

analyses in terms of *discrete* decay rate spectra. The resolution theorem of Part III shows that the "lines" could be somewhat broader, but the breadth could scarcely be comparable with the separation between the components.

Although only two materials have been examined at

low temperatures it is noteworthy that in either case the proportion of energy channelled through very fast phosphorescent processes is increased at low temperatures. At first sight this is hard to reconcile with the greater rigidity of selection rules to be expected at low temperatures.

## Theory of Impurity Resistance in Metals\*

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A many-body technique is developed for the calculation of the dc resistivity of a Fermi fluid in the presence of a few, randomly scattered, fixed, impurities. A certain class of graphs yields an expression for the conductivity which is similar in form to the standard classical transport coefficient; but the decay time is determined by the scattering of single-particle-like excitations at the Fermi surface by screened impurities. A propagator method similar to that used in field theory is employed throughout the paper, and the perturbation-theoretic interpretation of this method is examined in some detail.

### I. INTRODUCTION

IN this paper we shall examine a many-particle formulation of the theory of impurity resistance in metals. The emphasis will be placed on an attempt to understand the role played by the electron-electron interactions. In order to do this most effectively, we shall adopt the simplest possible model which retains the essential features of interest in the physical system. In particular, we shall consider a dense Fermi gas of electrons moving in the presence of a uniform, positively charged, background and a few randomly scattered impurities. These impurities are fixed in the metal and are charged. Such a system is known to have a finite dc conductivity.

The present calculation will be further restricted in two ways. In the first place, we shall work only at zero temperature. Secondly, we shall consider only a relatively simple term in the conductivity which, as we shall see, yields a result similar in form to the standard classical expression for the transport coefficient. Our physical picture will be that of electrons accelerated by the external field and scattered by the impurities. Our "electrons," however, will turn out to be single-particle-like excitations of the Fermi fluid, and the impurities will be screened. It is hoped that the methods developed here will be useful in extending the calculation to finite temperatures and in estimating the higher order effects of electron correlations.

The first part of the development will be the derivation of a formal expression for the linear response of the system to a uniform electric field. The result, which is a special case of Kubo's formula,<sup>1</sup> has a simple interpretation in terms of many-particle graphs. It then will be

shown that the simplest class of these graphs leads to an expression for the conductivity very similar to the Greenwood-Peierls formula,<sup>2</sup> but generalized to include the many-electron effects mentioned above. This derivation is contained in Secs. II, III, and IV. Section V contains a discussion of the process of renormalization in many-body problems which is necessary for the interpretation of the results of Sec. IV.

The actual evaluation of the conductivity will be performed here using a method developed by Edwards.<sup>3</sup> In Sec. VI the relevant features of Edwards' technique will be reviewed and generalized somewhat. In Secs. VII and VIII we shall make a detailed analysis of certain terms which appear and finally exhibit an explicit expression for the conductivity.

### II. FORMAL EXPRESSION FOR THE CONDUCTIVITY

In order to calculate the conductivity, we take the system of electrons and impurities in its ground state  $\Psi_0$  and slowly turn on a uniform electric field  $\mathbf{E}(t)$ . It is convenient to describe this field mathematically by the vector potential  $\mathbf{A} = -(c/\alpha)e^{i\alpha t}\mathbf{E}$ , which yields

$$\mathbf{E}(t) = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} = \mathbf{E}e^{i\alpha t}.$$

The conductivity  $\sigma$  then follows from examination of the current produced by  $\mathbf{E}$  at time  $t=0$  in the limit  $\alpha \rightarrow +0$ .

To first order in  $\mathbf{E}$ , the state  $\Psi(t=0)$  is given by

$$\Psi(0) = \Psi_0 - i \int_{-\infty}^0 dt e^{iHt} H'(t) e^{-iHt} \Psi_0 + \dots, \quad (2-1)$$

\* Supported in part by the Office of Naval Research.

<sup>1</sup> R. Kubo, J. Phys. Soc. Japan 12, 570-586 (1957).

<sup>2</sup> D. A. Greenwood, Proc. Phys. Soc. (London) 71, 585 (1958).

