$ (i.e., $\zeta\sim$ finite) appears to be more important (due to the Fermi factors), this will be shown to be negligible at the end of this appendix. Thus using (16), (B11) and (B16), and approximating to the lowest order in $\beta\hbar\omega$,[19]

$$\left.\begin{array}{c} f^{(-)\prime}(E_n^\lambda) \\ {[f^{(-)}(E_n^\lambda+\hbar\omega)-f^{(-)}(E_n^\lambda)]/\hbar\omega} \end{array}\right\} \cong e^{-\beta\lambda}e^{-\beta(\epsilon_n-E_p)},$$

one obtains

$$F_{xy}(\hbar\omega+i0) = -\frac{Z_p^0}{Z}\sum_{mn}\{-x_n[i\beta\hbar\omega\Phi_{nn}e^{-\beta(\epsilon_n-E_p)}+\beta y_n e^{-\beta(\epsilon_n-E_p)}]-ix_m\beta\hbar\omega\Phi_{mn}e^{-\beta(\epsilon_m-E_p)}\}, \tag{C3}$$

In the above ϵ_μ is the renormalized electronic energy given by $E_\mu^\lambda = \epsilon_\mu - E_p + \lambda$ [cf. Eq. (8)]. Inserting the solution of (15), namely,

$$\Phi_{nn} = \frac{y_n(1-2\Gamma_m/i\hbar\omega)}{-i\hbar\omega+\Gamma}, \quad \Phi_{mn} = \frac{-2\Gamma_m y_n/i\hbar\omega}{-\hbar\omega+\Gamma} \quad [\Gamma = 2(\Gamma_n+\Gamma_m)] \tag{C4}$$

into (C3), one obtains

$$F_{xy}(\hbar\omega+i0) = -\frac{Z_p^0}{Z}\sum_{mn}\frac{\beta}{-i\hbar\omega+\Gamma}\{2x_m y_n\Gamma_m e^{-\beta(\epsilon_m-E_p)}-2x_n y_n\Gamma_n e^{-\beta(\epsilon_n-E_p)}\}, \tag{C5}$$

which in view of the detailed balance condition $\Gamma_m e^{-\beta\epsilon_m} = \Gamma_n e^{-\beta\epsilon_n}$ leads to (18).

It remains to be shown, however, that the off-resonance contribution from $\zeta \ll \lambda$ is negligible. To show this one substitutes (B15) and (B17) into (C1) and rearranges terms:

$$F_{xy}(\hbar\omega+i0) = -\lim_{\beta\lambda\to\infty}\frac{Z_p^0 e^{\beta\lambda}}{Z}\sum_{mn}\Bigg\{x_n\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi i}\frac{(2/\hbar)[f^{(-)}(\zeta)-f^{(-)}(\zeta+\hbar\omega)]\Gamma(\zeta-E_m^\lambda)\Phi_{mn}}{[\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)][\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)]}$$

$$+\frac{y_n f^{(-)}(\zeta)}{\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)}\ \frac{2i\Gamma(\zeta-E_m^\lambda)}{[\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)][\zeta-E_{n\lambda}^{(0)}-G_n(\zeta+i0)]}$$

$$+\frac{y_n f^{(-)}(\zeta+\hbar\omega)}{\zeta-E_{n\lambda}^{(0)}-G_n(\zeta-i0)}\ \frac{2i\Gamma(\zeta+\hbar\omega-E_m^\lambda)}{[\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega-i0)][\zeta+\hbar\omega-E_{n\lambda}^{(0)}-G_n(\zeta+\hbar\omega+i0)]}\Bigg]$$

$$+x_m\int_{-\infty}^{\infty}\frac{d\zeta}{2\pi i}\ \frac{(2/\hbar)[f^{(-)}(\zeta)-f^{(-)}(\zeta+\hbar\omega)]\Gamma(\zeta-E_n^\lambda)\,\Phi_{nn}}{[\zeta-E_{m\lambda}^{(0)}-G_m(\zeta-i0)][\zeta+\hbar\omega-E_{m\lambda}^{(0)}-G_m(\zeta+\hbar\omega+i0)]}\Bigg\}\ . \qquad (C6)$$

The imaginary part of the self-energy, $\Gamma(\zeta-E_\mu^\lambda)$ vanishes for $E_\mu^\lambda-\zeta>x_D$ due to the absence of the phonon density of states. Therefore there is no contribution to the integrations in (C6) from the region $\psi\ll\lambda$.

