

Tin is an exception probably because of its complicated electronic structure and the complexity of the induced field, discussed above. The very large induced fields in Au and Re<sup>17</sup> dissolved in Fe are probably particularly significant, as both elements have 6s electrons with associated large fields. The internal field in atomic copper in the  $4s^2S_{1/2}$  state is  $1.3 \times 10^6$  G and that of atomic gold in the  $6s^2S_{1/2}$  state is  $21 \times 10^6$  G. These fields can be derived by using Eq. (15.5) in Ref. 36 and appropriate data from atomic spectroscopy.<sup>38,39</sup> Thus the internal fields of Cu and Au in Fe would correspond to 16% and 7% polarization of the conduction electrons, respectively. The internal field in atomic Ag in the  $5s^2S_{1/2}$  state is  $4.9 \times 10^6$  G.<sup>40</sup> It would be interesting to determine the induced field at Ag atoms dissolved in Fe, which should be  $\sim 400$  kG by analogy with Cu and Au.

<sup>38</sup> R. Ritschl, Z. Physik **79**, 1 (1932).

<sup>39</sup> R. E. Sheriff and D. Williams, Phys. Rev. **82**, 651 (1951).

<sup>40</sup> G. Wessel and H. Lew, Phys. Rev. **92**, 641 (1953).

*Notes added in proof.* (a) Dr. A. de Shalit (private communication) has informed us that newer data on transition rates in Au<sup>197</sup> would lower the core-excitation estimate of  $\mu_{77}$  from +0.60 nm to about the experimental value of +0.37 nm. From calculations on the quasiparticle model, L. Kisslinger and R. A. Sorensen have also predicted a very low value ( $\sim 0.12$  nm) for this moment (private communication).

(b) The unusual low-field behavior of our samples was reversible. If this behavior is the result of spin orientation, a more significant zero-field splitting may be obtained by extrapolating back the high-field slopes. We acknowledge a discussion of this point with Dr. R. J. Elliott.

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## Perturbation Theoretic Calculation of Polaron Mobility\*

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The low-temperature drift mobility of the polaron is calculated in perturbation theory with the aid of the Kubo formula. The result is  $\mu = \mu_0(1 - \alpha/6)$ , where  $\mu_0$  is the weak coupling mobility  $\mu_0 = (e/2\alpha\omega m) \exp(\hbar\omega/kT)$ . A comparison is made with the perturbation expansion of various intermediate coupling mobility theories. The expansion of Osaka,  $\mu = \mu_0(1 - 0.173\alpha + \dots)$ , agrees most closely with the exact perturbation expansion. It is concluded that the Osaka formula is probably the best in the intermediate coupling range  $\alpha < 6$ . It is explicitly shown to lowest nontrivial order in  $\alpha$  that various quasiparticle concepts are valid, viz., that  $\mu = e\tau/m^*$ , and that the electron density is a momentum integral over  $f(E(\mathbf{p}))$ .

### I. INTRODUCTION

THE drift mobility of a slow electron in the conduction band of a polar crystal has been the subject of much theoretical investigation.<sup>1-9</sup> There exist a large number of expressions for the low-temperature drift mobility, which unfortunately differ considerably in the experimentally interesting range<sup>10,11</sup> of coupling

constant ( $\alpha \sim 3$ ). This spread of results is illustrated for several representative theories in Fig. 1. Notice that at  $\alpha = 3$ , the results of Low and Pines differ from the results of Schultz by a factor of 6. Clearly it would be desirable to find out which of the various theories is most reliable. We attack the problem here by obtaining a perturbation expansion of the mobility in a power series in the coupling constant; we then compare the exact perturbation expansion with the power series expansion of the various intermediate coupling theories. This is done in the belief that the best intermediate coupling theory is likely to have a power series expansion which corresponds quite closely to the exact expansion.

Thus, the main body of this paper is concerned with finding the first nontrivial term in the expansion of the

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<sup>1</sup> A. Morita, Science Rep. Tohoku Univ. **38**, 1 (1954); A. Morita, C. Horie, and K. Hasegawa, *ibid.* **38**, 158 (1954).

<sup>2</sup> F. E. Low and D. Pines, Phys. Rev. **98**, 414 (1955); see also T. D. Lee, F. E. Low, and D. Pines, *ibid.* **90**, 297 (1953).

<sup>3</sup> T. D. Schultz, MIT Tech. Report No. 9, 1956 (unpublished).

<sup>4</sup> T. D. Schultz, Phys. Rev. **116**, 526 (1960).

<sup>5</sup> Y. Osaka, Progr. Theoret. Phys. (Kyoto) **25**, 517 (1961).

<sup>6</sup> F. Garcia-Moliner, Phys. Rev. **130**, 2290 (1963).

<sup>7</sup> R. P. Feynman, R. H. Hellwarth, C. K. Iddings, and P. M. Platzman, Phys. Rev. **127**, 1004 (1962).

