Mobility of Polarons

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(Received 2 September 1965)

The dc mobility of electrons is considered for scattering by acoustical and optical phonons. It is shown that the vertex terms (ladder diagrams) in the mobility integral can be partially summed to all orders of perturbation theory. These vertex terms are shown to be important for acoustic-phonon scattering. The sum of the ladder diagrams yields an effective energy width (inverse lifetime) with the $1-\cos\theta$ term, in agreement with transport theory. For polar coupling to optical phonons, the ladder diagrams can still be summed but are shown to be unimportant at low temperatures.

I. INTRODUCTION

A MANY-body calculation of most transport phenomena requires the evaluation of a two-particle correlation function.[1] This, in practice, separates into finding a one-particle Green's function and the vertex function. The one-particle Green's function is typically obtained by finding the lowest order terms in the self-energy. But finding the vertex function has been an enigma. In some cases, it is approximated by its lowest corrections, such as in Fig. 1(b). In other cases, one has to sum the ladder diagrams of Fig. 1 in order to find the correct result.

The calculation of polaron dc mobility limited by acoustical-phonon scattering is an example of when the ladder diagrams must be summed.[2-4] The purpose of the present study is to actually calculate and sum parts of the ladder diagrams of Fig. 1. In Sec. II, a prescription is derived whereby a vertex correction of any configuration of phonons may be written down by inspection. This allows one to take any vertex term and immediately sift out its largest contribution. In the low-temperature ($T\rightarrow 0$) and weak-coupling limit, the important terms in the ladder diagram can then be summed.

This procedure is applied to acoustical-phonon interactions in Sec. III. Starting from the Kubo[5] equation for the mobility, and by making several approximations, the most important terms in the ladder diagram are summed. This summation yields the *transport* equation result for the mobility; the transport form has the $(1-\cos\theta)$ term in the scattering integral. This result establishes the connection between the Kubo and transport forms of the mobility evaluation. The approximations, which are introduced to relate the transport and Kubo formulations, provide insight into the areas of applicability of the transport result.

The vertex corrections to the dc mobility for scattering by optical phonons is examined in Sec. IV. Langreth and Kadanoff[3] recently calculated the low-temperature mobility of electrons in polar crystals. They found that the diagram of Fig. 1(a) gave a mobility contribution $\sim\alpha^{-1}$, while Fig. 1(b) gave one $\sim\alpha^0$, and rightly predicted that other diagrams were either $\sim\alpha^{-1}$ or unimportant. We have calculated the mobility terms of order α^{-1} and α^0 from all of the diagrams in Fig. 1 and Fig. 3. These additional vertex terms, which may be summed to all orders, add correction terms $\sim(T/\omega_0)^{1/2}$ and are unimportant at low temperatures.

II. VERTEX TERMS

The dc mobilities will be calculated using the Kubo formalism. It is easiest to use the Matsubara[6] Green's functions. Following Abrikosov, Gorkov, and Dzyaloshinski,[1] the mobility at finite temperatures is found by evaluating the current-current Green's function:

$$P(\mathbf{r}-\mathbf{r}',\tau-\tau')=\tfrac{1}{3}\langle T_\tau \mathbf{j}(\mathbf{r},\tau)\cdot\mathbf{j}(\mathbf{r}',\tau')\rangle\,. \quad (2.1)$$

In Fourier transform space, this means evaluating

$$P(k)=-\frac{e^2}{3\beta m^2}\sum_{p_n}\int\frac{d^3p}{(2\pi)^3}\mathcal{G}(p)\mathcal{G}(p+k)\mathbf{p}\cdot\boldsymbol{\Gamma}(p,k)\,, \quad (2.2)$$

where p and k stand for four-vectors $p=(\mathbf{p},ip_n)$, etc., and $\beta=1/k_BT$. The Green's function and self-energy are

$$\mathcal{G}(p)=[ip_n-\epsilon_p-\Sigma(p)]^{-1}, \quad (2.3a)$$

$$\Sigma(p)=-T\sum_{q_n}\int\frac{d^3q}{(2\pi)^3}\mathcal{G}(p+q)\mathfrak{D}(q)\Gamma(p,q)\,, \quad (2.3b)$$

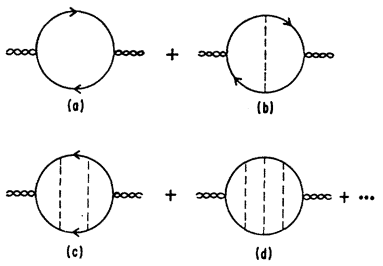

FIG. 1. Vertex diagrams discussed in the text. These are the ladder diagrams.