<sup>3</sup> S. F. Edwards, Phil. Mag. 3, 33, 1020 (1958).

where  $H$  is the complete Hamiltonian for the electrons interacting among themselves and with the impurities. According to the above prescription,  $H'$  is given by

$$H'(t) = -\frac{e}{mc} \mathbf{A} \cdot \mathbf{P} = -\frac{e}{m\alpha} e^{\alpha t} \mathbf{E} \cdot \mathbf{P}, \quad (2-2)$$

where  $\mathbf{P}$  is the total momentum operator for the electrons. The resulting current density at  $t=0$  is:

$$\begin{aligned} \mathbf{j} &= \frac{e}{m\Omega} \left\langle \Psi(0) \left| \left( \mathbf{P} - \frac{e}{c} \mathbf{A} N \right) \right| \Psi(0) \right\rangle \\ &= -\frac{ie^2}{m^2\alpha\Omega} \int_{-\infty}^0 e^{\alpha t} dt \langle \Psi_0 | [\mathbf{P}(0), \mathbf{P}(t) \cdot \mathbf{E}] | \Psi_0 \rangle \\ &\quad + \frac{e^2 n_e}{m\alpha} \mathbf{E} + \text{terms of higher order in } \mathbf{E}. \end{aligned} \quad (2-3)$$

Here  $\Omega$  is the volume of the system,  $n_e = N/\Omega$  is the number-density of electrons, and  $\mathbf{P}(t) = e^{iHt} \mathbf{P} e^{-iHt}$ .

The conductivity tensor  $\sigma_{\mu\nu}$  is defined by:

$$j_\mu = \sum_{\nu=1}^3 \sigma_{\mu\nu} E_\nu. \quad (2-4)$$

Since our system is effectively isotropic, we need calculate only  $\sigma$ , the average diagonal element of  $\sigma_{\mu\nu}$ . Using this definition and Eq. (2-3), it is convenient to write the expression for  $\sigma$  in the form:

$$\sigma = \lim_{\alpha \rightarrow +0} \left\{ \frac{2e^2}{3m^2\alpha\Omega} \text{Im} \int_{-\infty}^0 e^{\alpha t} dt \langle \Psi_0 | \mathbf{P}(0) \cdot \mathbf{P}(t) | \Psi_0 \rangle + \frac{e^2 n_e}{m\alpha} \right\}. \quad (2-5)$$

Equation (2-5) is the formal starting point of our theory. Note that the matrix element which appears has the form of an auto-correlation coefficient whose time dependence we may expect to resemble a decaying exponential. Unlike Kubo, however, we do not calculate an ensemble average for this coefficient. Rather, we perform our calculation at zero temperature and, following Kohn and Luttinger<sup>4</sup> and Edwards,<sup>3</sup> average over random configurations of the impurities.

To begin the evaluation of the matrix element in (2-5), we introduce the standard unitary operator,  $U(t, t')$ , defined by the perturbation series:

$$\begin{aligned} U(t, t') &= 1 + \sum_{n=1}^{\infty} (-i)^n \int_{t'}^t dt_1 \cdots \int_{t'}^{t_{n-1}} dt_n \\ &\quad \times [V_I(t_1) \cdots V_I(t_n)], \end{aligned} \quad (2-6)$$

where

$$V_I(t) = e^{iH_0 t} V e^{-iH_0 t} e^{-\alpha|t|} \quad (2-7)$$

is the interaction representation of  $V = H - H_0$  includ-

ing both the electron-electron and electron-impurity interactions.  $H_0$  is the kinetic energy operator for the electrons. Its lowest eigenstate is the Fermi vacuum,  $\Phi_0$ .  $U$  has the properties:

$$U(t, t') = U^\dagger(t', t); \quad (2-8)$$

$$e^{-iHt} = e^{-iH_0 t} U(t, 0); \quad (2-9)$$

and

$$\Psi_0 = U(0, -\infty) \Phi_0. \quad (2-10)$$

We also introduce the second-quantized representation of  $\mathbf{P}$  in terms of free-particle eigenstates:

$$\mathbf{P} = \sum_{\mathbf{k}} \mathbf{k} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \quad (2-11)$$

where  $a_{\mathbf{k}}^\dagger$  and  $a_{\mathbf{k}}$  are the creation and annihilation operators for plane-wave states of momentum  $\mathbf{k}$ . Thus,

$$\begin{aligned} \langle \Psi_0 | \mathbf{P}(0) \cdot \mathbf{P}(t) | \Psi_0 \rangle &= \sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') \langle \Phi_0 | U^\dagger(\infty, -\infty) U(\infty, 0) \\ &\quad \times a_{\mathbf{k}}^\dagger a_{\mathbf{k}} U(0, t) a_{\mathbf{k}'}^\dagger(t) a_{\mathbf{k}'} U(t, -\infty) | \Phi_0 \rangle. \end{aligned} \quad (2-12)$$

The operator  $U^\dagger(\infty, -\infty)$  has the usual effect of factoring out the vacuum fluctuations, leaving only linked graphs in (2-12).

### III. GRAPHICAL ANALYSIS

The analysis of (2-12) in terms of graphs follows according to the rules of Goldstone<sup>5</sup> or Hubbard.<sup>6</sup> In general, any graph has the form of a linked vacuum-to-vacuum fluctuation which interacts twice with the external field at times  $t$  and  $0$ . We shall denote these field interactions by dotted, wavy lines running off the diagram. Since the external field is uniform, these interactions carry no momentum. A Coulomb interaction between two electrons will be represented by a solid wavy line, and an interaction with an impurity by a straight dotted line ending at an "x" to mark the position of a fixed scattering center. Time runs in the vertical direction.