<sup>8</sup> D. J. Howarth and E. H. Sondheimer, Proc. Roy. Soc. (London) **A219**, 53 (1953).

<sup>9</sup> L. P. Kadanoff, Phys. Rev. **130**, 1364 (1963).

<sup>10</sup> See F. C. Brown in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Oliver and Boyd Ltd., Edinburgh,

1963), pp. 323-355, for a summary of the values of  $\alpha$  expected for various different materials.

<sup>11</sup> Reference 6 summarizes experimental mobility data on the intermediate coupling materials AgCl and AgBr.

mobility. Green's function techniques<sup>12,13</sup> are used for this purpose. In Sec. II the self-energy of the one-particle Green's function is expanded in a power series in  $\alpha$ . In Sec. III, the Kubo formula<sup>14</sup> for the mobility is expanded in terms of the one-particle Green's function, and the mobility is then obtained to the first nontrivial order. Finally, in Sec. IV we compare our exact perturbation expansion with the various intermediate coupling theories.

## II. EXPANSION OF THE SELF-ENERGY

We begin with the Fröhlich<sup>15,16</sup> Hamiltonian for the single electron in the crystal:

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

We eliminate the electron-phonon interaction in favor of a retarded "electron-electron" interaction<sup>17</sup>

$$\begin{aligned} V(1-1') &= V^>(1-1') \quad \text{for } it_1 > it_1', \\ &= V^<(1-1') \quad \text{for } it_1 < it_1', \end{aligned} \quad (2)$$

with

$$V^>(\mathbf{r}, t) = V^<(\mathbf{r}, -t) = -i \frac{\alpha}{r\sqrt{2}} [(\bar{N}+1)e^{-it} + \bar{N}e^{it}]. \quad (3)$$

Here  $\bar{N} = [e^\beta - 1]^{-1}$  is the equilibrium number of phonons in the state  $\mathbf{q}$ . In this paper, we shall restrict ourselves to the case in which  $1/\beta$ , the temperature measured in energy units, is much smaller than the phonon energy. Then  $\bar{N} \approx e^{-\beta} \ll 1$ .

In this section, we shall find the spectral weight function for the one-electron Green's function,

$$A(\mathbf{p}, \omega) = \frac{\Gamma(\mathbf{p}, \omega)}{[\omega - p^2/2 - \text{Re}\Sigma(\mathbf{p}, \omega)]^2 + [\Gamma(\mathbf{p}, \omega)/2]^2} \quad (4)$$

by expanding the self-energy,

$$\Sigma(\mathbf{p}, p_0) = \int \frac{d\omega' \Gamma(\mathbf{p}, \omega')}{2\pi p_0 - \omega'}, \quad (5)$$

in a power series in  $\alpha$ . Since there is only one particle in the crystal, we can make use of a variety of simplifica-

<sup>12</sup> P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).

<sup>13</sup> L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962).

<sup>14</sup> R. Kubo, Can. J. Phys. **34**, 1274 (1956).

<sup>15</sup> H. Fröhlich, Advan. Phys. **3**, 325 (1954).

<sup>16</sup> We follow the notation of R. P. Feynman [Phys. Rev. **97**, 660 (1955)] in using units in which  $\hbar$ , the electron band mass, and the phonon frequency are all set equal to unity.

<sup>17</sup> This retarded interaction was used at zero temperature by V. M. Galitskii and A. B. Migdal, Zh. Eksperim. i Teor. Fiz. **34**, 139 (1958) [translation: Soviet Phys.—JETP **7**, 96 (1958)] and A. B. Migdal, *ibid.* **34**, 1438 (1958) [translation: *ibid.* **7**, 996 (1958)]. It has been applied to the finite temperature polaron problem by R. D. Puff and G. D. Whitfield in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Oliver and Boyd Ltd., Edinburgh, 1963), pp. 171–190.

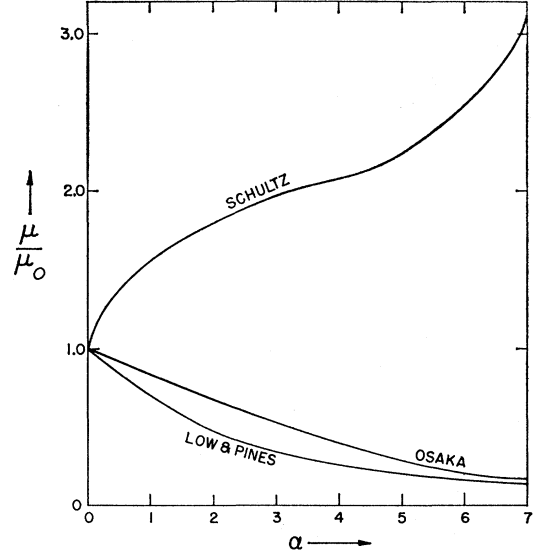


FIG. 1. Comparison of various mobility theories. Here  $\mu/\mu_0$  is the predicted mobility divided by the weak coupling mobility [ $\mu_0 = e/(2\alpha\bar{N}m\omega)$ ].

