

Study of transport in a strongly correlated electron system*

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The electronic transport in a strongly correlated electron system is studied at a low concentration c (c is unity for a filled band), using a single s -band Hubbard model. Employing a T -matrix approximation for the electron-electron interaction, we give a rigorous microscopic derivation of the ac Boltzmann transport equation for intraband electron transitions in a nondegenerate limit. The result is applied to the calculation of dc and ac conductivity in several situations: in two and three dimensions, the mobility is inversely proportional to the electron concentration to the lowest order in c . In the simple cubic lattice the mobility is larger roughly by a factor c^{-1} than that of a hole in an otherwise half-filled band treated earlier by Brinkman and Rice. The resistivity arises from the umklapp process of the electron-electron scattering. The ac conductivity shows a Drude-Lorentz type behavior characteristic of metallic conduction. In one dimension with nearest-neighbor hopping, the dc conductivity becomes infinite within a two-particle T -matrix approximation. The effect of many-particle scattering to this result is discussed. We also study how the above infinity is avoided by introducing a small second-nearest-neighbor or interchain electron transfer. The dc transverse conduction for the latter anisotropic case is also investigated. The interband optical absorption is also treated for degenerate and nondegenerate systems. In making a two-particle T -matrix approximation, we find a result obtained earlier by Kubo, using decoupling approximations.

I. INTRODUCTION

The electronic properties of solids with narrow bands are characterized by strong Coulomb interactions between electrons. Hubbard¹ and Kanamori² approximated the electron-electron interaction by an intrasite Coulomb repulsion U , using the Wannier representation. The Hubbard model [cf. (2.1)] incorporates the above form of the Coulomb repulsion as well as the kinetic energy, and contains the basic features of the problem where the electronic correlation plays an important role.

Recently Brinkman and Rice (BR),³ and Ohata and Kubo,⁴ studied the mobility of an extra electron or a hole in an otherwise half-filled, nearest-neighbor hopping Hubbard band with $U = \infty$. Eswaran and Kimball⁵ generalized the moment method of Ohata and Kubo⁴ to an arbitrary electron and impurity concentrations. The interband optical absorption has been investigated by Kubo⁶ for an arbitrary electron density, using the decoupling approximation of Hubbard.^{1a} The basic approximations used in these works are of nonperturbative nature. Path-counting methods are employed in the above cited dc calculations,³⁻⁵ so that an extension of these theories beyond the nearest-neighbor electron transfer and $U = \infty$ limit becomes very complicated. It is also very difficult to apply the retracing-path-summation method of BR³ to an electron density other than the one treated by them.

In this paper we use a different approach. One asks whether one can develop a systematic perturbation theory of ac and dc electron transport of

the Hubbard model. The basic difficulty of such a problem in a strong-coupling narrow-band Hubbard model lies in the fact that there is no suitable perturbation parameter. If one tries to use the kinetic energy as a perturbation in the site representation, then the standard perturbation method cannot be applied, because Wick's theorem is not available. At low electron concentration c limit, however, one may treat the electronic repulsion as a "perturbation," namely, as a scattering potential. In this limit it is sufficient to consider only the two-particle scattering, which can be solved exactly. As is well known, the effect of three-particle scattering is of order c smaller (c is unity for a filled band). The strength of the effective two-particle interaction becomes of order of the kinetic energy, namely, the bandwidth B , when $U \gg B$, because the electrons avoid each other at the cost of the kinetic energy.²

In the present approach the resistivity, namely, the momentum dissipation, occurs through the electron-electron umklapp scattering. The kinetic energy is included in the zeroth order, so that a general band structure can be treated readily. Furthermore, if one wishes, one can include other types of scattering such as electron-phonon, electron-impurity interactions. However, the present paper will be restricted to a pure Hubbard model. The result of the present treatment is valid at a low electron concentration, so that it is complementary to that of BR.³

For the main part of the paper, namely, up to Sec. VI, we treat dc and intraband transitions. The two-particle T -matrix approximation of

Kanamori² is employed. We are interested in a strongly correlated system, where the gap between the two subbands is large compared with $k_B T$, so that only the lower band is occupied. The present theory is also valid in the weakly interacting region ($U \ll B$). The external frequency ν is assumed to be small (i.e., $\hbar\nu \ll B$), allowing only the intraband transitions. For the above system, we give a rigorous microscopic derivation of the Boltzmann equation, starting from Kubo's formalism. To establish the Boltzmann equation, one has to assume that the system is at high temperature (i.e., $k_B T \gg \epsilon_F$; ϵ_F is the Fermi energy), namely, that the system is nondegenerate. This leads to a smallness parameter λ , which is given by the larger of the ratios xy^{-1} : $x = \hbar\nu$, $\Gamma \sim cB$ [cf. (3.16b)], and $y = B, k_B T$. In the dc limit, this corresponds to the requirement that the mean free path of the electron is larger than the de Broglie wavelength, a well-known criterion for the validity of the Boltzmann equation. The present analysis becomes exact in the dc limit at zero concentration.

The result is applied to the calculation of dc conductivity and intraband absorption in several situations: In two and three dimensions, the mobility is inversely proportional to the electronic concentration to the lowest order in c . This reflects simply the fact that the electron-electron unklapp mean free path is inversely proportional to the electron concentration. The ac conductivity shows a Drude-Lorentz-type behavior characteristic of metallic conduction. In one dimension with nearest-neighbor electron transfer only, BR³ and Beni *et al.*⁷ found for a single hole or an extra electron in an otherwise half-filled band that the conductivity is infinite in the limit $U = \infty$. In the present treatment, we find that the effective two-particle unklapp scattering strength vanishes for an arbitrary value of U , leading to an infinite conductivity. The physical picture of this one-dimensional anomaly is discussed. It is also shown that the two-particle approximation is insufficient in this case, and the effect of many-particle interactions is discussed. We study how the one-dimensional anomaly is avoided by introducing an interchain or a second-nearest-neighbor electron transfer. We also calculate the dc transverse conductivity of an anisotropic system.

The interband optical absorption ($\hbar\nu \simeq U$) is also studied for a low-density system. Using a T -matrix approximation, we find a result obtained by Kubo⁶ earlier by using decoupling approximations.

Up to Sec. VI we treat the intraband transition for a high-temperature nondegenerate system and assume $\hbar\nu \ll B$. In Sec. II we establish the basic

preliminaries. The conductivity is expressed in terms of a correlation function. In Sec. III we discuss the one-particle Green's function, the self-energy part, and the T -matrix approximation. In Sec. IV the correlation function is expressed in terms of a vertex function. An integral equation (i.e., vertex equation) for the vertex function is given. In Sec. V the vertex equation is evaluated and the Boltzmann equation is obtained. The basic results of Secs. II-V are summarized in Sec. VI, where we solve the Boltzmann equation in the dc limit for several situations, using a variational method. The ac conductivity is also obtained, using a perturbation method. The interband optical absorption is treated in Sec. VII. Finally, in Sec. VIII a discussion of the result is given.

II. FORMALISM

In this section we set up the basic formalism. The Hubbard Hamiltonian has the form

$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad (2.1)$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ denote, respectively, the creation and destruction operators for an electron in a Wannier state localized at site i with spin σ , and $n_{j\sigma}$ is the number operator (i.e., $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$). The first term represents the tunneling of electrons from site j to i with a transfer integral t_{ij} which depends only on their vector separation [i.e., $t_{ij} = t(\vec{r}_i - \vec{r}_j)$]. The second term represents the repulsive Coulomb interaction between two electrons of opposite spins on the same site. Obvious vector notations will be suppressed frequently.