[1] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).
[2] K. Baumann and J. Ranninger, Ann. Phys. (N. Y.) **20**, 157 (1962).
[3] D. C. Langreth and L. P. Kadanoff, Phys. Rev. **133**, A1070 (1964). This article, and Ref. 4, contain references to other polaron mobility calculations.
[4] *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Plenum Press, New York, 1962).
[5] R. Kubo, Can. J. Phys. **34**, 1274 (1956).
[6] T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955).

and the vertex functions are defined in the usual way. The retarded Green's function is obtained by the analytical continuation $ip_n \to \epsilon + i\delta$:

$$\mathcal{G}(\mathbf{p},ip_n) \xrightarrow[ip_n \to \epsilon+i\delta]{} G_R(\mathbf{p},\epsilon)\,, \tag{2.4a}$$

$$P(k,i\omega_n) \xrightarrow[i\omega_n \to \omega+i\delta]{} P_R(\mathbf{k},\omega)\,. \tag{2.4b}$$

The spectral function is

$$A(p,\epsilon) = -2\,\mathrm{Im}G_R(p,\epsilon)\,. \tag{2.5}$$

The density of the electrons is assumed small enough that they do not affect the phonons, and $D(q)$ can be replaced by $D^{(0)}(q)$.

The mobility is found by using the above definitions to evaluate $P(k)$. This immediately gives the retarded function $P_R(k,\omega)$, and the dc mobility is given by[1]

$$\mu = (en_0)^{-1} \lim_{\omega \to 0,\, \mathbf{k} \to 0} \omega^{-1}\,\mathrm{Im}P_R(\mathbf{k},\omega)\,, \tag{2.6}$$

where n_0 is the density of electrons. The limit $\mathbf{k} \to 0$ presents no problem and will be taken in the starting equation (2.2).

In actually calculating a mobility for a given electron-phonon interaction, the self-energies are usually evaluated by considering just the lowest order diagrams. This hopefully gives a reasonably accurate Green's function to use in (2.2). Assuming that a Green's function is known, the vector vertex term in (2.2) still has to be found. One method is to approximate $\boldsymbol{\Gamma}$ by its first term, $\boldsymbol{\Gamma}^{(0)} = \mathbf{p}$. The Matsubara sum over P_n can be evaluated, giving

$$P^{(0)}(i\omega_n) = \frac{e^2}{3m^2}\int \frac{d^3p}{(2\pi)^4} d\epsilon p^2 A(p,\epsilon) n_F(\epsilon) \times [\mathcal{G}(\mathbf{p},\epsilon+i\omega_n) + \mathcal{G}(\mathbf{p},\epsilon-i\omega_n)]\,. \tag{2.7}$$

The analytical continuation of $P(i\omega_n)$ to $P_R(\omega)$ just changes $\mathcal{G}$ to G_R. The lowest order contribution to the mobility is

$$\mu^{(0)}(\omega) = \frac{e}{6n_0m^2}\int \frac{d^3p\,d\epsilon}{(2\pi)^4} p^2 A(p,\epsilon) A(p,\epsilon+\omega) \times \left[\frac{n_F(\epsilon) - n_F(\epsilon+\omega)}{\omega}\right]. \tag{2.8a}$$

For nondegenerate systems, this reduces to ($\omega \to 0$)

$$\mu^{(0)} = \frac{e\beta}{6n_0m^2}\int \frac{d^3p\,d\epsilon}{(2\pi)^4} p^2 A(p,\epsilon)^2 n_F(\epsilon)\,. \tag{2.8b}$$

This is a well-known result.[2,3] The above derivation of (2.8) is very efficient. More importantly, the derivation of $\mu^{(n)}$ for an arbitrary number of phonons (n) in the vector vertex $\boldsymbol{\Gamma}^{(n)}$ is no more complicated than this derivation of the zeroth term.

When actually evaluating (2.8b) it is convenient to use the "quasiparticle approximation"

$$A(p,\epsilon)^2 \approx 4\pi \frac{\delta(\epsilon - E(p))}{\Gamma(p)} Z(p)\,, \tag{2.9}$$

where

$$\Gamma(p) = -2\,\mathrm{Im}\sum_R (p, E(p))\,, \tag{2.10a}$$

$$Z(p) = \left(1 - \frac{\partial}{\partial\epsilon}\mathrm{Re}\sum_R(p,\epsilon)\right)^{-1}\Bigg|_{\epsilon = E(p)}\,, \tag{2.10b}$$

and where $\sum_R$ is the retarded self-energy and $E(p)$ is the quasiparticle energy. Since $\Gamma(p)$ is proportional to the electron-phonon coupling constant g, then $\mu^{(0)} \sim g^{-1}$. For $g \ll 1$, one can write the mobility as a power series in g:

$$\mu = \frac{a_{-1}}{g} + a_0 g^0 + a_1 g + \cdots\,. \tag{2.11}$$

A perturbation theory is only useful if the mobility can be found after evaluating a few terms. One asks the question whether, after evaluating $\mu^{(0)}$, all terms of order g^{-1} have been evaluated. Unfortunately, the answer to that question is "no." This is demonstrated below by evaluating the major vertex corrections, which are the ladder diagrams indicated in Fig. 1.