tions appropriate to the low-density case. In general, single-electron propagation is described by the two functions  $G^>(\mathbf{p}, \omega)$  and  $G^<(\mathbf{p}, \omega)$  defined by

$$\begin{aligned} G^>(\mathbf{p}, \omega) &= A(\mathbf{p}, \omega)[1 - f(\omega)], \\ G^<(\mathbf{p}, \omega) &= A(\mathbf{p}, \omega)f(\omega), \\ f(\omega) &= [e^{\beta(\omega - \mu)} + 1]^{-1}, \end{aligned} \quad (6)$$

where  $\mu$  is the chemical potential.<sup>18</sup> However, in the low-density limit,  $\beta\mu \rightarrow -\infty$ ,  $f(\omega) \ll 1$ , and

$$\begin{aligned} G^>(\mathbf{p}, \omega) &\approx A(\mathbf{p}, \omega) \\ G^<(\mathbf{p}, \omega) &\approx A(\mathbf{p}, \omega)e^{-\beta(\omega - \mu)} \ll G^>(\mathbf{p}, \omega). \end{aligned} \quad (7)$$

Thus, in the evaluation of  $\Sigma$ , we shall set  $G^<(\mathbf{p}, \omega) = 0$ .

With this simplification,  $\Sigma(1-1')$  may more easily be expanded in a power series in  $\alpha$ . This expansion to second order is diagrammatically indicated in Fig. 2. Here, the solid lines represent the free propagator

$$\begin{aligned} G_0(1, 1') &= -i \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{r}_1 - \mathbf{r}_1') - i\frac{1}{2}p^2(t_1 - t_1')} \\ &= 0 \quad \text{for } it_1 > it_1', \\ &= 0 \quad \text{for } it_1 < it_1', \end{aligned} \quad (8)$$

while the dashed lines represent the retarded potential  $V$ . The first-order diagram, indicated in Fig. 2(a), gives

$$\Sigma_1(1-1') = iV(1-1')G_0(1-1')$$

or

$$\Sigma_1(\mathbf{p}, p_0) = \int \frac{d\omega' \Gamma_1(\mathbf{p}, \omega')}{2\pi p_0 - \omega'}, \quad (9)$$

<sup>18</sup> Although we use the symbol  $\mu$  for both the mobility and the chemical potential, no confusion should arise.

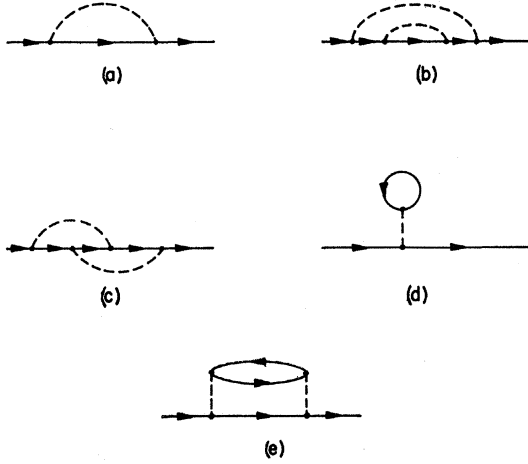


FIG. 2. Diagrams for the self-energy. We calculate the effects of diagrams 2(a), 2(b), and 2(c), but not of 2(d) or 2(e), since the latter necessarily vanish when the density goes to zero.

with

$$\Gamma_1(\mathbf{p}, \omega) = \int \frac{d^3 p'}{(2\pi)^3} \frac{2^{3/2} \pi \alpha}{(\mathbf{p} - \mathbf{p}')^2} [\bar{N} \delta(\omega + 1 - p'^2/2) + (\bar{N} + 1) \delta(\omega - 1 - p'^2/2)]. \quad (10)$$

Physically,  $\Gamma(\mathbf{p}, \omega)$  represents the rate of emission and absorption of phonons by a hypothetical electron of momentum  $\mathbf{p}$  and energy  $\omega$ . Below a certain threshold (here  $\omega = 1$ ) real emission processes are impossible, and  $\Gamma(\mathbf{p}, \omega)$  is very small because it is proportional to  $\bar{N}$ , the number of phonons available for absorption. In this region  $A(\mathbf{p}, \omega)$  is particularly simple. It is only large when  $\omega - p^2/2 - \text{Re}\Sigma(\mathbf{p}, \omega)$  nearly vanishes. The value of  $\omega$  for which this quantity vanishes is called  $E(\mathbf{p})$ , the quasiparticle energy. It obeys

$$E(\mathbf{p}) = p^2/2 + \text{Re}\Sigma(\mathbf{p}, E(\mathbf{p})). \quad (11)$$