One transforms (2.1) in a band representation to

$$H = \sum_{k\sigma} \epsilon_k n_{k\sigma} + \frac{U}{N} \sum_{k_1 k_2 k_3 k_4} \Delta(k_1 + k_2, k_3 + k_4) \times c_{k_3\uparrow}^\dagger c_{k_1\uparrow} c_{k_4\downarrow}^\dagger c_{k_2\downarrow}, \quad (2.2)$$

where $n_{k\sigma} \equiv c_{k\sigma}^\dagger c_{k\sigma}$, and N is the total number of sites. The destruction operator $c_{k\sigma}$ is given by

$$c_{k\sigma} = N^{-1/2} \sum_j \exp(-i\vec{r}_j \cdot \vec{k}) c_{j\sigma} \quad (2.3)$$

and the band energy is given by

$$\epsilon_k = - \sum_j \exp(i\vec{r}_j \cdot \vec{k}) t(\vec{r}_j). \quad (2.4)$$

Finally, $\Delta(k_1 + k_2, k_3 + k_4)$ in the second term of (2.2) denotes the Kronecker delta and is nonvanishing only when $\vec{k}_1 + \vec{k}_2 = \vec{k}_3 + \vec{k}_4 + \vec{g}$ (\vec{g} is a reciprocal-lattice vector).

The conductivity is given by⁸

$$\sigma_{xy}(\nu) = (e^2/i\Omega) [\mathfrak{F}_{xy}(\hbar\nu + i0) - \mathfrak{F}_{xy}(i0)] / \nu, \quad (2.5)$$

where $e, \Omega, i0$ are, respectively, the charge of an electron, volume of the crystal, and a positive imaginary infinitesimal. $\mathfrak{F}_{xy}(\hbar\nu + i0)$ is the analytic continuation ($\omega_r \rightarrow \hbar\nu + i0$) of the velocity-velocity correlation function

$$\mathfrak{F}_{xy}(\omega_r) = \int_0^\beta e^{\omega_r u} \mathfrak{F}_{xy}(u) du \quad (\beta^{-1} \equiv k_B T). \quad (2.6)$$

The boson "frequency" is given by $\omega_r = 2\pi i r \beta^{-1}$ (r is an integer), and

$$\mathfrak{F}_{xy}(u) = \langle T v_x(u) v_y \rangle. \quad (2.7)$$

Here T is the time-ordering operator and $v_x(u)$ is in the Heisenberg representation [i.e., $v_x(u) = e^{uH} v_x e^{-uH}$]. The angular bracket denotes the grand canonical thermodynamic average. The expression for the velocity operator in band repre-

sentation is

$$v_x = \sum_{k\sigma} v_k^x n_{k\sigma}; \quad v_k^x = \hbar^{-1} \frac{\partial \epsilon_k}{\partial k_x}. \quad (2.8)$$

III. T -MATRIX AND SELF-ENERGY PART

As is mentioned in the Introduction, it is sufficient to consider only two-particle scattering at a low electron concentration. When the Coulomb repulsion is very strong, one has to go beyond the first Born approximation by incorporating the modification of the wave functions to all orders in U . As a result, one obtains a smaller effective repulsion due to the fact that electrons avoid each other, as the correlation becomes large. The above approximation is known as a two-particle T -matrix approximation.

The T matrix K is shown in Fig. 1(a) as the shaded area and is given by^{2,9,10}

$$K(p_1, p_2; p_3, p_4) = N^{-1} U - \beta N^{-1} U \sum_q S(p_1 - q) S(p_2 + q) K(p_1 - q, p_2 + q; p_3, p_4), \quad (3.1)$$

where S is a dressed temperature Green's function (represented by solid lines) defined in (3.5) below, and p_i, q are four momenta given by $p_i = (\vec{k}_i, \xi_{i_i})$, $q = (\vec{q}, \omega_m)$. Here \vec{k}_i, \vec{q} are wave vectors and ω_m, ξ_{i_i} are, respectively, boson "frequency" and fermion "frequency," i.e., $\xi_{i_i} = \beta^{-1}(2l+1)\pi i + \mu$. m, l are integers and μ is the chemical potential. It is understood in (3.1) that

$$p_1 + p_2 = p_3 + p_4. \quad (3.2)$$

The wave vectors are conserved to within a reciprocal-lattice vector. The momentum-independent electron repulsion U is represented by dotted lines in Fig. 1. One then obtains from (3.1)

$$K(p_1, p_2; p_3, p_4) = N^{-1} U [1 + L(p_1 + p_2)]^{-1}, \quad (3.3)$$

where

$$L(p_1 + p_2) = \beta^{-1} N^{-1} U \sum_q S^0(p_1 - q) S^0(p_2 + q). \quad (3.4)$$

Here the full propagators are replaced by the bare propagators S^0 in accordance with the two-particle approximation. The full Green's function is

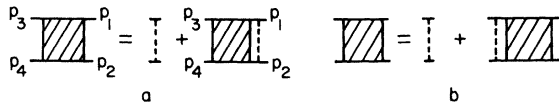


FIG. 1. Two equivalent definitions of T matrix.

given for $p = (\vec{k}, \xi_l)$ by

$$S(p) = [\xi_l - \epsilon_k - G_k(\xi_l)]^{-1}. \quad (3.5)$$

We shall frequently write $S(p) = S_k(\xi_l)$. This kind of notation will be used throughout. The self-energy part $G_k(\xi_l)$ is shown in Fig. 2:

$$G(p) \equiv G_k(\xi_l) = \beta^{-1} \sum_{p_1} K(p_1, p; p_1, p) S^0(p_1). \quad (3.6)$$

The total number of electrons N_e is related to the full Green's function by

$$\begin{aligned} N_e &= \sum_{k\sigma} \langle T c_{k\sigma}^\dagger(+0) c_{k\sigma} \rangle \\ &= 2\beta^{-1} \sum_{kl} S_k(\xi_l) \exp(+0 \times \xi_l). \end{aligned} \quad (3.7)$$

The l summation can be converted^{9,10} into an integration in the complex ξ plane by using the analytical properties of S_k :

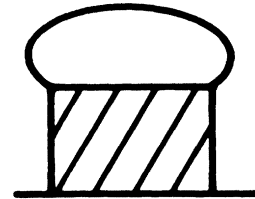


FIG. 2. Self-energy part.