A generalized vertex diagram is indicated in Fig. 2, where the various phonon lines can be connected in all possible combinations For n phonons, the vector vertex is

$$\mathbf{p}\cdot\boldsymbol{\Gamma}^{(n)} = (-)^n\beta^{-n} \sum_{q_{1n}q_{2n}\cdots} \int \frac{d^3q_1\cdots d^3q_n}{(2\pi)^{3n}} \times V(q_1)\cdots V(q_n)\mathbf{p}\cdot(\mathbf{p}+\mathbf{q}_1+\cdots\mathbf{q}_n) \times \mathfrak{F}^{(n)}(p,\, p+q_1,\, p+q_1+q_2,\cdots) \times D^{(0)}(q_1)D^{(0)}(q_2)\text{—}D^{(0)}(q_n)\,, \tag{2.12a}$$

$$\mathfrak{F}^{(n)} = \mathcal{G}(p+k)\mathcal{G}(p+k+q_1')\cdots \times \mathcal{G}(p)\mathcal{G}(p+q_1)\cdots\,. \tag{2.12b}$$

Terms in the mobility proportional to the density of electrons are ignored. When the Matsubara sum is taken over phonon frequencies q_n, there are terms proportional

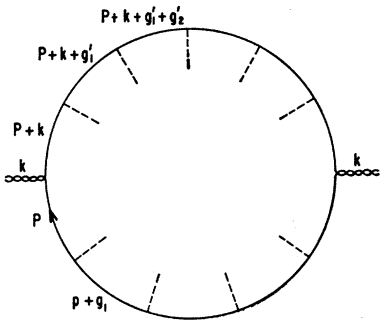

FIG. 2. A generalized vertex diagram used in deriving (2.14). The phonon lines can be connected in any fashion.

to the phonon occupation numbers n_q and n_q+1, and also terms proportional to the electron density. Ignoring the latter terms, the vector vertex becomes

$$\mathbf{p}\cdot\boldsymbol{\Gamma}^{(n)}=\int\frac{d^3q_1d^3q_n}{(2\pi)^{3n}}V(q_1)\cdots V(q_n)\mathbf{p}\cdot(\mathbf{p}+\mathbf{q}_1\cdots\mathbf{q}_n)$$
$$\times[N_{q1}N_{q2}\cdots N_{qn}]\mathfrak{F}^{(n)},$$
$$\mathfrak{F}^{(n)}=\mathcal{G}(\mathbf{p}+\mathbf{k},ip_n+i\omega_n)$$
$$\times\mathcal{G}(\mathbf{p}+\mathbf{k}+\mathbf{q}',ip_n+i\omega_n\pm\omega_q')\cdots$$
$$\times\mathcal{G}(\mathbf{p},ip_n)\mathcal{G}(\mathbf{p}+\mathbf{q}_1,ip_n\pm\omega_q)\cdots. \quad (2.13)$$

In (2.13), $Nq=n_q$ or n_q+1, corresponding to $\pm\omega_q$, where all possible combinations of $\pm$ signs are taken, representing all possible combinations of phonon absorption and emission.

By inserting (2.13) in our prescription (2.6) for finding the mobility, the n-phonon combination is

$$\mu^{(n)}=\frac{2}{3}\frac{e}{n_0}\frac{\beta}{m^2}\int\frac{d^3pd\epsilon}{(2\pi)^4}n_F(\epsilon)$$
$$\times\int\frac{d^3q_1'''d^3q_n}{(2\pi)^{3n}}V(q_1)\cdots V(q_n)\mathbf{p}$$
$$\cdot(\mathbf{p}_1+\cdots\mathbf{q}_n)F_R^{(n)}Nq_1Nq_2\cdots Nq_n, \quad (2.14a)$$
$$F_R^{(n)}=\{\mathrm{Im}G_R(\mathbf{p},\epsilon)G_R(\mathbf{p}+\mathbf{q}',\epsilon\pm\omega_q)\cdots\}$$
$$\times\{\mathrm{Im}G_R(\mathbf{p},\epsilon)G_R(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)\cdots\}. \quad (2.14b)$$

In (2.14b), all of the G_R for one electron line of Fig. 2 are in one bracket, the other line in the other bracket. By using these equations, the vertex correction to the mobility for any configuration of phonons can be written down by inspection. For the ladder diagrams of Fig. 1, this reduces to

$$F_R^{(n)}=\{\mathrm{Im}G_R(\mathbf{p},\epsilon)G_R(\mathbf{p}+\mathbf{q}_1,\epsilon\pm\omega_{q1})\cdots\}^2. \quad (2.14c)$$