In the region  $\omega \sim E(\mathbf{p})$ ,  $A(\mathbf{p}, \omega)$  has the form

$$A(\mathbf{p}, \omega) = z(\mathbf{p}) \frac{[\tau(\mathbf{p})]^{-1}}{[\omega - E(\mathbf{p})]^2 + [2\tau(\mathbf{p})]^{-2}}, \quad (12)$$

where  $\tau(\mathbf{p})$  is the quasiparticle lifetime defined by

$$\tau(\mathbf{p}) = z(\mathbf{p}) \Gamma(\mathbf{p}, E(\mathbf{p})). \quad (13)$$

The quantity  $z(\mathbf{p})$ , called the wave function renormalization constant, is defined by

$$z(\mathbf{p}) = \left[ 1 - \frac{\partial}{\partial \omega} \text{Re}\Sigma(\mathbf{p}, \omega) \right]^{-1} \Big|_{\omega = E(\mathbf{p})}. \quad (14)$$

For  $\omega < E(0)$ ,  $\omega - p^2/2 - \text{Re}\Sigma(\mathbf{p}, \omega)$  can no longer vanish. In this region, we can neglect the appearance of  $\Gamma(\mathbf{p}, \omega)$

in the denominator of Eq. (4), so that

$$A(\mathbf{p}, \omega) = \frac{\Gamma(\mathbf{p}, \omega)}{[\omega - p^2/2 - \text{Re}\Sigma(\mathbf{p}, \omega)]^2} \quad \text{for } \omega < E(0). \quad (15)$$

We shall be most concerned with the low-momentum quasiparticle states ( $p^2/2 \sim \beta^{-1} \ll 1$ ), since these are the states which are appreciably excited at low temperature. We can determine the properties of these quasiparticles to first order in  $\alpha$  by applying Eqs. (9) and (10) to find that for small  $\mathbf{p}$  and  $\omega$

$$\text{Re}\Sigma(\mathbf{p}, \omega) = -\alpha [1 + \frac{1}{2}\omega - \frac{1}{6}p^2]. \quad (16)$$

Using Eq. (11), we recover the well-known results that for  $p^2/2 \ll 1$ ,

$$E(\mathbf{p}) = -\alpha + p^2/2m^* + O(p^4) \quad (17)$$

with

$$m^* = 1 + \alpha/6, \quad (18)$$

while the wave function renormalization constant is for small  $p$ ,

$$z(0) = 1 - \alpha/2. \quad (19)$$

We shall need Eqs. (17), (18), and (19) in our later discussion of the polaron mobility. It will also be necessary for us to have an expression for the density of electrons

$$\begin{aligned} n &= \int \frac{d^3 p}{(2\pi)^3} \int \frac{d\omega}{2\pi} G^<(\mathbf{p}, \omega) \\ &= \int \frac{d^3 p}{(2\pi)^3} \int \frac{d\omega}{2\pi} \frac{e^{-\beta(\omega - \mu)}}{2\pi} A(\mathbf{p}, \omega), \end{aligned} \quad (20)$$

which is correct to the first order in  $\alpha$ . To obtain this expression, we notice that the factor  $e^{-\beta(\omega - \mu)}$  highly weights the integrand in Eq. (20) for small values of  $\omega$ . We split the integral into two parts: For  $\omega > E(0)$  we use Eq. (12) to express  $A(\mathbf{p}, \omega)$ , because the temperature factor cuts out all contributions from energies appreciably greater than the minimum quasiparticle energy,  $E(0)$ . Then

$$\begin{aligned} n &= \int \frac{d^3 p}{(2\pi)^3} \int_{E(0)}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-\beta(\omega - \mu)} z(0)}{2\pi} \\ &\quad \times \left\{ \frac{\tau^{-1}(0)}{[\omega - E(\mathbf{p})]^2 + [2\tau(0)]^{-2}} \right\} + \int \frac{d^3 p}{(2\pi)^3} \\ &\quad \times \int_{-\infty}^{E(0)} \frac{d\omega}{2\pi} \frac{e^{-\beta(\omega - \mu)} \Gamma(\mathbf{p}, \omega)}{[\omega - p^2/2 - \text{Re}\Sigma(\mathbf{p}, \omega)]^2}. \end{aligned} \quad (21)$$

In the limit as  $\tau \rightarrow \infty$ , we can replace the  $\{ \}$  in Eq. (21) by  $2\pi\delta(\omega - E(\mathbf{p}))$ . To first order in  $\alpha$ , we can replace  $\Gamma(\mathbf{p}, \omega)$  in the second term by the  $\Gamma_1(\mathbf{p}, \omega)$  defined by Eq. (10), and neglect the  $\text{Re}\Sigma(\mathbf{p}, \omega)$  in the denominator of the second term. Then, we find after

some integration that

$$n = \int \frac{d^3 p}{(2\pi)^3} e^{-\beta[E(\mathbf{p}) - \mu]}. \quad (22)$$

[Although we have verified Eq. (22) only to first order in  $\alpha$ , it appears from preliminary calculations that

it is in fact valid to all orders in  $\alpha$  in this low-temperature situation. However, we shall only need it to first order here.]