$$N_e = 2 \int_{-\infty}^{\infty} \rho(\xi) f(\xi) d\xi, \quad (3.8)$$

$$\rho(\xi) = \frac{1}{\pi} \text{Im} \sum_k S_k(\xi - i0),$$

where $f(\xi)$ is the Fermi function, and Im is the imaginary part of what follows. The factor 2 indicates the spin degeneracy. We assume a random spin configuration up to Sec. VII. An extension to an arbitrary spin configuration is trivial. The quantity $\rho(\xi)$ is to be identified with the single-particle density of states. It is shown in (3.16) that the self-energy part is of order c . Therefore, the full Green's function S_k in (3.8) can be replaced by a free Green's function S_k^0 in the limit $c \ll 1$, yielding

$$N_e = 2 \sum_k f_k, \quad f_k \equiv f(\epsilon_k). \quad (3.9)$$

At high temperature, namely, when $-\beta\epsilon_k$ is not large and at low concentration ($c \equiv N_e/2N \ll 1$) one obtains

$$f_k = \exp[-\beta(\epsilon_k - \mu)] \sim c \ll 1. \quad (3.10a)$$

It is clear that

$$f(\xi) \sim c \quad \text{if } -\beta\xi \lesssim 1. \quad (3.10b)$$

We shall also frequently use a similar relation for the boson occupation function:

$$N(\xi - 2\mu) \equiv (e^{\beta(\xi - 2\mu)} - 1)^{-1} \approx e^{-\beta(\xi - 2\mu)} \sim c^2 \quad \text{if } -\beta\xi \lesssim 1. \quad (3.11)$$

The summation on boson frequency in (3.4) can also be converted into an integration in the complex ω plane, yielding

$$L(p_1 + p_2) = -N^{-1}U \sum_q [1 - f(\epsilon_{k_1 - q}) - f(\epsilon_{k_2 + q})] \\ \times S_{k_2 + q}^0(\zeta_{I_1} + \zeta_{I_2} - \epsilon_{k_1 - q}). \quad (3.12)$$

Terms proportional to the Fermi function in (3.12) are unimportant for the intraband transitions. However, they should be maintained for the interband transitions treated in Sec. VII. To simplify the notation, we introduce

$$K(p_1, p_2; p_3, p_4) \equiv K_{1234}(\zeta_{I_1} + \zeta_{I_2}). \quad (3.13)$$

Here the subscripts 1234 stand for the momenta k_1, k_2, k_3 , and k_4 . The function $K_{1234}(z)$ has a cut along a segment of the $\text{Im}(z) = 0$ axis near the lower band. For a large value of U (i.e., $U \gg B$), it has another cut near the upper band (i.e., $z \approx U$). This cut corresponds to the excitations in the upper Hubbard band, and will not be considered for the present analysis, until we come to Sec. VII.

The self-energy part of (3.6) can also be computed in a straightforward manner, yielding

$$G_k(\zeta_I) = \sum_{k_1} f_{k_1} K_{1010}(\epsilon_{k_1} + \zeta_I), \quad (3.14)$$

where terms of order c^2 are dropped. The subscript "0" in K_{1010} stands for \vec{k} . Defining

$$G_k(\zeta - i0) = M_k(\zeta) + i\Gamma_k(\zeta), \quad (3.15)$$

we observe the following properties of the self-energy part:

$$\Gamma_k(\zeta) = 0 \quad \text{if } |\zeta| > \frac{3}{2}B, \quad (3.16a)$$

$$M_k(\zeta), \Gamma_k(\zeta) \text{ are of order } cB. \quad (3.16b)$$

These properties are used frequently in Sec. V.

IV. VERTEX EQUATION AND CORRELATION FUNCTION

In this section we evaluate the correlation function. For this purpose, a vertex equation is derived using the T -matrix approximation. The vertex equation is shown in Fig. 3. The external field vertex parts are represented by black dots with wiggly lines.⁹⁻¹¹ The latter indicates the external field lines. The external-field vertex parts (designated as Λ) are given by an integral equation:

$$\Lambda_\sigma(p, p_\omega) = -\beta^{-2} \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p) S(p_1) S(p_{1\omega}) S(p_2) S(p_3) K(p_3, p_\omega; p_2, p_{1\omega}) \Lambda_\sigma(p_1, p_{1\omega}) \\ - \beta^{-2} \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p) S(p_1) S(p_2) S(p_{2\omega}) S(p_3) K(p_3, p_\omega; p_{2\omega}, p_1) \Lambda_{-\sigma}(p_2, p_{2\omega}) \\ + \beta^{-1} \sum_{p_3} K(p_3, p_\omega; p_{3\omega}, p) S(p_3) S(p_{3\omega}) \Lambda_{-\sigma}(p_3, p_{3\omega}) + v_k^*, \quad (4.1)$$

where $p_\omega \equiv (\vec{k}, \zeta_I + \omega_r)$, etc., and σ indicates the spin, which will be suppressed hereafter. The vertex function $\Lambda(p, p_\omega)$, has cuts along the axes $\text{Im}(\zeta_I) = 0, \text{Im}(\zeta_I + \omega_r) = 0$ in the complex ζ_I plane.

It is convenient to define a quantity

$$\Phi(p, p_\omega) = i\hbar \Lambda(p, p_\omega) [\omega_r + G(p) - G(p_\omega)]^{-1}. \quad (4.2)$$

Then

$$S(p)S(p_\omega)\Lambda(p, p_\omega) = -i\hbar^{-1}[S(p) - S(p_\omega)]\Phi(p, p_\omega). \tag{4.3}$$

One rewrites (4.1) as

$$\begin{aligned} (i\hbar)^{-1}[\omega_r + G(p) - G(p_\omega)]\Phi(p, p_\omega) &= v_k^x - \frac{1}{i\hbar\beta^2} \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p)S(p_2)S(p_3)K(p_3, p_\omega; p_2, p_{1\omega})\Phi(p_1, p_{1\omega})[S(p_1) - S(p_{1\omega})] \\ &\quad - \frac{1}{i\hbar\beta^2} \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p)S(p_1)S(p_3)K(p_3, p_\omega; p_{2\omega}, p_1)\Phi(p_2, p_{2\omega})[S(p_2) - S(p_{2\omega})] \\ &\quad + \frac{1}{i\hbar\beta} \sum_{p_3} K(p_3, p_\omega; p_{3\omega}, p)\Phi(p_3, p_{3\omega})[S(p_3) - S(p_{3\omega})]. \end{aligned} \tag{4.4}$$

In the Appendix we derive a useful relationship:

$$G(p) - G(p_\omega) = -\beta^2 \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p)S(p_2)S(p_3)K(p_3, p_\omega; p_2, p_{1\omega})[S(p_1) - S(p_{1\omega})], \tag{4.5}$$

which, substituted into (4.4), yields

$$\begin{aligned} (i\hbar)^{-1}\omega_r\Phi(p, p_\omega) - v_k^x &= -\frac{1}{i\hbar\beta^2} \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p)S(p_2)S(p_3)K(p_3, p_\omega; p_2, p_{1\omega})[\Phi(p_1, p_{1\omega}) - \Phi(p, p_\omega)][S(p_1) - S(p_{1\omega})] \\ &\quad - \frac{1}{i\hbar\beta^2} \sum_{p_1 p_2 p_3} K(p_2, p_1; p_3, p)S(p_1)S(p_3)K(p_3, p_\omega; p_{2\omega}, p_1)\Phi(p_2, p_{2\omega})[S(p_2) - S(p_{2\omega})] \\ &\quad + \frac{1}{i\hbar\beta} \sum_{p_3} K(p_3, p_\omega; p_{3\omega}, p)\Phi(p_3, p_{3\omega})[S(p_3) - S(p_{3\omega})]. \end{aligned} \tag{4.6}$$

The above equation will lead to the Boltzmann transport equation. The quantity $\Phi(p, p_\omega)$ becomes the distribution function, when analytically continued to the real axis. The term proportional to $\Phi(p, p_\omega)$ on the right-hand side of (4.6) arises from the self-energy parts through (4.5) and will eventually constitute the scattering-out rate.