Let us consider first those graphs in which no electron-electron interactions occur. Two such graphs are drawn in Fig. 1. It is important to note that a graph like 1(b) must be included even though it appears that here we are measuring the momentum of a state which

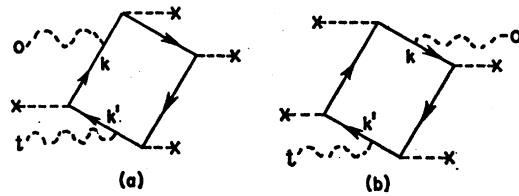


FIG. 1. Some graphs which contribute to  $\sigma$ . No electron-electron interactions are included.

<sup>5</sup> J. Goldstone, Proc. Roy. Soc. (London) A239, 267 (1957).

<sup>6</sup> J. Hubbard, Proc. Roy. Soc. (London) A240, 539 (1957).

<sup>4</sup> W. Kohn and J. M. Luttinger, Phys. Rev. 108, 590 (1957).

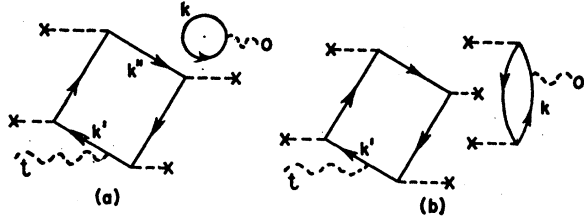


FIG. 2. Some two-loop graphs which do not contribute to  $\sigma$ . Formally, these diagrams are included in Eq. (2-12); but their net contribution vanishes.

is unoccupied. The significance of this graph is that it cancels out the violation of the Pauli principle which occurs in Fig. 2(a) when  $\mathbf{k} = \mathbf{k}'$ .

Strictly speaking, Fig. 2(a) is a "linked" graph according to the above discussion—it contains no vacuum fluctuations. It is apparent, however, that its contribution to  $\sigma$  vanishes when summed over  $\mathbf{k}$  and  $\mathbf{k}'$  with the weight factor  $(\mathbf{k} \cdot \mathbf{k}')$ , since the graph is invariant under the replacement of  $\mathbf{k}$  by  $-\mathbf{k}$ . This is a special case of the theorem which states that all graphs of the form of Fig. 2(b) make zero contribution to  $\sigma$ . Working back from Eq. (2-12), we find that the matrix element for the sum of all such two-loop graphs reduces to:

$$\sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') \langle \Psi_0 | a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} | \Psi_0 \rangle \langle \Psi_0 | a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} | \Psi_0 \rangle = 0, \quad (3-1)$$

which vanishes because there is no net current in the ground state for any configuration of impurities.

Graphs of the kind shown in Fig. 1 may be expressed in terms of the free-electron propagator  $S_F(\mathbf{k}, t' - t)$  defined by:

$$S_F(\mathbf{k}, t' - t) = \lim_{\alpha \rightarrow +0} \begin{cases} \exp[-i\epsilon_{\mathbf{k}}(t' - t) - \alpha|t' - t|], & t' > t, \quad \epsilon_{\mathbf{k}} > \epsilon_F \\ -\exp[-i\epsilon_{\mathbf{k}}(t' - t) - \alpha|t' - t|], & t' < t, \quad \epsilon_{\mathbf{k}} \leq \epsilon_F, \end{cases} \quad (3-2)$$

where  $\epsilon_{\mathbf{k}} = k^2/2m$ , and  $\epsilon_F$  is the Fermi energy  $k_F^2/2m$ . The limit  $\alpha \rightarrow 0$  is understood to be taken after performing the time integrations. Introducing the field of the impurities  $V_{\text{imp}}$  [see Eq. (6-1) for the precise form of this quantity], we may construct the function  $S_1(\mathbf{k}', \mathbf{k}, t' - t)$ ,

$$S_1(\mathbf{k}', \mathbf{k}, t' - t) = S_F(\mathbf{k}, t' - t) \delta_{\mathbf{k}, \mathbf{k}'} - i \int_{-\infty}^{\infty} S_F(\mathbf{k}', t' - t_1) \times (V_{\text{imp}})_{\mathbf{k}', \mathbf{k}} S_F(\mathbf{k}, t_1 - t) dt_1 + \dots, \quad (3-3)$$

which describes the propagation of an electron starting with momentum  $\mathbf{k}$  at time  $t$  through any number of interactions to a state with momentum  $\mathbf{k}'$  at time  $t'$ . That is,  $S_1$  is the sum of graphs shown in Fig. 3.