The form (2.14c) is clarified by listing the lowest terms:

$$F_R^{(0)}=\tfrac{1}{4}A(p,\epsilon)^2, \quad (2.15a)$$
$$F_R^{(1)}=\tfrac{1}{4}\{-A(p,\epsilon)\,\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)$$
$$-\mathrm{Re}\,G_R(p,\epsilon)A(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)\}^2, \quad (2.15b)$$
$$F_R^{(2)}=\tfrac{1}{4}\{-A(p,\epsilon)\,\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)$$
$$\times\mathrm{Re}\,G_R(p+q+q',\epsilon\pm\omega_q\pm\omega_{q'})$$
$$-\mathrm{Re}\,G_R(\mathbf{p},\epsilon)A(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)$$
$$\times\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q}+\mathbf{q}',\epsilon\pm\omega_q\pm\omega_{q'})$$
$$-\mathrm{Re}\,G_R(\mathbf{p},\epsilon)\,\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)$$
$$\times A(\mathbf{p}+\mathbf{q}+\mathbf{q}',\epsilon\pm\omega_q\pm\omega_{q'})$$
$$+\tfrac{1}{4}A(\mathbf{p},\epsilon)A(\mathbf{p}+\mathbf{q},\epsilon\pm\omega_q)$$
$$\times A(\mathbf{p}+\mathbf{q}+\mathbf{q}',\epsilon\pm\omega_q\pm\omega_{q'})\}^2. \quad (2.15c)$$

The term $F^{(0)}$ just gives the lowest order term $\mu^{(0)}$ in (2.8). The one-phonon term (2.15b), Fig. 1(b), was previously given by Langreth and Kadanoff. The prescription (2.14) for writing down the contribution of an arbitrary ladder diagram is quite simple. This will allow the important terms in the ladder diagram to be summed to all orders. This is done in the following sections for both acoustical and optical phonons.

It was noted above that the quasiparticle approximation would be used for evaluating $A(p,\epsilon)^2$. A similar approximation must be used for $[\mathrm{Re}\,G_R(p,\epsilon)]^2$. Noting the identity

$$[\mathrm{Re}\,G_R(p,\epsilon)]^2=+A(p,\epsilon)/\Gamma(p)-\tfrac{1}{4}A(p,\epsilon)^2, \quad (2.16)$$

it is clear that $(\mathrm{Re}\,G_R)^2$ has the property of a delta function. But there is an additional nonsingular property which is important. This leads to the approximation

$$[\mathrm{Re}\,G_R(p,\epsilon)]^2=\frac{2\pi\delta(\epsilon-E(p))Z(p)}{2\Gamma(p)}$$
$$+P^2\frac{1}{[\epsilon-E(p)]^2}Z(p)^2. \quad (2.17)$$

The notation P^2 means "principle part squared"; the singular behavior of the denominator, which causes the first term, is ignored in the second term.

III. DC MOBILITY; ACOUSTICAL PHONONS

The zeroth-order term for the mobility is obtained by combining (2.8) and (2.9):

$$\mu^{(0)}=\frac{e\beta}{3n_0m^2}\int\frac{d^3p}{(2\pi)^3}\frac{p^2}{\Gamma(p)}n_F(E(p))Z(p). \quad (3.1)$$

As pointed out by Baumann and Ranninger,[2] this is usually a bad approximation to the electronic mobility from acoustic scattering. This form has the wrong energy width. From a transport equation analysis, one knows that the usual energy width integral should have a factor of

$$1-\cos\theta=-\mathbf{p}\cdot\mathbf{q}/p^2 \quad (3.2)$$

for scattering from $\mathbf{p}\to\mathbf{p}+\mathbf{q}$. It is convenient to define a transport self-energy and the corresponding energy width

$$\Sigma_T^{(1)}(p)=T\sum_{qn}\int\frac{d^3q}{(2\pi)^3}V(q)$$
$$\times(\mathbf{p}\cdot\mathbf{q}/p^2)\mathcal{G}(p+q)D^{(0)}(q), \quad (3.3a)$$
$$\Gamma_T(p)=-2\,\mathrm{Im}\,\Sigma_T(\mathbf{p},E(p))>0. \quad (3.3b)$$

Setting the un-normalization factor $Z(p)$ equal to unity, the mobility from the transport equation is

$$\mu_T^{(0)}=\frac{e\beta}{3n_0m^2}\int\frac{d^3p}{(2\pi)^3}\frac{p^2}{\Gamma_T(p)}n_F(E(p)). \quad (3.4)$$

The two forms $\mu^{(0)}$ and $\mu_T^{(0)}$ are quite different since $\Gamma(p)$ and $\Gamma_T(p)$ are different. For example, for piezoelectric electron-phonon scattering, $\Gamma_T(p)$ is well be-

haved on the mass shell ($E(p)\to\epsilon_p$), while $\Gamma(p)$ diverges logarithmically in this limit.[7]

It will now be shown how one can derive the transport result (3.4) from the Kubo formalism. Under certain conditions, one can get (3.4) by summing the ladder diagrams of Fig. 1. The first two conditions are (1) that the phonon energy is neglected ($\omega_q=0$, elastic scattering), and (2) that only induced phonon terms are important ($Nq+1\approx Nq\gg 1$). Both of these conditions are also assumed in deriving (3.4) from the usual transport equation. The third condition (3) is that the quasiparticle approximation (as defined in Sec. II) is valid.