So far, we have obtained  $n$ ,  $m^*$ ,  $z(0)$ , and  $E(0)$  to first order in  $\alpha$ . However, we shall need  $\tau^{-1}(0)$  to order  $\alpha^2$ . Therefore, the contributions of Figs. 2(b) and 2(c) to  $\Gamma(\mathbf{p}, \omega)$  must be evaluated. Figure 2(b) gives

$$\Sigma_{2b} > (1-1') = - \int d^3 \bar{r}_1 \int_{t_1'}^{t_1} d\bar{t}_1 \int d^3 \bar{r}_1' \int_{t_1'}^{t_1} d\bar{t}_1' V > (\bar{\mathbf{1}} - \bar{\mathbf{1}}') V > (1-1') G_0 > (1-\bar{\mathbf{1}}) G_0 > (\bar{\mathbf{1}} - \bar{\mathbf{1}}') G_0 > (\bar{\mathbf{1}}' - 1'), \quad (23)$$

which has the Fourier transform

$$\begin{aligned} \Gamma_{2b}(\mathbf{q}, \omega) &= \int d^3 r \int_{-\infty}^{\infty} dt e^{-i\mathbf{p} \cdot \mathbf{r} + i\omega t} i \Sigma_{2b} > (\mathbf{r}, t) \\ &= \text{Re} \int \frac{d^3 p}{(2\pi)^3} \int \frac{d^3 p'}{(2\pi)^3} \frac{16\pi^3 \alpha^2 \bar{N}}{(\mathbf{p}-\mathbf{q})^2 (\mathbf{p}-\mathbf{p}')^2} \left\{ \delta(\omega - p'^2/2) \left[ \frac{1}{(\omega+1-p^2/2+i\epsilon)^2} + \frac{1}{(\omega-1-p^2/2+i\epsilon)^2} \right] \right. \\ &\quad \left. + \left[ \frac{\partial}{\partial \omega} \delta(\omega+1-p^2/2) \right] \frac{1}{\omega-p^2/2} + \left[ \frac{\partial}{\partial \omega} \delta(\omega-1-p^2/2) \right] \frac{1}{\omega-p^2/2} \right\} + O(\bar{N}^2), \quad (24) \end{aligned}$$

where  $\epsilon$  is an infinitesimal. Similarly Fig. 2(c) gives

$$\Sigma_{2c} > (1-1') = - \int d^3 \bar{r}_1 \int_{t_1'}^{t_1} d\bar{t}_1 \int d^3 \bar{r}_1' \int_{t_1'}^{t_1} d\bar{t}_1' V > (1-\bar{\mathbf{1}}') V > (\bar{\mathbf{1}} - \bar{\mathbf{1}}') G_0 > (1-\bar{\mathbf{1}}) G_0 > (\bar{\mathbf{1}} - \bar{\mathbf{1}}') G_0 > (\bar{\mathbf{1}}' - 1') \quad (25)$$

and

$$\begin{aligned} \Gamma_{2c}(\mathbf{q}, \omega) &= \mathcal{P} \int \frac{d^3 p}{(2\pi)^3} \int \frac{d^3 p'}{(2\pi)^3} \frac{32\pi^3 \alpha^2 \bar{N}}{(\mathbf{p}-\mathbf{q})^2 (\mathbf{p}'-\mathbf{q})^2} \left\{ \delta(\omega - (\mathbf{p}+\mathbf{p}'-\mathbf{q})^2/2) \frac{1}{\omega+1-p^2/2} \frac{1}{\omega-1-p'^2/2} \right. \\ &\quad \left. + \delta(\omega+1-p^2/2) \frac{1}{\omega-1-p'^2/2} \frac{1}{\omega - (\mathbf{p}+\mathbf{p}'-\mathbf{q})^2/2} + \delta(\omega-1-p'^2/2) \frac{1}{\omega+1-p^2/2} \frac{1}{\omega - (\mathbf{p}+\mathbf{p}'-\mathbf{q})^2/2} \right\} + O(\bar{N}^2), \quad (26) \end{aligned}$$

where  $\mathcal{P}$  indicates that the integrals are to be interpreted in the principal value sense.

To second order in  $\alpha$ ,  $\tau^{-1}(0)$  contains the sum  $\Gamma_{2b}(0,0) + \Gamma_{2c}(0,0)$ . Notice that the first terms in the  $\{ \}$  of Eqs. (24) and (26) each produce discontinuities at  $\omega=0$ ,  $\mathbf{q}=0$ . Each term contributes for  $\omega>0$  and  $\mathbf{q}=0$ ; neither contributes for  $\omega<0$ . However, as Schultz<sup>3</sup> has pointed out, these discontinuities cancel in the sum  $\Gamma_{2b}(\mathbf{q}, \omega) + \Gamma_{2c}(\mathbf{q}, \omega)$ . Therefore, we may safely eliminate them by evaluating  $\Gamma_{2b}$  and  $\Gamma_{2c}$  for  $\omega$  just less than zero. Then we find after performing the integrals that

$$\Gamma_{2b}(0, \omega) |_{\omega=0^-} = -2\alpha \bar{N} [\frac{1}{2}\pi\alpha], \quad (27)$$

and

$$\Gamma_{2c}(0, \omega) |_{\omega=0^-} = 2\alpha \bar{N} [\frac{1}{2}\pi\alpha]. \quad (28)$$