The correlation function is given by

$$\mathfrak{F}_x(\omega_r) = -\beta^{-1} \sum_p v_k^x S(p)S(p_\omega)\Lambda(p, p_\omega) = \frac{-1}{i\hbar\beta} \sum_p v_k^x [S(p) - S(p_\omega)]\Phi(p, p_\omega). \tag{4.7}$$

Defining

$$\Phi_k(\zeta) = \Phi_k(\zeta - i0, \zeta + \hbar\nu + i0), \tag{4.8a}$$

$$\Phi_k^\pm(\zeta) = \Phi_k(\zeta \pm i0, \zeta + \hbar\nu \pm i0), \tag{4.8b}$$

one evaluates (4.7) slightly above the real axis (i.e., $\omega_r = \hbar\nu + i0$):

$$\begin{aligned} \mathfrak{F}_x(\hbar\nu + i0) &= \frac{1}{2\pi\hbar} \sum_k v_k^x \int_{-\infty}^{\infty} d\zeta \left([f(\zeta) - f(\zeta + \hbar\nu)]\Phi_k(\zeta)\mathfrak{S}_k(\zeta; \hbar\nu) \right. \\ &\quad \left. - f(\zeta) \sum_{\pm} (\pm)\Phi_k^\pm(\zeta)\mathfrak{S}_k^\pm(\zeta; \hbar\nu) + [f(\zeta + \hbar\nu) - f(\zeta)]\Phi_k^-(\zeta)\mathfrak{S}_k^-(\zeta; \hbar\nu) \right), \end{aligned} \tag{4.9}$$

where

$$\mathfrak{S}_k(\zeta; \hbar\nu) = S_k(\zeta - i0) - S_k(\zeta + \hbar\nu + i0), \quad \mathfrak{S}_k^\pm(\zeta; \hbar\nu) = S_k(\zeta \pm i0) - S_k(\zeta + \hbar\nu \pm i0). \tag{4.10}$$

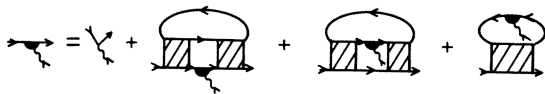


FIG. 3. Vertex equation.

It is now clear that to evaluate the correlation function, one has to solve for $\Phi_k(\zeta)$, $\Phi_k^\pm(\zeta)$ from the integral equation (4.6). To this end we evaluate (4.6) using λ (defined in the Introduction) as a perturbation parameter. This is an extremely complicated and lengthy task, so that we give only

a brief description of the important steps and basic approximations, omitting the details. The computation is carried out in Sec. V. The basic results are summarized in (6.1)–(6.4) of Sec. VI.

V. EVALUATION OF THE CORRELATION FUNCTION: BOLTZMANN EQUATION

In this section we evaluate the vertex equation (4.6), and the correlation function (4.9), using a standard technique such as given in Refs. 9–11. A fundamental approximation is given by¹⁰

$$-i\nu\Phi_k^\pm(\zeta) = v_k^x[1 + B_k^\pm(\zeta)] + O(\lambda^2), \tag{5.2a}$$

$$-i\nu\Phi_k(\zeta) = v_k^x + \frac{2\pi}{\hbar} \sum_{k_1 k_2 k_3} (f_1 + f_2 - 1) [f_3 + N(\zeta + \epsilon_3 - 2\mu)] [\Phi_k(\zeta) + \Phi_3 - \Phi_1 - \Phi_2] \times |K_{2130}(\zeta + \epsilon_3 - i0)|^2 \delta(\zeta + \epsilon_3 - \epsilon_1 - \epsilon_2) + O(\lambda), \tag{5.2b}$$

where $\epsilon_i = \epsilon_{k_i}$, $f_i = f(\epsilon_i)$, $\Phi_i = \Phi_{k_i}(\epsilon_i)$, and $\delta(x)$ is a δ function. In (5.2a) $B_k^\pm(\zeta)$ are certain functions which are of order λ and have the following property:

$$B_k^+(\zeta) - B_k^-(\zeta) = O(\lambda^2) \text{ if } |\zeta| > \frac{3}{2} B. \tag{5.3}$$

Terms proportional to f_1, f_2 , and $N(\zeta + \epsilon_3 - 2\mu)$ in (5.2b) are of lower order, and may be dropped. However, they are maintained for later convenience. In deriving (5.2), use is made, for the last term on the right-hand side of (4.6), of a relationship

$$K_{3030}(\zeta + \epsilon_3 - i0) - K_{3030}(\zeta + \epsilon_3 + i0) = - \sum_{k_1 k_2} 2\pi i (f_1 + f_2 - 1) |K_{2130}(\zeta + \epsilon_3 - i0)|^2 \times \delta(\zeta + \epsilon_3 - \epsilon_1 - \epsilon_2) + O(\lambda).$$

$$-i\nu\Phi_k f_k' k_B T = v_k^x f_k' k_B T + \frac{2\pi}{\hbar} \sum f_k f_3 f_1^{(+)} f_2^{(+)} (\Phi_k + \Phi_3 - \Phi_1 - \Phi_2) |K_{2130}(\epsilon_k + \epsilon_3 - i0)|^2 \delta(\epsilon_k + \epsilon_3 - \epsilon_1 - \epsilon_2). \tag{5.5}$$

Equations (5.4) and (5.5) are the central results of this section. The Boltzmann equation (5.5) has been derived for a nondegenerate system, where $f_i \ll 1$. It is not clear whether this equation will remain valid at low temperature and low density, where the system is degenerate.

$$S_k(\zeta + \hbar\nu \pm i0) \approx S_k^0(\zeta \pm i0) + [\hbar\nu - G_k(\zeta + \hbar\nu \pm i0)] \times S_k^{0'}(\zeta \pm i0) + O(\lambda^2), \tag{5.1}$$

where prime means a first derivative with respect to the argument, and can roughly be replaced by B^{-1} or β for an order-of-magnitude estimate. Therefore the second term is of order λ . The perturbation parameter λ is defined in the Introduction. The expression in (5.1) is correct, only when this function is multiplied by a smoothly varying function, which is then integrated in ζ .

Using (3.10)–(3.16), (4.8), and (5.1), one performs the ζ_{i_i} summations on the right-hand side of (4.6). The result is given by

The above equation followed directly from (3.6) and (4.5). The structural similarity between (4.6) and (5.2) is now clear.