Assuming these three conditions, the important terms in the ladder diagrams will now be summed. The first term is (2.15b)

$$F_R^{(1)}=\tfrac{1}{4}\{A(\mathbf{p},\epsilon)^2\,\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon)^2 +\mathrm{Re}\,G_R(\mathbf{p},\epsilon)^2A(\mathbf{p}+\mathbf{q},\epsilon)^2 +2A(\mathbf{p},\epsilon)A(\mathbf{p}+\mathbf{q},\epsilon) \times\mathrm{Re}\,G_R(\mathbf{p},\epsilon)\,\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon)\}\,. \quad (2.15b')$$

Since our interest is in vertex terms of order unity, only the A^2 and $\mathrm{Re}\,G_R^2$ terms are important. Also, $Z(p)$ will be set equal to unity. In $\mathrm{Re}\,G_R^2$, only the singular part of (2.17) is used. Considering only these terms gives

$$F_R^{(1)}\simeq\tfrac{1}{4}A(p,\epsilon)^2 2\pi\frac{\delta(\epsilon-E(\mathbf{p}+\mathbf{q}))}{\Gamma(\mathbf{p}+\mathbf{q})}\,. \quad (2.15b'')$$

Using this form in (2.14a) gives for the first ladder diagram

$$\mathbf{p}\cdot\Gamma L^{(1)}=p^2\Lambda_a(\epsilon)\,, \quad (3.5a)$$

$$\Lambda_a(\epsilon)=\frac{1}{p^2}\int\frac{d^3q}{(2\pi)^3}V(q)2Nq2\pi \times\frac{\delta(\epsilon-E(\mathbf{p}+\mathbf{q}))}{\Gamma(\mathbf{p}+\mathbf{q})}\mathbf{p}\cdot(\mathbf{p}+\mathbf{q})\,, \quad (3.5b)$$

$$\Lambda_a(\epsilon)=[\Gamma(\epsilon)-\Gamma_T(\epsilon)]/\Gamma(\epsilon)\,. \quad (3.5c)$$

The notation $\Gamma(\epsilon)$ and $\Gamma_T(\epsilon)$ mean (2.10a) and (3.3b) for $\epsilon=E(p)$. Similarly, the two-phonon ladder diagrams give

$$F_R^{(2)}=\tfrac{1}{4}A(p,\epsilon)^2 2\pi\frac{\delta(\epsilon-E(\mathbf{p}+\mathbf{q}))}{\Gamma(\mathbf{p}+\mathbf{q})} \times 2\pi\frac{\delta(\epsilon-E(\mathbf{p}+\mathbf{q}+\mathbf{q}'))}{\Gamma(\mathbf{p}+\mathbf{q}+\mathbf{q}')}\,. \quad (3.6)$$

In evaluating this and other higher order diagrams, the chain rule must be used. This integration rule, valid for $|\mathbf{p}|=|\mathbf{k}|$, is that

$$\int\frac{d^3q}{(2\pi)^3}V(q)2Nq2\pi\frac{\delta(\epsilon-E(\mathbf{k}+\mathbf{q}))}{\Gamma(\mathbf{k}+\mathbf{q})} \times\mathbf{p}\cdot(\mathbf{k}+\mathbf{q})=\mathbf{p}\cdot\mathbf{k}\Lambda_a(\epsilon)\,. \quad (3.7)$$

[7] See Appendix.

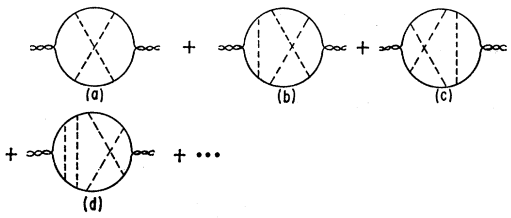

FIG. 3. Vertex diagrams discussed in Sec. IV.

From this rule it can be seen immediately that the important vertex term from the two-phonon diagram (3.6) is

$$\mathbf{p}\cdot\Gamma_L^{(2)}=p^2\Lambda_a(\epsilon)^2\,. \quad (3.8)$$

When one evaluates the equivalent terms from higher order ladder diagrams, there results the series

$$\mathbf{p}\cdot\Gamma_L=p^2[1+\Lambda_a+\Lambda_a^2+\Lambda_a^3+\cdots] \quad (3.9a)$$

or

$$\mathbf{p}\cdot\Gamma_L=p^2/(1-\Lambda_a)\,. \quad (3.9b)$$

The integrand for the mobility integral now has the form

$$A(p,\epsilon)^2\frac{p^2}{1-\Lambda_a}=p^2\frac{2\pi\delta(\epsilon-E(p))}{\Gamma_T(p)}\,. \quad (3.10)$$

This is the desired result. Starting from the Kubo formalism, the contributions to the vertex of order unity have been summed for the ladder diagram. Under the three conditions listed above, the Kubo formalism does give the transport equation form of the mobility.