Thus, the second-order contributions to  $\tau^{-1}(0)$  from the diagrams 2(b) and 2(c) exactly cancel, so that to second order, only  $\Gamma_1(\mathbf{p}, \omega)$  contributes to  $\tau^{-1}(0)$ . From Eq. (13)

$$\tau^{-1}(0) = z(0) \Gamma_1(0, E(0)), \quad (29)$$

and near  $\omega=0$ , Eq. (10) implies that

$$\Gamma_1(0, \omega) = 2\alpha \bar{N} [1 - \omega/2],$$

so that

$$\tau^{-1}(0) = 2\alpha \bar{N} + O(\alpha^2). \quad (30)$$

The inverse quasiparticle lifetime contains no corrections of order  $\alpha^2$ .

### III. CALCULATION OF THE MOBILITY

To calculate the mobility, we use the Kubo<sup>14</sup> formula

$$\mu = \frac{e\beta}{6n} \int_{-\infty}^{\infty} dt \int d^3 r \langle \mathbf{j}(\mathbf{r}, t) \cdot \mathbf{j}(\mathbf{0}, 0) \rangle, \quad (31)$$

where  $\mathbf{j}(\mathbf{r}, t)$  is the momentum current, given in terms of the Heisenberg field operators by

$$\mathbf{j}(\mathbf{r}, t) = -\frac{1}{2} i [\psi^\dagger(\mathbf{r}, t) \nabla \psi(\mathbf{r}, t) - \nabla \psi^\dagger(\mathbf{r}, t) \psi(\mathbf{r}, t)]. \quad (32)$$

The correlation function in Eq. (31) can be expressed in terms of the two-particle Green's function  $G_2$  as

$$\begin{aligned} \langle T(\mathbf{j}(\mathbf{r}_1, t_1) \cdot \mathbf{j}(\mathbf{r}_2, t_2)) \rangle \\ = \frac{1}{2} (\nabla_1 - \nabla_1') \cdot (\nabla_2 - \nabla_2') G_2(1, 2; 1', 2') |_{1'-1^+, 2'-2^+}. \quad (33) \end{aligned}$$

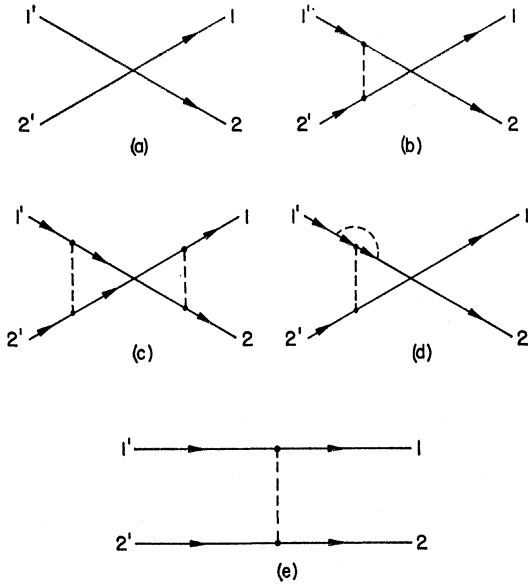


FIG. 3. Diagrams for  $G_2(1,2; 1',2')$ . Here the solid lines are  $G$ 's, not  $G_0$ 's. Figure 3(a) contributes a  $1/\alpha$  term to  $\mu$ . Figure 3(b) is of order  $\alpha^0$ ; 3(c) and 3(d) are of order  $\alpha$ . Figure 3(e) is of the order of the density squared and may be neglected.

Therefore, Eq. (31) becomes

$$\mu = \frac{e\beta}{24n} \int_{-\infty}^{\infty} dt_1 \int d^3r_1 (\nabla_1 - \nabla_{1'}) \cdot (\nabla_2 - \nabla_{2'}) G_2^>(1,2; 1',2') |_{1'=1^+, 2'=2^+=0}. \quad (34)$$

Here the  $G_2^>$  is a reminder that we should use the form of  $G_2$  appropriate for  $it_1 > it_2$ .