In terms of  $S_1$  we have:

$$\sigma = \lim_{\alpha \rightarrow +0} \left\{ -\frac{4e^2}{3m^2\Omega\alpha} \text{Im} \sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') \int_{-\infty}^0 e^{\alpha t} dt \times [S_1(\mathbf{k}', \mathbf{k}, -t) S_1(\mathbf{k}, \mathbf{k}', t)] + \frac{e^2 n_e}{m\alpha} \right\}, \quad (3-4)$$

where the quantity in square brackets is understood to be averaged over random configurations of the impurities. The extra factor 2 accounts for electrons of both spins, and the minus sign is required by the definition of the propagator [see Eq. (4-2)]. In the absence of electron-electron interactions, Eq. (3-4) is still an exact expression for  $\sigma$ .

The many-body effects which we shall consider in this paper are those which may be included by using the true single-electron propagator  $S$  instead of  $S_1$  in Eq. (3-4). Figure 4 shows a graph illustrating the three principal kinds of resulting corrections to a term in  $S_1$  whose basic structure is that of Fig. 3(b). At (a) we have added an electron self-energy part which takes into account the fact that the particle is moving in the presence of all the other electrons. At (b) we have included the polarization of the electron gas due to the impurities. (There also will be similar terms in which the impurity interaction appears to higher orders.) Since the impurities are fixed, these terms just represent the static screening calculated by Langer and Vosko<sup>7</sup> and others.<sup>8</sup> Finally, at (c), we have indicated a vertex correction in which an exchange interaction takes place between the incident electron and the screening cloud surrounding the impurity.

#### IV. THE TIME INTEGRATION

The formula which we wish to evaluate now is:

$$\sigma = \lim_{\alpha \rightarrow +0} \left\{ -\frac{4e^2}{3m^2\Omega\alpha} \text{Im} \sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') \int_{-\infty}^0 e^{\alpha t} dt \times [S(\mathbf{k}', \mathbf{k}, -t) S(\mathbf{k}, \mathbf{k}', t)] + \frac{e^2 n_e}{m\alpha} \right\}. \quad (4-1)$$

It turns out that a knowledge of the spectral properties

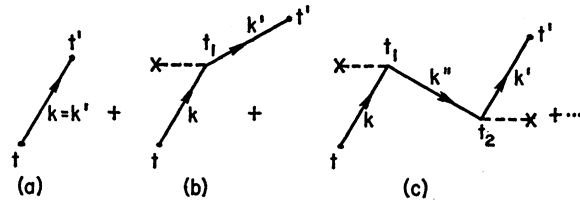


FIG. 3. Some typical terms in  $S_1$ , the one-electron propagator without many-body corrections.

<sup>7</sup> J. Langer and S. Vosko, J. Phys. Chem. Solids **12**, 196 (1960).

<sup>8</sup> J. J. Quinn, R. A. Ferrell, and A. A. Maradudin (unpublished).

of  $S$  enables us to perform the time integration in this expression.

The spectral representation of  $S$  may be derived from the formula<sup>9</sup>:

$$S(\mathbf{k}, \mathbf{k}', t-t') = T \langle \Psi_0 | e^{iHt} a_{\mathbf{k}} e^{-iH(t-t')} a_{\mathbf{k}'}^\dagger e^{-iHt'} | \Psi_0 \rangle, \quad (4-2)$$

where  $T$  is the time-ordering operator which includes a change of sign upon permutation. Introducing complete sets of  $N+1$  particle states  $\Psi_S$  and  $N-1$  particle states  $\Psi_{S'}$ , and taking the Fourier transform, we get:

$$\begin{aligned} S(\mathbf{k}, \mathbf{k}', \omega) &= \frac{1}{2\pi} \lim_{\epsilon \rightarrow +0} \int_{-\infty}^{\infty} S(\mathbf{k}, \mathbf{k}', t) e^{i\omega t - \epsilon|t|} dt \\ &= \frac{1}{2\pi i} \lim_{\epsilon \rightarrow +0} \left\{ \int_{\mu}^{\infty} \frac{A(\mathbf{k}, \mathbf{k}', x)}{x - \omega - i\epsilon} dx + \int_{-\infty}^{\mu} \frac{B(\mathbf{k}, \mathbf{k}', x)}{x - \omega + i\epsilon} dx \right\}, \end{aligned} \quad (4-3)$$

where

$$A(\mathbf{k}, \mathbf{k}', x) = \sum_S \langle \Psi_0 | a_{\mathbf{k}} | \Psi_S \rangle \langle \Psi_S | a_{\mathbf{k}'}^\dagger | \Psi_0 \rangle \delta(E_S - E_0 - x), \quad (4-4)$$

and

$$B(\mathbf{k}, \mathbf{k}', x) = \sum_{S'} \langle \Psi_0 | a_{\mathbf{k}'}^\dagger | \Psi_{S'} \rangle \langle \Psi_{S'} | a_{\mathbf{k}} | \Psi_0 \rangle \delta(E_{S'} - E_0 + x). \quad (4-5)$$