IV. DC MOBILITY; OPTICAL PHONONS

The Kubo formalism is very suited to evaluating mobilities limited by optical-phonon scattering. At low temperatures and for weak coupling, the correct mobility is given by the first few terms indicated in Fig. 1. Because the phonon scattering is inelastic, the transport equation derivation of the mobility is far more difficult.[8]

There have been many past calculations of mobilities in polar crystals.[3,4] Langreth and Kadanoff[3] have recently calculated the mobility using a Green's-function approach. In terms of the polar coupling constant α, they found that the diagram of Fig. 1(a) contributed $\mu^{(0)}\sim\alpha^{-1}$, while the one-phonon term Fig. 1(b) contributed $\mu^{(1)}\sim\alpha^0$. This is generating a series of the type (2.11), for $g=\alpha$. The present investigation shows that Fig. 1(c) has two terms of order α^0. However, these two contributions cancel in the important leading term, so that the net correction is of order $(T/\omega_0)^{1/2}$. The optical-phonon frequency is ω_0. The diagram Fig. 3 also contributes a mobility term of α^0 which is of order $(T/\omega_0)^{1/2}$. There are also vertex corrections of order unity arising from each ladder diagram. These terms are of order (T/ω_0) as $T\to 0$ and are not important. This analysis examines *every term* in the vertex which con-

[8] D. J. Howarth and E. H. Sondheimer, Proc. Roy. Soc. (London) A219, 53 (1953).

tributes a mobility correction of order α^{-1} or α^0. Our optical-phonon results, which are briefly outlined below, confirm the Langreth-Kadanoff (LK) result.

The term $\mu^{(0)}\sim\alpha^{-1}$ comes directly from (3.1). This gives[9]

$$\mu^{(0)}=(e\tau^{(0)}/m^2)m^*Z(0)^2, \tag{4.1}$$

where the quasiparticle lifetime is

$$\tau^{-1}(0)=\Gamma(0,E(0))Z(0). \tag{4.2}$$

The lifetime has been evaluated to order α^2 by LK.

We now consider the effect of the ladder diagrams, Fig. 1, on this result. Since only vertex corrections of unity are desired,[10] just the singular part of $(\mathrm{Re}\,G_R)^2$ are now considered. The first correction to (4.1) comes from the two-phonon diagram Fig. 1(c). The important term in $F_R^{(2)}$ (2.15c) is

$$F_R^{(2)}\simeq\tfrac{1}{16}A(p,\epsilon)^2N(N+1)A(\mathbf{p}+\mathbf{q},\epsilon+\omega_0)^2 \times A(\mathbf{p}+\mathbf{q}+\mathbf{q}',\epsilon)^2, \tag{4.3}$$

where N is the thermal occupation number for phonons. When this is integrated over phonon coordinates, the vertex contribution is

$$\mathbf{p}\cdot\boldsymbol{\Gamma}^{(2)}=p^2\Lambda_0(\epsilon), \quad 0<\epsilon<\omega_0, \tag{4.4a}$$

$$\Lambda_0(\epsilon)=\frac{\left[1-\dfrac{\epsilon+\omega_0/2}{(\epsilon(\epsilon+\omega_0))^{1/2}}\ln\dfrac{(\epsilon+\omega_0)^{1/2}+\sqrt{\epsilon}}{(\epsilon+\omega_0)^{1/2}-\sqrt{\epsilon}}\right]^2}{\left[\ln\dfrac{(\epsilon+\omega_0)^{1/2}+\sqrt{\epsilon}}{(\epsilon+\omega_0)^{1/2}-\sqrt{\epsilon}}\right]^2}. \tag{4.4b}$$

For small energies, this goes as

$$\lim_{\epsilon\to0}\Lambda_0(\epsilon)=(4/9)(\epsilon/\omega_0). \tag{4.5}$$

Considering the sum of all even-phonon ladder diagrams generates the series, valid for $0<\epsilon<\omega_0$,

$$\mathbf{p}\cdot\boldsymbol{\Gamma}=p^2(1+\Lambda_0+\Lambda_0^2+\Lambda_0^3\cdots)=p^2/1-\Lambda^0(\epsilon). \tag{4.6}$$

Because of the low-energy limit of $\Lambda_0(\epsilon)$, (4.5), this vertex correction is only of order (T/ω_0), and does not change the main result (4.1). This behavior contrasts sharply with the acoustic-phonon scattering derived in Sec. III, where the vertex caused a major change in the results.