To evaluate Eq. (34), we shall expand  $G_2$  in a power series in  $G$  and  $V$ . This expansion is indicated in Fig. 3. It should be noted that we cannot expand  $G_2$  in terms of  $G_0$  and  $V$  because  $\mu$  is proportional to  $\alpha^{-1}$ , and hence the  $G_0$  expansion cannot converge. For most systems, even the expansion in  $V$  and  $G$  will converge very slowly.<sup>19</sup> Fortunately this convergence is particularly rapid for the case of low-temperature optical phonon scattering. For small  $\alpha$ , Fig. 3(a) gives the contribution of the scattering out of the beam term in the standard Boltzmann equation. It is of order  $\alpha^{-1}$ . Figures 3(b) and 3(c) give parts of the scattering back into the beam term. At high temperatures they too would be of order  $\alpha^{-1}$ . However, at low temperatures the scattering back into the beam term does not contribute to the mobility to lowest order in  $\alpha$ .<sup>9</sup> Therefore, Figs. 3(b) and 3(c) are not of order  $\alpha^{-1}$  at low temperatures;

<sup>19</sup> For example, in a system of electrons interacting with acoustical phonons, an infinite set of diagrams must be summed to get results correct to order  $\alpha^{-1}$ . The application of the Kubo formula to such a system is discussed in detail by J. Ranninger in *Polarons and Excitons*, edited by C. G. Kuper and G. D. Whitfield (Oliver and Boyd Ltd., Edinburgh, 1963), pp. 202-210.

instead they are of order  $\alpha^0$  and  $\alpha^1$ , respectively. This especially rapid convergence of the perturbation theory simplifies our calculation considerably. We wish to calculate  $\mu$  to order  $\alpha^0$ . We must calculate the contributions from Figs. 3(a) and 3(b), but we can safely neglect Figs. 3(c), 3(d), and all higher order diagrams.

Figure 3(a) gives a contribution to the mobility which is

$$\begin{aligned} \mu_a &= \frac{e\beta}{24n} \int_{-\infty}^{\infty} dt_1 \int d^3r_1 (\nabla_1 - \nabla_{1'}) \cdot (\nabla_2 - \nabla_{2'}) \\ &\quad \times G^>(1-2') G^<(2-1') |_{1'=1^+, 2'=2^+=0} \\ &= \frac{e\beta}{6n} \int \frac{d^3p}{(2\pi)^3} \int \frac{d\omega}{2\pi} p^2 [A(\mathbf{p}, \omega)]^2 e^{-\beta(\omega - \mu)}. \end{aligned} \quad (35)$$

The predominant contributions to Eq. (35) come for  $\mathbf{p}=0$ ,  $\omega \approx E(\mathbf{p})$ . In this region we can write

$$[A(\mathbf{p}, \omega)]^2 = [z(\mathbf{p})]^2 \frac{[\tau(\mathbf{p})]^2}{\{[\omega - E(\mathbf{p})]^2 + [2\tau(\mathbf{p})]^2\}^2},$$

which becomes in the limit of large  $\tau$

$$[A(\mathbf{p}, \omega)]^2 = 4\pi\tau(\mathbf{p}) [z(\mathbf{p})]^2 \delta(\omega - E(\mathbf{p})). \quad (36)$$

Hence, Eq. (35) may be written as

$$\begin{aligned} \mu_a &= \frac{e\beta}{6n} \int \frac{d^3p}{(2\pi)^3} p^2 2\tau(0) [z(0)]^2 e^{-\beta(E(\mathbf{p}) - \mu)} \\ &= e\tau(0) [z(0)]^2 m^*, \end{aligned} \quad (37)$$

where we have used Eq. (22) in going from the first line to the second line of Eq. (37). We express  $m^*$ ,  $z$ , and  $\tau$  with the aid of Eqs. (18), (19), and (30), respectively, to find

$$\mu_a = (e/2\alpha\bar{N}) [1 - \frac{5}{6}\alpha]. \quad (38)$$

The next contribution to the mobility comes from Fig. 3(b), which gives

$$\begin{aligned} G_2^b(1,2; 1',2') &= -i \int_0^{-i\beta} d\bar{1} \int_0^{-i\beta} d\bar{1}' G(1-\bar{1}) \\ &\quad \times G(\bar{1}-2') V(\bar{1}-\bar{1}') G(2-\bar{1}') G(\bar{1}'-1'). \end{aligned} \quad (39)$$

For  $t_1 = t_{1'}$  and  $t_2 = t_{2'} = 0$ ,

$$\begin{aligned} G_2^b(1,2; 1',2') &= -i \int_0^{t_1} d\bar{1} \int_{t_1}^{-i\beta} d\bar{1}' G^>(1-\bar{1}) \\ &\quad \times G^>(\bar{1}-2') V^<(\bar{1}-\bar{1}') G^<(2-\bar{1}') G^>(\bar{1}'-1') \end{aligned} \quad (40)$$

plus terms of order  $[G^<]^2$ , which we neglect. We substitute Eq. (40) into Eq. (34), and find after considerable algebra that Eq. (40) makes a contribution to the

mobility which is

$$\begin{aligned} \mu_b = & \frac{e\beta}{3n} \int \frac{d\omega}{2\pi} \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} \frac{2^{3/2}\pi\alpha}{(\mathbf{p}-\mathbf{p}')^2} \mathbf{p} \cdot \mathbf{p}' e^{-\beta(\omega-\mu)} \{ \bar{N} A(\mathbf{p},\omega) \operatorname{Re}G(\mathbf{p}',\omega+1) [A(\mathbf{p},\omega) \operatorname{Re}G(\mathbf{p}',\omega+1) \\ & + \operatorname{Re}G(\mathbf{p},\omega) A(\mathbf{p}',\omega+1)] + (\bar{N}+1) A(\mathbf{p},\omega) \operatorname{Re}G(\mathbf{p}',\omega-1) [A(\mathbf{p},\omega) \operatorname{Re}G(\mathbf{p}',\omega-1) + \operatorname{Re}G(\mathbf{p},\omega) A(\mathbf{p}',\omega-1)] \}, \quad (41) \end{aligned}$$

where

$$\operatorname{Re}G(\mathbf{p},\omega) = \mathcal{P} \int \frac{d\omega' A(\mathbf{p},\omega')}{2\pi \omega - \omega'}.$$