The chemical potential,  $\mu$ , is defined by

$$\mu = \lim_{N \rightarrow \infty} [E_0(N+1) - E_0(N)]; \quad (4-6)$$

and  $E_0(N)$ ,  $E_S(N+1)$ , etc., are exact eigenvalues of  $H$  for  $N$ ,  $N+1$  particle systems.

The function  $S$  may be defined throughout the complex  $\omega$  plane by writing:

$$S(\mathbf{k}, \mathbf{k}', \omega) = \frac{1}{2\pi i} \left\{ \int_{\mu}^{\infty} \frac{A(\mathbf{k}, \mathbf{k}', x)}{x - \omega} dx + \int_{-\infty}^{\mu} \frac{B(\mathbf{k}, \mathbf{k}', x)}{x - \omega} dx \right\}. \quad (4-7)$$

This equation actually defines two analytic functions  $S$ : one which is analytic in the upper half  $\omega$  plane, the

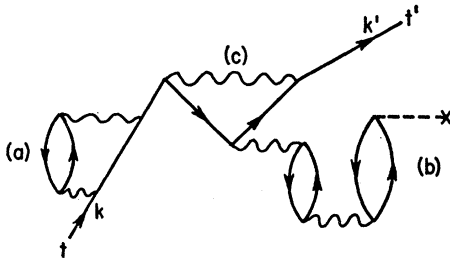


FIG. 4. Some many-body corrections to  $S_1$ .

<sup>9</sup> For a more complete discussion, see V. M. Galitskii and A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) 34, 189 (1958) [translation: Soviet Phys.-JETP 34(7), 96 (1958)].

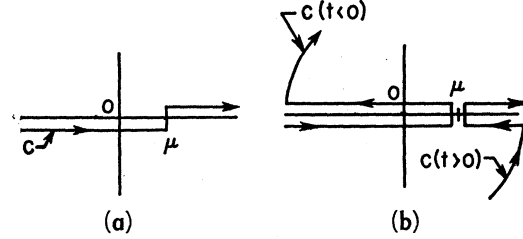


FIG. 5. (a) The contour  $C$ . (b) Allowed distortions of  $C$  for positive and negative  $t$  in Eq. (4-9).

other analytic in the lower half plane. There is a cut along the real axis, the discontinuity across this cut being given by the spectral functions  $A$  and  $B$ . Equation (4-3) then tells us that, along the real axis, we must take:

$$S(\mathbf{k}, \mathbf{k}', \omega) = \lim_{\epsilon \rightarrow +0} \begin{cases} S(\mathbf{k}, \mathbf{k}', \omega + i\epsilon), & \omega > \mu \\ S(\mathbf{k}, \mathbf{k}', \omega - i\epsilon), & \omega < \mu. \end{cases} \quad (4-8)$$

That is:

$$S(\mathbf{k}, \mathbf{k}', t) = \int_C S(\mathbf{k}, \mathbf{k}', \omega) e^{-i\omega t} d\omega, \quad (4-9)$$

where the contour  $C$  is defined in Fig. 5(a). For values of  $t > 0$ , we may close  $C$  in the lower half plane; for  $t < 0$ , we close in the upper half plane. Since  $S$  is analytic everywhere off the real axis, these contours may be distorted as shown in Fig. 5(b). In this way we recover our original expression for  $S(\mathbf{k}, \mathbf{k}', t)$ .

Inserting Eq. (4-9) into (4-1) and distorting the contours as described, we find:

$$\begin{aligned} \sigma &= \lim_{\alpha \rightarrow +0} \left\{ -\frac{4e^2}{3m^2\Omega\alpha} \operatorname{Im} \int_{-\infty}^0 e^{\alpha t} dt \int_{\mu}^{\infty} e^{i\omega_1 t} d\omega_1 \right. \\ &\quad \left. \times \int_{-\infty}^{\mu} e^{-i\omega_2 t} d\omega_2 \mathcal{G}(\omega_1, \omega_2) + \frac{e^2 n_e}{m\alpha} \right\}, \end{aligned} \quad (4-10)$$

where:

$$\begin{aligned} \mathcal{G}(\omega_1, \omega_2) &= \lim_{\epsilon \rightarrow +0} \sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') [S(\mathbf{k}', \mathbf{k}, \omega_1 + i\epsilon) - S(\mathbf{k}', \mathbf{k}, \omega_1 - i\epsilon)] \\ &\quad \times [S(\mathbf{k}, \mathbf{k}', \omega_2 - i\epsilon) - S(\mathbf{k}, \mathbf{k}', \omega_2 + i\epsilon)] \\ &= - \sum_{\mathbf{k}, \mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') A(\mathbf{k}', \mathbf{k}, \omega_1) B(\mathbf{k}, \mathbf{k}', \omega_2). \end{aligned} \quad (4-11)$$