The one-phonon vertex gives the term $\mu^{(1)}\sim\alpha^0$. From (2.15b), the relevant vertex term is

$$\mathbf{p}\cdot\boldsymbol{\Gamma}^{(1)}(\mathbf{p},\epsilon)=2\int\frac{d^3q}{(2\pi)^3}V(q) \times\mathbf{p}\cdot(\mathbf{p}+\mathbf{q})\,\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon-\omega_0)^2. \tag{4.7}$$

This is most easily evaluated by noting the identities

$$\mathbf{p}\cdot\boldsymbol{\Gamma}^{(1)}(\mathbf{p},\epsilon)=2p^2\frac{\partial}{\partial\epsilon_p}\mathrm{Re}\,\Sigma^{(1)}(p,\epsilon) =-2p^2\frac{\partial}{\partial\epsilon}\mathrm{Re}\,[\Sigma^{(1)}(p,\epsilon)-\Sigma_T^{(1)}(p,\epsilon)]. \tag{4.8}$$

This gives the LK result for the leading term

$$\mathbf{p}\cdot\boldsymbol{\Gamma}^{(1)}(\mathbf{p},\epsilon)=p^2\frac{\alpha}{3}(1+O(\epsilon/\omega_0)). \tag{4.9}$$

There are additional corrections to this result arising from other ladder diagrams. Summing all ladder diagrams of odd number of phonon terms, the additional factor is $(1-\Lambda_0(\epsilon))^{-1}$ as in (4.6), which is a negligible contribution to (4.9).

The two-phonon terms, Fig. 1(c), are now examined for mobility contributions of order α^0. The two important terms are

$$F_R^{(2)}=\tfrac{1}{4}A(\mathbf{p},\epsilon)^2\frac{A(\mathbf{p}+\mathbf{q}+\mathbf{q}'\epsilon)}{\Gamma(\mathbf{p}+\mathbf{q}+\mathbf{q}'\epsilon)} \times[\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon-\omega_0)^2+\mathrm{Re}\,G_R(\mathbf{p}+\mathbf{q},\epsilon+\omega_0)^2].$$

The contribution of these terms to the mobility may be found exactly in the quasiparticle approximation. The first term gives a vertex term of $p^2\alpha(\pi/6)\times[1+O((\epsilon/\omega_0)^{1/2})]$. In evaluating the second term, the double principle part definition of (2.17) is used. The singular part of this term has already been included in the $\mu^{(0)}$ vertex correction (4.3). After doing the integrals, the leading term is $-p^2\alpha\pi/6$, which just cancels the first term. The additional terms $\sim(\epsilon/\omega_0)^{1/2}$ are of order $(T/\omega_0)^{1/2}$ and may be neglected. The diagram of Fig. 3(a) also provides a term smaller by $(T/\omega_0)^{1/2}$ and is unimportant when $T\to0$. The remaining vertex terms of Figs. 1 and 3 just add a $(1-\Lambda_0(\epsilon))^{-2}$ factor to these $(T/\omega_0)^{1/2}$ corrections.

This accounting of vertex terms includes *all terms* in the mobility of order α^{-1} and α^0. All of the ladder diagrams which contribute terms of order α^{-1} or α^0 have been evaluated and have been shown not to be important as $T\to0$. This confirms the Langreth-Kadanoff result

$$\mu=e\tau(0)(m^*/m^2)Z(0)^2(1+2/3\alpha).$$

V. DISCUSSION

The above results shown that the important parts of the ladder diagrams in the polaron mobility calculation can be summed to all orders. An important part of summing these diagrams is being able to easily write down the vertex correction for any particular diagram. This turns out to be quite simple when one uses the Matsubara method as developed by Abrikosov *et al.*

[9] In this section, the definitions of m^*, $Z(p)$, N, etc., parallel those of Langreth and Kadanoff, Ref. 3.

[10] This means that we also set $Z(p)=1$.

The ladder diagrams are very important for acoustical-phonon interactions. When the phonon scattering can be treated as elastic, and when the quasiparticle approximation is justified, the transport result is valid. The quasiparticle approximation ($\Gamma \ll T$) should generally be valid for piezoelectric electron-phonon interactions.[11–13] The width of the spectral function is given in the Appendix as $\Gamma \sim gT(\epsilon_s/\epsilon_p)^{1/2}$, so the approximation is valid for thermal electrons when $T > g^2\epsilon_s$. This is about 0.5°K in CdS, which has one of the strongest piezoelectric electron-phonon interactions. Neglecting the phonon energy is not a serious error, since these energies are less than the spectral width for $g > 1$.

Note added in proof. Green's-function methods have also recently been applied to electron mobility in metals by T. Holstein [Ann. Phys. (N. Y.) **29** (1964)] and G. M. Eliashberg (Zh. Eksperim. i. Teor. Fiz. **41**, 1241 (1961) [English transl.: Soviet Phys.—JETP **14**, 886 (1962)]).

APPENDIX

The analytical forms for the lowest order self-energy and vertex diagrams are listed below. Results are given for optical phonons, polar coupling, and for acoustical phonons, piezoelectric coupling. Some of the results are well known, but are included for completeness.