Results obtained so far enable us to evaluate the correlation function given in (4.9). After using (5.1)–(5.3), and (3.10) in (4.9), one obtains

$$\frac{\mathcal{F}_x(\hbar\nu + i0) - \mathcal{F}_x(0)}{i\nu} = - \sum_k f_k' \Phi_k v_k^x + O(\lambda), \tag{5.4}$$

where $\Phi_k = \Phi_k(\epsilon_k)$. The result in (5.4) arises solely from the first term on the right-hand side of (4.9). Other terms in (4.9) give lower-order contributions. Finally using an identity ($f^{(+)} = 1 - f$),

$$f^{(+)}(x)f(x+y) = N(y)[f(x) - f(x+y)],$$

one rewrites (5.2b) as

VI. BOLTZMANN EQUATION AND THE CONDUCTIVITY
In Sec. V we established the Boltzmann equation:

$$-i\nu\Phi_k f_k' = v_k^x f_k' + \frac{1}{k_B T} \sum_{k_1 k_2 k_3} (\Phi_k + \Phi_{k_1} - \Phi_{k_2} - \Phi_{k_3}) \times P_{k k_1}^{k_2 k_3} + O(\lambda^2), \tag{6.1}$$

with the transition rate given by

$$P_{kk_3}^{k_1 k_2} = (2\pi/\hbar) f_k f_1 f_2^{(+)} f_3^{(+)} |K_{3210}(\epsilon_k + \epsilon_1 - i0)|^2 \times \delta(\epsilon_k + \epsilon_1 - \epsilon_2 - \epsilon_3). \quad (6.2)$$

Here $f_1^{(+)} = 1 - f(\epsilon_1) \simeq 1$, $\epsilon_1 = \epsilon_{k_1}$, and the quantity K_{3210} contains the crystal momentum-conservation factor $\Delta(k + k_1, k_2 + k_3)$. The perturbation parameter λ is defined in the Introduction. The conductivity is given from (2.5) and (5.45) by

$$\sigma_x = -\frac{2e^2}{\Omega} \sum_k f'_k \Phi_k v_k^x + O(\lambda), \quad (6.3)$$

where the factor 2 arises from the spin degeneracy. The above results are valid to lowest order in the smallness parameters c defined in the Introduction. The Fermi function f_k becomes a Maxwell-Boltzmann factor of order c in the present nondegenerate limit. The T matrix is given, inserting the momentum conservation factor explicitly, by

$$\rho = \frac{1}{4k_B T \Omega} \frac{2\pi}{\hbar} 2 \sum_{kk_1 k_2 k_3} (\Phi_k + \Phi_1 - \Phi_2 - \Phi_3)^2 f_k f_1 f_2^{(+)} f_3^{(+)} |K_{3210}(\epsilon_k + \epsilon_{k_1} - i0)|^2 \times \delta(\epsilon_k + \epsilon_1 - \epsilon_2 - \epsilon_3) \left(\frac{e}{\Omega} 2 \sum_k v_k^x \Phi_k f'_k \right)^{-2}, \quad (6.6)$$

where the factor 2 in front of the momentum summations accounts for the spin degeneracy. The solution of the Boltzmann equation (6.1) gives the minimum value for ρ in (6.6).

Usually one takes $\Phi_k = v_k^x$ or k_x as a trial function when the field is in the x direction. For the former choice, one may rewrite (6.6) in a more illuminating fashion by making use of the symmetry property of $P_{kk_i}^{k_2 k_3}$ with respect to the interchange of indices $k, k_1 \leftrightarrow k_2, k_3$, and assuming a cubic symmetry of the crystal for convenience:

$$\sigma(0) = \rho^{-1} = ne^2 \tau_{\text{eff}} / m^*. \quad (6.7)$$

Here n is the electron density (i.e., $n = N_e / \Omega = 2cN / \Omega$), m^* is the effective mass:

$$\frac{1}{m^*} = -\frac{1}{cN} \sum_k f'_k (v_k^x)^2, \quad (6.8a)$$

and τ_{eff}^{-1} is the effective relaxation rate:

$$\tau_{\text{eff}}^{-1} = \frac{m^*}{6cN^2 k_B T} \sum_{kk_1} f_k f_1 (\vec{v}_k + \vec{v}_1)^2 \tau_{k, k_1}^{-1}, \quad (6.9)$$

where the transport relaxation rate is given by

$$K_{3210}(\epsilon_k + \epsilon_{k_1} - i0) = UN^{-1} \Delta(k + k_1, k_2 + k_3) \times [1 + L_{k+k_1}(\epsilon_k + \epsilon_{k_1})]^{-1}, \quad (6.4)$$

where

$$L_{k+k_1}(z) = -UN^{-1} \sum_{k_5 k_6} \frac{\Delta(k + k_1, k_5 + k_6)}{z - \epsilon_{k_5} - \epsilon_{k_6} - i0}. \quad (6.5)$$

As is mentioned in the Introduction, the correlation effect reduces the effective Coulomb repulsion to $U_{\text{eff}} \sim B$ for large U (i.e., $U \gg B$) except for a one-dimensional anomaly to be discussed later.

A. dc conductivity

In the following we study the dc conductivity of the system. The resistivity is given, using a variational principle,¹² by the minimum of the following trial resistivity:

$$\tau_{k, k_1}^{-1} = N \sum_{k_2 k_3} (f_k f_1)^{-1} \times \left(1 - \frac{(\vec{v}_k + \vec{v}_1) \cdot (\vec{v}_2 + \vec{v}_3)}{(\vec{v}_k + \vec{v}_1)^2} \right) P_{kk_1}^{k_2 k_3}. \quad (6.10)$$

The velocity transfer factor

$$1 - [(\vec{v}_k + \vec{v}_1) \cdot (\vec{v}_2 + \vec{v}_3)] / (\vec{v}_k + \vec{v}_1)^2$$

measures the degree of the momentum transfer during each collision and is a characteristic of electronic transport relaxation. At high temperature ($\beta B \ll 1$) one obtains for a nearest-neighbor tight-binding cubic lattice

$$1/m^* = (1/2k_B T)(2ta/\hbar)^2, \quad (6.8b)$$

where a, t are the lattice constant, and the transfer integral.

1. Mobility in three dimension

In two or three dimensions, the effective Coulomb repulsion becomes approximately U_{eff}^2

$= U^2[1 + (UB^{-1}\chi)^2]^{-1}$, which reduces to $U_{\text{eff}} = \chi^{-1}B$ when $U \gg B$ (χ is of order unity). The physical meaning of this is discussed already. According to (6.9) the relaxation time is inversely proportional to the electron density, as is expected and the conductivity given in (6.7) is finite at zero concentration. In a nearest-neighbor simple-cubic tight-binding band, one obtains for $z=6$,

$a \approx 3 \text{ \AA}$, and $\beta B \ll 1$:

$$\begin{aligned} \mu &= e\tau_{\text{eff}}/m^* = (ea^2/\hbar) \frac{1}{8} \pi \beta t c^{-1} I^{-1} \\ &\approx (0.2\beta z t) c^{-1} I^{-1} \quad (\text{cm}^2/\text{V sec}) \end{aligned} \quad (6.11)$$

and

$$\tau_{\text{eff}} = (\pi\hbar/8t) c^{-1} I^{-1}, \quad (6.12)$$

where

$$\begin{aligned} I = \sum_{\vec{g}} (2\pi)^3 \int \int \int_{-\pi}^{\pi} \frac{d^3\theta}{(2\pi)^3} \cdots \int \int \int_{-\pi}^{\pi} \frac{d^3\theta_3}{(2\pi)^3} & [\sin\theta^x(\sin\theta^x + \sin\theta_1^x - \sin\theta_2^x - \sin\theta_3^x)] \left(\frac{1}{F(\vec{\theta}, \vec{\theta}_1)} \right)^2 \\ & \times \delta \left(\sum_{\alpha=x,y,z} (\cos\theta^\alpha + \cos\theta_1^\alpha - \cos\theta_2^\alpha - \cos\theta_3^\alpha) \right) \delta(\vec{\theta} + \vec{\theta}_1 - \vec{\theta}_2 - \vec{\theta}_3 - \vec{g}a). \end{aligned} \quad (6.13)$$

Here $F(\vec{\theta}, \vec{\theta}_1) = (2t/U) |L_{k+k_1}(\epsilon_k + \epsilon_{k_1})|$; $\vec{\theta} = \vec{k}a$, etc. The quantity in the parentheses of (6.11) corresponds to the mobility of a single hole obtained by BR.³ Although it is very difficult to evaluate the dimensionless parameter I , it is not likely to be too much different from order unity. In fact, an approximate computer estimate gives $I \approx 0.6$.