Furthermore, from (4-4) and (4-5) we see that:

$$A^*(\mathbf{k}, \mathbf{k}', \omega) = A(\mathbf{k}', \mathbf{k}, \omega), \quad B^*(\mathbf{k}, \mathbf{k}', \omega) = B(\mathbf{k}', \mathbf{k}, \omega); \quad (4-12)$$

thus  $\mathcal{G}(\omega_1, \omega_2)$  is real. Now we may perform the time integration and take the imaginary part in (4-10). The result is:

$$\begin{aligned} \sigma &= \lim_{\alpha \rightarrow +0} \left\{ \frac{4e^2}{3m^2\Omega\alpha} \int_{\mu}^{\infty} d\omega_1 \int_{-\infty}^{\mu} d\omega_2 \right. \\ &\quad \left. \times \frac{\omega_1 - \omega_2}{(\omega_1 - \omega_2)^2 + \alpha^2} \mathcal{G}(\omega_1, \omega_2) + \frac{e^2 n_e}{m\alpha} \right\}. \end{aligned} \quad (4-13)$$

The next step in the derivation is to take the limit  $\alpha \rightarrow 0$ . The expression in brackets in (4-13) may be considered expanded in powers of  $\alpha$ , the leading term being proportional to  $\alpha^{-1}$ . If  $\sigma$  is to be finite, the coefficient of this first term must vanish. (That is, it must vanish in the exact expression for  $\sigma$  including all of the many-body corrections.) Thus we shall identify  $\sigma$  with the finite term in (4-13).<sup>10</sup> This is:

$$\sigma = \lim_{\alpha \rightarrow +0} -\frac{4e^2}{3m^2\Omega} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\mu} d\omega_2 \times \frac{2\alpha(\omega_1 - \omega_2)}{[(\omega_1 - \omega_2)^2 + \alpha^2]^2} \mathcal{G}(\omega_1, \omega_2). \quad (4-14)$$

Integrating by parts, we have:

$$\begin{aligned} \sigma &= \lim_{\alpha \rightarrow +0} -\frac{4e^2}{3m^2\Omega} \int_{-\infty}^{\infty} d\omega_1 \left\{ \frac{\alpha}{(\omega_1 - \mu)^2 + \alpha^2} \mathcal{G}(\omega_1, \mu) \right. \\ &\quad \left. - \int_{-\infty}^{\mu} \frac{\alpha}{(\omega_1 - \omega_2)^2 + \alpha^2} \frac{\partial \mathcal{G}}{\partial \omega_2} d\omega_2 \right\} \\ &= -\frac{4\pi e^2}{3m^2\Omega} \int_{-\infty}^{\infty} d\omega_1 \delta(\omega_1 - \mu) \mathcal{G}(\omega_1, \mu) \\ &= -\frac{2\pi e^2}{3m^2\Omega} \mathcal{G}(\mu, \mu). \quad (4-15) \end{aligned}$$

The final form of Eq. (4-15) contains the expected result that, at zero temperature, only those electrons whose energies lie exactly at the top of the Fermi sea contribute to the current. Here the result has been extended to include an important class of many-electron corrections.

In the special case of noninteracting electrons, (4-15) reduces easily to the Greenwood-Peierls formula. Let " $h$ " be the Hamiltonian for a single electron interacting with the impurities. We shall denote the eigenstates of  $h$  by  $|n\rangle$ , and the eigenstates of the momentum operator,  $\mathbf{p}$ , by  $|\mathbf{k}\rangle$ . Then  $S_1$  is given by

$$S_1(\mathbf{k}, \mathbf{k}', \omega) = \frac{1}{2\pi i} \left\langle \mathbf{k} \left| \frac{1}{h - \omega} \right| \mathbf{k}' \right\rangle; \quad (4-16)$$

and

$$A(\mathbf{k}, \mathbf{k}', x) = B(\mathbf{k}, \mathbf{k}', x) = \langle \mathbf{k} | \delta(h - x) | \mathbf{k}' \rangle, \quad (4-17)$$