A. Optical Phonons: Polar Coupling

The lowest order self-energy[4] is

$$\Sigma^{(1)}(p) = -\beta^{-1} \sum_{q_n} \int \frac{d^3q}{(2\pi)^3} V(q) D(q) G(p+q) , \tag{A1}$$

$$\Sigma^{(1)}(p) = -\alpha \frac{\omega_0^{3/2}}{\sqrt{\epsilon_p}} \left\{ N \sin^{-1}\left(\frac{\epsilon_p}{\epsilon_p - \omega_0 - ip_n}\right)^{1/2} + (N+1) \sin^{-1}\left(\frac{\epsilon_p}{\epsilon_p + \omega_0 - ip_n}\right)^{1/2} \right\} . \tag{A2}$$

The transport self-energy is

$$\Sigma_T^{(1)}(p) = \beta^{-1} \sum_{q_n} \int \frac{d^3q}{(2\pi)^3} V(q) \frac{p \cdot q}{p^2} D^{(0)}(q) G(p+q) , \tag{A3}$$

$$\Sigma_T^{(1)}(p) = \frac{\alpha}{2}\left(\frac{\omega_0}{\epsilon_p}\right)^{3/2} \left\{ N \left[(\epsilon_p(-\omega_0 - ip_n))^{1/2} - (\epsilon_p - \omega_0 - ip_n) \sin^{-1}\left(\frac{\epsilon_p}{\epsilon_p - \omega_0 - ip_n}\right)^{1/2} \right] + (N+1) \left[(\epsilon_p(\omega_0 - ip_n))^{1/2} - (\epsilon_p + \omega_0 - ip_n) \times \sin^{-1}\left(\frac{\epsilon_p}{\epsilon_p + \omega_0 - ip_n}\right)^{1/2} \right] \right\} . \tag{A4}$$

[11] A. R. Hutson, J. Appl. Phys. Suppl. **32**, 2287 (1961).
[12] G. D. Mahan and J. J. Hopfield, Phys. Rev. Letters **12**, 241 (1964).
[13] Y. Osaka, J. Phys. Soc. Japan **19**, 2347 (1964).

B. Acoustical Phonons: Piezoelectric Coupling

The lowest order self-energy is

$$\Sigma^{(1)}(p) = -\frac{\bar{g}^2}{\beta} \sum_{q_n} \int \frac{d^3q}{(2\pi)^3} D^{(0)}(q) G(p+q) . \tag{A5}$$

In this form, the piezoelectric interaction has been assumed to be isotropic, with

$$D^{(0)}(q) = -\frac{1}{q_n^2 + \omega_q^2} , \tag{A6a}$$

$$\bar{g}^2 = 4\pi g \hbar^2 C s^3 , \tag{A6b}$$

$$g = \frac{e^2}{\epsilon_0 \hbar C s} \langle K^2 \rangle , \tag{A6c}$$

where $\langle K^2 \rangle$ is the average of the square of the electromechanical coupling constant. The dimensionless constant g is a convenient coupling parameter for the piezoelectric interaction. After doing the Matsubara sum q_n in (A5),

$$\Sigma^{(1)}(p) = \frac{\bar{g}^2}{(2\pi)^3} \int d^3q \, \frac{1}{2\omega_q} \times \left[\frac{N_q}{ip_n - \epsilon(\mathbf{p}+\mathbf{q}) + \omega_q} + \frac{N_q + 1}{ip_n - \epsilon(\mathbf{p}+\mathbf{q}) - \omega_q} \right] . \tag{A7}$$

This can be evaluated in the high-temperature limit, $N_q + 1 \approx T \approx \omega_q$, which is valid even at helium temperature. Defining $\epsilon_s = mCs^2/2$, this becomes[12,13]

$$\Sigma^{(1)}(p) = \frac{g}{\beta} \sqrt{\left(\frac{\epsilon_s}{\epsilon_p}\right)} \left\{ \sin^{-1}\left(\frac{\sqrt{\epsilon_p} + \sqrt{\epsilon_s}}{(\epsilon_p - ip_n)^{1/2}}\right) + \sin^{-1}\left(\frac{\sqrt{\epsilon_p} - \sqrt{\epsilon_s}}{(\epsilon_p - ip_n)^{1/2}}\right) \right\} . \tag{A8}$$

The transport self-energy (A3) evaluated in the high-temperature limit, is

$$\Sigma_T^{(1)}(p) = \frac{-g}{2\beta} \frac{\sqrt{\epsilon_s}}{\epsilon_p^{3/2}} \left\{ (\epsilon_p - ip_n) \times \left[\sin^{-1}\frac{\sqrt{\epsilon_p} + \sqrt{\epsilon_s}}{(\epsilon_p - ip_n)^{1/2}} + \sin^{-1}\frac{\sqrt{\epsilon_p} - \sqrt{\epsilon_s}}{(\epsilon_p - ip_n)^{1/2}} \right] - (\sqrt{\epsilon_p} + \sqrt{\epsilon_s})(\epsilon_p - ip_n - (\sqrt{\epsilon_p} - \sqrt{\epsilon_s})^2)^{1/2} - (\sqrt{\epsilon_p} - \sqrt{\epsilon_s})(\epsilon_p - ip_n - (\sqrt{\epsilon_p} + \sqrt{\epsilon_s})^2)^{1/2} \right\} . \tag{A9}$$