2. Nearest-neighbor-hopping Hubbard chain

The numerical evaluation of (6.6) is comparatively simple and interesting for a nearest-neighbor-hopping Hubbard chain. Taking $\Phi_k = k$, one finds that only the umklapp process ($k+k_1 = k_2+k_3+g$, $g = \pm 2\pi/a, \pm 4\pi/a$) contributes to the resistivity. Using $\epsilon_k = -2t \cos ka$, one rewrites the energy conservation factor of (6.6) as

$$\begin{aligned} \delta(\epsilon_k + \epsilon_1 - \epsilon_2 - \epsilon_3) \\ = \delta[4t \cos \frac{1}{2}(k+k_1)a \sin \frac{1}{2}(k-k_3)a \sin \frac{1}{2}(k_1-k_3)a], \end{aligned} \quad (6.14)$$

where momentum conservation and trigonometric addition theorems have been used repeatedly. It is sufficient to consider $g = 2\pi/a, 4\pi/a$. The δ function of (6.14) is nonzero when its argument vanishes. Let us consider the zeros of the factor $\sin \frac{1}{2}(k-k_3)a$; for $k-k_3=0$, k_1 and k_2 are restricted to $k_1 = \pi/a$, and $k_2 = -\pi/a$, leading to a contribution of order $1/N \rightarrow 0$. For $k-k_3 = 2\pi/a$, one has $k = \pi/a$, and $k_3 = -\pi/a$ so that this contribution vanishes similarly as $1/N$. In the same way the zeros of the second sine factor of (6.14) are unimportant. The cosine factor of (6.14) vanishes when $k+k_1 = \pi/a$, and this root gives a meaningful contribu-

tion to the U process. This corresponds to the situation where two electrons jump across the Brillouin zone in the same direction. However, it should be noted that when $k+k_1 = \pi/a$, the denominator of (6.4) diverges and NK_{3210} vanishes. Namely, the effective Coulomb repulsion vanishes, and the resistivity becomes zero. Physically, the two particles move with the same group velocities when $k+k_1 = \pm \pi/a$, and they do not interact in our local interaction model. However, one has to make a self-energy correction (of order c) to $L_{k+k_1}(z)$ in (6.5). Namely, a full propagator should be used on the right-hand side of (3.12). At the same time various three-particle scattering corrections to the diagrams in Fig. 3 should be made. Noting from (3.14) that U is always larger than the self-energy part, one finds for umklapp process

$$|K_{3210}(\epsilon_k + \epsilon_1 - i0)| \sim N^{-1} \Delta(k+k_1, k_2+k_3) c B \xi,$$

where $\xi = 1$ for a strong correlation ($U \gg B$) and $\xi = (U/B)^2$ for a weak correlation ($U \ll B$). Inserting the above equation into (6.6), the resistivity becomes of order c^2 . However, as can be seen from (6.3), the present formula for the resistivity is valid only to the zeroth order in c , the three-particle and many-particle interactions contributing to higher-order terms. Therefore we can only conclude that the resistivity is of order c or higher for an arbitrary value of U . It should be mentioned at this point that, when $U/B = \infty$, the electrons are generally believed to behave as spinless Fermions⁷ for the present nearest-neighbor-hopping Hubbard chain, giving rise to an infinite dc conductivity. This would mean in our case that all the higher-order terms (in c) in the resistivity cancel out exactly for $U/B = \infty$.

3. Effect of second-nearest-neighbor or interchain electron transfer to nearest-neighbor-hopping Hubbard chain

If the strength of the second-nearest-neighbor electron transfer (t_2) or the interchain transfer (t_\perp) is sufficiently large such that $t_2, t_\perp \gg ct\xi$, then the self-energy correction is unimportant and the two-particle scattering approximation is valid. In the following we consider first the effect of t_2 , and write $\epsilon_k = -\cos k - \epsilon \cos 2k$ ($2t=1, a=1, \epsilon=t_2/t$). We assume here that $c \ll |\epsilon| \ll 1$, and take $\Phi_k = v_k$. It can readily be shown that only the U process contributes to the resistivity. Introducing a coordinate transformation $\theta_0 = \frac{1}{2}(k+k_1), \theta = \frac{1}{2}(k_2+k_3), \phi_0 = \frac{1}{2}(k-k_1)$, and $\phi = \frac{1}{2}(k_2-k_3)$, where $\theta_0 = \theta + \frac{1}{2}g$ and g is a reciprocal-lattice vector, and using energy conservation, one obtains

$$L_{k+k_1}(\epsilon_k + \epsilon_1) = \frac{-i(|\sin\phi_0| + |\sin\phi|)}{4|\epsilon \cos 2\theta_0 (\cos\phi \cos \frac{1}{2}g - \cos\phi_0) \sin\phi_0 \sin\phi|}.$$

At this point we assume that $U \gg 2|\epsilon|$. Using the above result in (6.6), one obtains to the lowest order in ϵ and in high-temperature limit (i.e., $\beta B \ll 1$),

$$\mu = (ea^2/\hbar) \beta 2t/\epsilon^2 c I_1,$$

where

$$I_1 = 64 \int_0^\pi \int_0^\pi \frac{1}{2} d\phi_0 d\phi \frac{|\cos\phi - \cos\phi_0|^3 \sin^2\phi_0 \sin^2\phi}{(\sin\phi + \sin\phi_0)^2} = 0.47.$$

Therefore the mobility is larger than that in a simple cubic lattice by a factor $2/\epsilon^2$. The interchain transfer has a similar effect and the mobility has the form $\mu \propto (ea^2/\hbar)(\beta 2t/\epsilon_\perp^2 c)$ where $\epsilon_\perp = t_\perp/t$.

4. Transverse mobility in an anisotropic system

One now considers the transverse conduction in an anisotropic system, where the transverse (i.e., the interchain) transfer integral t_\perp is much smaller than the nearest-neighbor intrachain transfer t . In this limit, the momentum summations on the right-hand side of (6.6) in the transverse direction are decoupled from those in the longitudinal direction. As a result, the transverse resistivity becomes proportional to the imaginary part of the self-energy part ($\Gamma \sim ct$) and inversely proportional to the electron lifetime ($\tau = \hbar/\Gamma$). Using $\Phi_k = v_k$ in (6.6), and assuming $U \gg B$, and $\beta B \ll 1$, one obtains for the transverse mobility

$$\mu_t = (ea_y^2/\hbar) \pi \beta t_\perp^2 / 8ct, \quad (6.15)$$

where a_y is the interchain distance.