We neglect the terms in Eq. (41) proportional to  $\bar{N}$  and notice that the only important contribution to Eq. (41) comes from the term involving  $[A(\mathbf{p},\omega)]^2$ , which we evaluate with the aid of Eq. (36). Thus,

$$\begin{aligned} \mu_b = & \frac{e\beta}{3n} (2^{5/2}\pi\alpha) \tau(0) \int \frac{d^3p}{(2\pi)^3} \int \frac{d^3p'}{(2\pi)^3} \frac{\mathbf{p} \cdot \mathbf{p}'}{(\mathbf{p}-\mathbf{p}')^2} \\ & \times \left[ \frac{1}{1+p'^2/2} \right]^2 e^{-\beta(p'^2/2-\mu)} + O(\alpha). \quad (42) \end{aligned}$$

Hence, finally,

$$\mu_b = \frac{2}{3} \alpha e \tau(0) = (e/2\alpha\bar{N}) \frac{2}{3} \alpha, \quad (43)$$

and

$$\mu = \mu_a + \mu_b = \mu_0(1 - \alpha/6), \quad (44)$$

where  $\mu_0$  is the weak coupling mobility  $[\mu_0 = e/2\alpha\bar{N}]$ .

Again, we see a verification of the quasiparticle

picture which would predict

$$\mu = \frac{e\tau(0)}{m^*} = \frac{e}{2\alpha\bar{N}} [1 - \alpha/6 + O(\alpha^2)]. \quad (45)$$

We have explicitly verified that  $e\tau(0)/m^*$  is a correct expression for the mobility in the first nontrivial order in  $\alpha$ ; as mentioned earlier, however, preliminary calculations indicate that the quasiparticle picture of the polaron is generally valid at low temperatures for the description of polaron states with energies below the phonon emission threshold, so that  $e\tau(0)/m^*$  is probably correct to all orders in  $\alpha$  at low temperatures. However, these speculations about the correctness of the quasiparticle picture are irrelevant to our main purpose here: the derivation of a perturbation theoretic formula for the mobility, as given by Eq. (44). This result is an exact perturbation expansion of the mobility which is appropriate for weak coupling,  $\alpha/6 \ll 1$ , and low temperatures,  $\beta^{-1} \ll 1$ . The next corrections to this formula will be terms  $\mu_0\beta^{-1}$  and  $\mu_0(\alpha/6)^2$  times numerical coefficients of order unity. Equation (44) is then inappropriate in the intermediate coupling domain  $\alpha \sim 6$ .

#### IV. CONCLUSIONS

One possible criterion for the reliability of a weak and intermediate coupling polaron mobility theory is that its expansion in powers of  $\alpha$  correspond quite closely with the exact expansion. We have thus computed the first nontrivial term (proportional to  $\alpha$ ) in the expansion of  $\mu/\mu_0$  for the various theories; the results are displayed in Table I. We see immediately that, according to the above criterion, the mobility formula which was originally derived by Osaka (and recently derived in another way by one of us) is exceedingly good. The coefficient of the  $\alpha$  term of  $\mu/\mu_0$  given by Osaka differs from the exact coefficient by only about 4%. For this reason, we conclude that the Osaka formula is probably the most reliable low-temperature mobility result that we presently have.

TABLE I. Expansion of the various mobility theories in powers of  $\alpha$ .<sup>a</sup>

Underlying theory	Mobility theory	$\mu/\mu_0$ for $\alpha=3$	$\mu/\mu_0$ for $\alpha \rightarrow 0$
Lee, Low, and Pines	Low and Pines	0.34	$1 - 0.500\alpha$
Feynman model	Osaka (Kadanoff)	0.53	$1 - 0.173\alpha$
	Schultz	2.0	$1 + 1.05\alpha$
	Garcia-Moliner <sup>b</sup>	0.39	$1 - 0.250\alpha$
Perturbation theory	Morita <sup>b</sup>	0.1	$1 - 2.22\alpha$
	Present theory		$1 - 0.167\alpha$

<sup>a</sup> The dc mobility of Ref. 7 is not included in this table, because it has the wrong temperature dependence in the low-temperature limit.

<sup>b</sup> In theories which do not specify  $m^*$ , we have used the Feynman-model values calculated by Schultz (Ref. 4).