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[1](a) M. Pollak and T. H. Geballe, Phys. Rev. **122**, 1742 (1961); (b)M. Pollak, Philos. Mag. **23**, 519 (1971).

[2]A. Aldea, Z. Phys. **244**, 206 (1971).

[3]J. Schnakenberg, Phys. Status Solidi **28**, 623 (1968).

[4]It may be remarked that $\vec{p}$ is invariant with respect to the canonical transformation of Ref. 3.

[5]The treatment in Ref. 2 based on the standard temperature-diagram technique of a grand-canonical ensemble of fermions includes, incorrectly, contributions from the unphysical states.

[6]A. A. Abrikosov, Physica (Utr.) **2**, 5 (1965).

[7]The disconnected diagrams turn out to be of the order $e^{-\beta\lambda}$ smaller. Therefore they are discarded.

[8]T. Holstein, Ann. Phys. (N.Y.) **29**, 410 (1964).

[9]We are assuming $\hbar\omega\sim\Gamma_j$, where Γ_j is the imaginary component of the electron self-energy part; as may be seen below [cf. Eq. (10)] and in Appendix A, Γ_j is proportional to J_{nm}^2 (in fact, more accurately also to $\langle B_{nm}\rangle^2$, which, in the weak-coupling approximation, appropriate to the physical situation in doped elemental semiconductors, may be equated to unity).

[10]In the weak-coupling approximation, $\Sigma_q u_q \ll 1$, so that (a) $\langle B_{mn}\rangle\to 1$, (b) in the expansion of the exponential of (6), terms of quadratic or higher order in the exponential argument may be discarded.

[11]Namely, (14a) and (14b), from which (15) are derived, are the algebraic equivalents of the diagrammatic equations of Fig. 4; these in turn are equivalent to the summation of the ladder diagrams to all orders in the number of rungs.

[12]The minus sign arises from closing the fermion loop.

[13]This can readily be obtained by using Abrikosov's method. This relation simply reflects the fact that "dressed" energy ϵ_μ replaces the "bare" energy $\epsilon_\mu^{(0)}$ as one includes the effect of the perturbation to the unperturbed electronic distribution function $Z_e^0\equiv Z^0/Z_p^0=e^{-\beta(\epsilon_m^{(0)}-E_p)}+e^{-\beta(\epsilon_n^{(0)}-E_p)}$.

[14]Our definition $\sigma(\omega)$ corresponds to their $\sigma(-\omega)$.

[15]$2\Gamma_n$ in this work corresponds to Γ_n in Ref. 2.

[16]This approximation is valid, because the low-frequency phonons $[\hbar\omega_q\sim(\epsilon_n^{(0)}-\epsilon_m^{(0)})]$ are important.

[17]The detailed manipulation leading to Eqs. (B1) are essentially identical to the procedure followed in Sec. III of Ref. 8 (especially pp. 441–443).

[18]Namely, the substitution of (B11) into (B3) yields (B10) directly. The replacement (B11) is also discussed in Ref. 8, Sec. III, especially pp. 443(bottom)–445(top). In our case, one does not have k integration as in Ref. 8. However, in its place, we have a ζ integration, in which factors other than the "resonance denominators" [left-hand side of (B11)] vary on an energy scale $\sim kT$. For the applicability of (B11) it is necessary and sufficient that (a) $\Gamma(\zeta')\ll kT$ and (b) $\hbar\omega M'(\zeta')\ll kT$. These are both valid from Appendix A.

[19] $f^{(-)\prime}(E_n^\lambda)$ arises from integration by parts of the second integral of (C2) after use of (B11).