It is to be mentioned that (6.1) is valid for an arbitrary value of t_\perp , and (6.15) for $t_\perp \ll t$. We give, now, a physical interpretation of (6.15) in two regimes, namely, $t \gg t_\perp \gg \Gamma$, and $t_\perp \ll \Gamma$. For the former case, one rewrites (6.15) as $\mu_t = e l_\perp / (m_t^* v_\perp)$, where $m_t^{*-1} = \frac{1}{2} \beta v_\perp^2 = \frac{1}{2} \beta (2t_\perp a_y / \hbar)^2$. The transverse mean free path [$l_\perp = \pi t_\perp a_y / (8ct)$] is much larger than the interchain distance, and (6.15) can be interpreted in terms of band conduction. For the latter situation, however, $l_\perp \ll a_y$, and the interchain hopping time is much larger than the electron lifetime (i.e., $\hbar t_\perp^{-1} \gg \tau$). Therefore each hopping is completely incoherent, and the transverse motion becomes diffusive. The mobility in (6.15) is proportional to the interchain hopping rate: $\mu_t \propto (\hbar^{-1} t_\perp \tau)^2 / \tau$. Here the numerator is the hopping probability during the electron lifetime τ . Therefore one moves from a band conduction regime into a diffusive conduction regime, as one decreases t_\perp . A similar situation exists in small polaron band conduction.¹³

B. ac conductivity

1. Three dimension

We discuss the linear response of the system to a high-frequency external field ($\nu \tau_{\text{eff}} \gg 1$). Here it is proper to treat the collision terms as a perturbation. The distribution function Φ_k is then given from (6.1) by

$$\Phi_k = \frac{v_k^x}{-i\nu} - \frac{\beta}{f'_k v^2} \sum_{k_1 k_2 k_3} (v_k^x + v_1^x - v_2^x - v_3^x) P_{kk_1}^{k_2 k_3}, \quad (6.16)$$

which, substituted in (6.3), yields

$$\sigma_x(\nu) = \sigma_x^{(0)} + \sigma_x^{(1)}, \quad (6.17)$$

where

$$\sigma_x^{(0)} = -ne^2 / im^* \nu \quad (6.18)$$

and

$$\sigma_x^{(1)} = ne^2 / m^* \nu^2 \tau_{\text{eff}}. \quad (6.19)$$

Here the effective relaxation rate is given by

$$\tau_{\text{eff}}^{-1} = \frac{m^*}{k_B T c N} \sum_{kk_1 k_2 k_3} v_k^x (v_k^x + v_1^x - v_2^x - v_3^x) P_{kk_1}^{k_2 k_3}. \quad (6.20)$$

One can easily reduce this result to the form given in (6.9) for a cubic system¹⁴ using the invariance of $P_{kk_1}^{k_2 k_3}$ with respect to the mutual interchange of the two incident wave vectors k, k_1 . The quantity $\sigma_x^{(0)}$ in (6.18) has the well-known form of the high-frequency conductivity of a collisionless electron

gas, and $\sigma_x^{(1)}$ in (6.19) constitutes the classical Drude-Lorentz contribution to the dissipative part of σ_x in the high-frequency region. Combining (6.18) and (6.19), one may interpolate

$$\sigma(\nu) = \sigma(0)(1 - i\nu\tau_{\text{eff}}^{-1})^{-1}. \quad (6.21)$$

The dc conductivity $\sigma(0)$ is given in (6.7) and was obtained from (6.6) by choosing a trial function $\Phi_k = v_k^x$. The result in (6.19) can also be obtained, using a non-Boltzmann-type approach¹⁵ in the region $k_B T \gg \hbar\nu \gg \tau_{\text{eff}}^{-1}$.

2. Nearest-neighbor-hopping Hubbard chain

It is seen from (6.20) that only the U process with $k+k_1 = \pm\pi$ contributes, and $\tau_{\text{eff}}^{-1} = 0$, as was in dc case. However, in view of (5.1) and (6.1), τ_{eff}^{-1} can be determined only up to $O(\hbar\nu)$ in the present treatment. Therefore, one concludes that $\sigma_x^{(1)} = O((\hbar\nu)^{-1})$. According to a different and improved treatment¹⁵ of this specific situation, $\sigma_x^{(1)}$ is independent of the external frequency and vanishes as $(B/U)^2$ for a large U .

VII. INTERBAND TRANSITIONS

When the external frequency corresponds to the separation of the two subbands, then interband optical absorption occurs. The lower band consists of electronic states in which the electron visits mainly the empty sites. On the other hand, for the upper band the electron runs over the occupied sites of the opposite spin. In this section, we assume that the system may be degenerate.

The single-particle excitation spectrum manifests itself through the poles of the full Green's function $S_k(\xi_l)$ given in (3.5). In Sec. III we found that when $\xi_l \approx \epsilon_k$, the self-energy part is small and constitutes a minor correction. However, when $\xi_l \approx U$, as is necessary to obtain the upper band spectrum, this is no longer true. In this case, the T matrix has a cut, as can be seen from (3.3), (3.12), and the self-energy part has to be treated explicitly. In this paper we confine ourselves to a certain simple approximation, which serves to reveal the nature of the decoupling approximations adopted in some existing theories^{1a,6}: To find the absorption and the Green's function of electrons with spin σ , we assume that each electron of spin σ moves in the system of electrons of spin $-\sigma$. Then using (3.3), and (3.12) in (3.14), one obtains for $\xi_l \sim U \gg B$

$$G_k^\sigma(\xi_l) = U\xi_l c_{-\sigma} / [\xi_l - U(1 - c_{-\sigma})], \quad (7.1)$$

where $c_\sigma \equiv N_\sigma^e/N$, and N_σ^e is the number of electrons with spin σ . This leads to

$$S_k^\sigma(\xi_l) = \frac{\xi_l - U(1 - c_{-\sigma})}{(\xi_l - \epsilon_k)(\xi_l - U) - U\epsilon_k c_{-\sigma}}, \quad (7.2)$$

which can be rewritten

$$S_k^\sigma(\xi_l) = \sum_{\alpha=1,2} \frac{A_{\alpha k}^\sigma}{\xi_l - E_{\alpha k}^\sigma}, \quad (7.3)$$

where

$$E_{\alpha k}^\sigma = \frac{1}{2} \{ \epsilon_k + U + (-1)^\alpha [(\epsilon_k + U)^2 - 4U\epsilon_k(1 - c_{-\sigma})]^{1/2} \} \quad (7.4)$$

and

$$A_{\alpha k}^\sigma = (-1)^\alpha [E_{\alpha k}^\sigma - U(1 - c_{-\sigma})] / (E_{2k}^\sigma - E_{1k}^\sigma). \quad (7.5)$$

These results were obtained by Hubbard^{1a} using a decoupling method. The above result is derived in the region $\xi_l \sim U$ near the upper band. The lower band value $E_{1k}^\sigma \approx \epsilon_k(1 - c_{-\sigma})$ is reasonable in view of (3.16b), although it should not be taken seriously.