Inserting these results into (4-15), we have

$$\begin{aligned} \sigma &= \frac{2\pi e^2}{3m^2\Omega} \sum_{\mathbf{k}, \mathbf{k}'} \langle \mathbf{k} | \delta(h - \mu) | \mathbf{k}' \rangle \langle \mathbf{k}' | \delta(h - \mu) | \mathbf{k} \rangle \\ &= \frac{2\pi e^2}{3m^2\Omega} \sum_{m, n} \sum_{\nu=1}^3 |\langle m | p_{\nu} | n \rangle|^2 \delta(E_n - E_m) \delta(E_n - \mu), \quad (4-18) \end{aligned}$$

<sup>10</sup> The coefficient of  $\alpha^{-1}$  is the current produced by an electric field  $\alpha E e^{i\alpha t}$  in the limit  $\alpha \rightarrow 0$ . This is nonzero for a free electron gas, but should vanish as soon as we insert some impurities. It ought to be possible to demonstrate this fact directly.

which is the zero temperature form of Greenwood's formula.

## V. SOME COMMENTS CONCERNING THE TRANSITION FROM PERTURBATION THEORY TO THE SPECTRAL REPRESENTATION

The perturbation-theoretic interpretation of Eq. (4-15) in the case of interacting electrons presents certain difficulties which must be handled rather carefully before proceeding to use this equation in the evaluation of  $\sigma$ . In particular, (4-15) depends critically upon the treatment of  $S$  in the neighborhood of its branch point at  $\omega = \mu$ . The value of  $\mu$  is not known *a priori*; and furthermore, any perturbation approximation to  $S$  may not have quite the same analytic properties as those exhibited for the exact propagator in Eq. (4-7). Thus we are required to find a self-consistent procedure for the actual evaluation of these many-body corrections to the conductivity.

For our purposes, it will be sufficient to consider the function  $S'(\mathbf{k}, \omega)$ , the one-electron propagator in the absence of impurities. Although the impurities may shift the chemical potential, we shall see that this shift enters into the conductivity only to high order in the impurity-density, and may be ignored.

To construct  $S'$  in perturbation theory, we start with the free-electron propagator  $S_F$  defined by Eq. (3-2). The Fourier transform of  $S_F$  is:

$$S_F(\mathbf{k}, \omega) = \frac{1}{2\pi i} \frac{1}{\epsilon_k - \omega - i\alpha_k}, \quad \alpha_k \rightarrow \begin{cases} +0 & \text{for } k > k_F \\ -0 & \text{for } k \leq k_F. \end{cases} \quad (5-1)$$

In the usual manner, we define the function  $\Sigma'(\mathbf{k}, \omega)$  to be the sum of all proper self-energy parts of  $S'$ . (A proper self-energy part is a diagram which is connected to the rest of the graph by two electron lines and cannot be broken into two such diagrams by cutting only a single internal electron line.) Then,

$$S'(\mathbf{k}, \omega) = \frac{1}{2\pi i} \frac{1}{\epsilon_k - \omega - i\alpha_k - \Sigma'(\mathbf{k}, \omega)}. \quad (5-2)$$

It is not by any means apparent that  $S'$  as constructed according to (5-2) has the analytic properties predicted by the spectral representation. In any finite order of this perturbation expansion,  $\Sigma'$  will have a branch point at  $\omega = \epsilon_F$  instead of at  $\omega = \mu$ . Furthermore, there seems to be no reason for performing  $\omega$  integrations along the contour  $C$ . In order to construct  $S'$  with the analytic properties required for use in our conductivity formula (4-15), we must perform a trick similar to mass renormalization in field theory. Such a procedure has been used recently by Luttinger and Ward<sup>11</sup> in examining the zero-temperature limit of their formulation of

<sup>11</sup> J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960). See also reference 13.

quantum statistics. We shall borrow heavily from their results.

Let us imagine for a moment that we can calculate  $\Sigma'$  exactly. Formally we may do this by drawing all proper skeleton self-energy parts and inserting the exact  $S'$  for each internal electron line. (A skeleton diagram is one in which all self-energy parts have been removed from the electron lines, a definition which is unambiguous for a self-energy graph.) Evaluation of any of these self-energy diagrams by means of the spectral representation of  $S'$  leads to the conclusion that  $\Sigma'(\mathbf{k}, \omega)$  is cut along the real axis and that the physical values of  $\omega$  are found along the contour  $C$ .