To find the interband absorption it is more convenient to use a formula

$$\sigma_{xy}(\nu) = -ne^2/im\nu + (e^2/i\nu\Omega)\mathcal{F}_{xy}(\hbar\nu + i0), \quad (7.6)$$

where \mathcal{F}_{xy} is given in (2.6). The main contribution of interband transition arises from the bubble diagram shown in Fig. 4, according to the approximations stated above. One then obtains

$$\mathcal{F}_{xy}(\omega_r) = \frac{-1}{\beta} \sum_{k\sigma} \sum_{\uparrow} v_k^x v_k^y S_k^\sigma(\xi_l) S_k^\sigma(\xi_l + \omega_r), \quad (7.7)$$

which can be evaluated using (7.3):

$$\mathcal{F}_{xy}(\omega_r) = - \sum_{k\sigma} \sum_{\alpha\alpha'} v_k^x v_k^y A_{\alpha k}^\sigma A_{\alpha' k}^\sigma \frac{f(E_{\alpha k}^\sigma) - f(E_{\alpha' k}^\sigma)}{\omega_r + E_{\alpha k}^\sigma - E_{\alpha' k}^\sigma}.$$

Using

$$\vec{\nabla}_k A_{\alpha k}^\sigma = \vec{V}_{\alpha k}^\sigma, \quad \vec{V}_{\alpha k}^\sigma \equiv \hbar^{-1} \nabla_k E_{\alpha k}^\sigma, \quad (7.8)$$

which are found readily from (7.3)–(7.5), one obtains from (7.6),

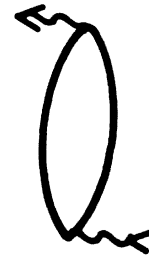


FIG. 4. Bubble diagram responsible for the interband absorption.

$$\text{Re}\sigma_{xy}(\nu) = \frac{\pi e^2}{\nu\Omega} \sum_{k\sigma} V_{1k}^{\sigma x} V_{2k}^{\sigma y} \times [f(E_{1k}^{\sigma}) - f(E_{2k}^{\sigma})] \sigma(\hbar\nu - E_{2k}^{\sigma} + E_{1k}^{\sigma}). \quad (7.9)$$

This coincides with the result obtained earlier by Kubo⁶ using a decoupling method. However, we believe that (7.9) is incorrect at a high-concentration limit. For example, (7.9) predicts⁶ an incorrect (narrower) optical-absorption width in a half-filled band limit (i.e., $c = \frac{1}{2}$).¹⁶

VIII. DISCUSSION

We have studied the ac and dc electronic conduction in a low-density interacting electron system described by the Hubbard model. Utilizing a T -matrix approximation, the Boltzmann equation is established for intraband transitions in a non-degenerate system. The interband absorption has also been considered: The two-particle T -matrix approximation gives a result which coincides with that obtained by Kubo,⁶ using a decoupling approximation.

The result of the intraband transitions is applied to the calculation of dc and ac conductivities in several situations: In two and three dimensions, the mobility is inversely proportional to the electronic concentration. This is due to the fact that the collision time is inversely proportional to the number of scatterers. The resistivity arises from the umklapp process of the electron-electron scattering. The electronic mobility for the simple cubic lattice is given approximately by $\mu = 0.6\mu_h c^{-1}$, where μ_h is the mobility of a hole in an otherwise half-filled band, as found by Brinkman and Rice.³ The magnitude of the conductivity is finite at zero concentration and is comparable with that of Eswaran and Kimball.⁵ The ac conductivity shows a Drude-Lorentz-type behavior

characteristic of metallic conduction.

In one dimension with nearest-neighbor electron transfer (t) only, the dc conductivity becomes infinite within the two-particle approximation. However, it is shown that the two-particle approximation is insufficient in this case, and many-particle interactions should be considered. Upon introducing many particle scattering, one finds that the resistivity does not vanish, but is of order c or higher, unlike in two or three dimensions, where it is independent of c at a low concentration. It is not clear from our study whether the resistivity vanishes to all orders in c for $U = \infty$, as the spinless Fermion model would predict. However, the present study reveals clearly that, for a nearest-neighbor-hopping Hubbard chain, one cannot use the conventional two-particle scattering form of Boltzmann equation, even for an arbitrarily weak scattering: many-particle scattering plays an important role.

The two-particle T -matrix approximation becomes valid for a sufficiently low frequency ($\hbar\nu \ll t_2, t_1$), if the second-nearest-neighbor electron transfer (t_2), or an interchain transfer (t_1) is sufficiently large compared with the many-body effect (i.e., $t_\alpha \gg ct\xi$, $\alpha = 2, \perp$). In this case, the effective electron-electron umklapp interaction becomes $U_{\text{eff}} = U$ and $U_{\text{eff}} \sim t_\alpha$ ($\alpha = 2, \perp$), respectively, in the weak (i.e., $U \ll |t_\alpha|$) and in the strong correlation limit (i.e., $U \gg |t_\alpha|$). For the latter, conductivity becomes independent of the electron concentration as in two or three dimensions, and increases as $(t/t_\alpha)^2$ for decreasing value of $|t_\alpha|$. Finally, a dc transverse conductivity for the latter extreme anisotropic case is also studied.

APPENDIX

In this Appendix we derive (4.5). From Figs. 1(a), and 1(b), one finds

$$K(p_2, p_1; p_3, p) = UN^{-1} - UN^{-1}\beta^{-1} \sum_q S(p_2 - q) S(p_1 + q) K(p_2 - q, p_1 + q; p_3, p) \quad (\text{A1a})$$

and

$$K(p_3, p_\omega; p_2, p_{1\omega}) = UN^{-1} - UN^{-1}\beta^{-1} \sum_q S(p_2 - q) S(p_{1\omega} + q) K(p_3, p_\omega; p_2 - q, p_{1\omega} + q). \quad (\text{A1b})$$

The right-hand side (RHS) of (4.5) is then given by

$$\begin{aligned} \text{RHS} = & -\beta^{-2} \sum K(p_2, p_1; p_3, p) S(p_2) S(p_3) S(p_1) UN^{-1} \left(1 - \beta^{-1} \sum_q S(p_2 - q) S(p_{1\omega} + q) K(p_3, p_\omega; p_2 - q, p_{1\omega} + q) \right) \\ & + \beta^{-2} UN^{-1} \sum \left(1 - \beta^{-1} \sum_q S(p_2 - q) S(p_1 + q) K(p_2 - q, p_1 + q; p_3, p) \right) S(p_2) S(p_3) S(p_{1\omega}) K(p_3, p_\omega; p_2, p_{1\omega}). \end{aligned} \quad (\text{A2})$$

The first term of the first large parentheses (designated as R_1) can be rewritten upon changing to $p_2 = p_3 - q, p_1 = p + q$ as

$$R_1 = G(p) - UN^{-1}\beta \sum_{p_3} S(p_3). \quad (\text{A3})$$

The first term of the second large parentheses (designated as R_3) can be rewritten similarly as

$$R_3 = -G(p_\omega) + UN^{-1}\beta^{-1} \sum_{p_3} S(p_3). \quad (\text{A4})$$

For the second term of the first large parentheses (R_2), we transform $p_2 - q = \bar{p}_2, p_{1\omega} + q = \bar{p}_{1\omega}$, obtaining

$$\begin{aligned} R_2 = & \beta^{-2} \sum K(\bar{p}_2 + q, \bar{p}_1 - q; p_3, p) \\ & \times S(\bar{p}_2 + q)S(p_3)S(\bar{p}_1 - q)UN^{-1}\beta^{-1} \\ & \times S(\bar{p}_2)S(\bar{p}_{1\omega})K(p_3, p_{1\omega}; \bar{p}_2, \bar{p}_{1\omega}). \end{aligned}$$

Upon transforming $\bar{p}_2 = p_2, q \rightarrow -q, \bar{p}_1 = p_1$, it is seen that R_2 cancels the second term of the second large parentheses. Combining (A3) and (A4) one obtains (4.5).

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