The same kind of graph-by-graph analysis indicates that, as long as the perturbation expansion is well behaved,  $\Sigma'$  is real at  $\omega = \mu$ . Physically this means that the single-particle-like state just at the surface of the Fermi sea does not decay. In perturbation theory, the phase space available for energy-conserving decay processes vanishes at  $\omega = \mu$ . The generality of this result is a crucial question in the theory of Fermi surfaces. On the assumption that the result is valid, Luttinger and Ward have shown that  $-\Sigma'(k_F, \mu)$  is exactly the shift in the chemical potential due to electron-electron interactions. That is:

$$-\Sigma'(k_F, \mu) = \mu - \epsilon_F = \delta\mu. \quad (5-3)$$

We now may reconstruct  $S'$  in the following way. Rearrange the Hamiltonian which describes the interacting electrons by adding  $\delta\mu$  to the kinetic energy term and subtracting it from the interaction term. Then use for the free-electron propagator:

$$S_\mu(\mathbf{k}, \omega) = \frac{1}{2\pi i} \frac{1}{\epsilon_k + \delta\mu - \omega - i\alpha_k}, \quad (5-4)$$

and include  $-\delta\mu$  in the perturbation expansion as if it were a constant external field. Calculating  $S'$  according to these rules, we find:

$$S' = \frac{1}{2\pi i} \frac{1}{\epsilon_k + \delta\mu - \omega - i\alpha_k - \Sigma''(\mathbf{k}, \omega)}, \quad (5-5)$$

where  $\Sigma''$  is the sum of all proper self-energy diagrams defined in the obvious way. Since this  $S'$  must be the same as that in Eq. (5-2), we must have

$$\Sigma''(\mathbf{k}, \omega) = \Sigma'(\mathbf{k}, \omega) + \delta\mu, \quad (5-6)$$

which is reasonable since  $\delta\mu$  by itself is the simplest possible proper self-energy part in the new sense.

By performing this formal renormalization, we recover the analytic properties of the spectral representation. If we use  $S_\mu$  instead of  $S_F$  for each free electron line, then any graph will have a branch point at  $\omega = \mu$  rather than at  $\omega = \epsilon_F$ . Furthermore, since  $i\alpha_k$  is important in the denominator of  $S_\mu$  only near the pole at  $\omega = \epsilon_k + \delta\mu$ , we may rewrite  $S_\mu$  by dropping  $i\alpha_k$  altogether and performing  $\omega$  integrations along the contour

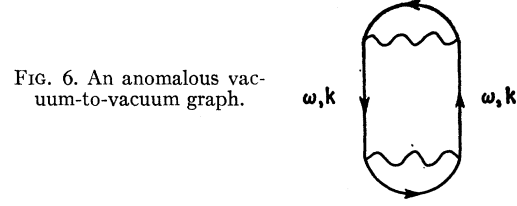


FIG. 6. An anomalous vacuum-to-vacuum graph.

$C$ . A similar contour method could not have been applied to  $S_F$  because it would have given rise to an anomalous delta function whenever  $C$  passed through a pole as it crossed the real axis. For example, the simple vacuum-to-vacuum diagram drawn in Fig. 6 is obviously zero if we use Eq. (5-1) because  $k$  cannot be both  $\leq k_F$  and  $> k_F$  at the same time. The contour method, on the other hand, would give rise to an integral of the form,

$$\begin{aligned} & \frac{1}{2\pi i} \int_{C_F} \frac{d\omega}{(\epsilon_k - \omega)^2} \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\epsilon_F} \frac{d}{d\omega} \left( \frac{1}{\epsilon_k - \omega + i\alpha} - \frac{1}{\epsilon_k - \omega - i\alpha} \right) d\omega \\ &= -\delta(\epsilon_k - \epsilon_F). \end{aligned} \quad (5-7)$$

Any such delta function which appears in the renormalized theory, however, always will be multiplied by  $\Sigma''(k_F, \mu)$ , which vanishes according to Eqs. (5-3) and (5-6). Thus the contour method is applicable after renormalization; and the resulting  $S'$  is in exact accord with the spectral representation to any order in the rearranged perturbation expansion.

Despite appearances, the calculation of  $S'$  as described above does not really require a knowledge of the exact value of  $\delta\mu$ . We may eliminate this number from actual computations by making the substitution  $\omega = \omega' + \delta\mu$  in Eqs. (5-4) and (5-5). The contour relevant for integrations in the  $\omega'$  plane now is simply  $C_F$  which crosses the real axis at  $\omega = \epsilon_F$  instead of at  $\omega = \mu$ . The  $\delta\mu$  which occurs in the form of an interaction may be handled by noting that, every time a proper self-energy part appears in a graph, there is a corresponding graph in which this proper part is replaced by  $-\delta\mu$ . It is self-consistent to evaluate this in the same approximation that was used for evaluation of the corresponding self-energy part. Using Eq. (5-3), we see that this is equivalent to subtracting from the self-energy part its value at  $k = k_F, \omega' = \epsilon_F$ . Thus we may construct the function  $S'(\mathbf{k}, \omega' + \delta\mu)$  by perturbation theory using the propagator

$$S_F(\mathbf{k}, \omega') = \frac{1}{2\pi i} \frac{1}{\epsilon_k - \omega'}, \quad (5-8)$$

and the contour  $C_F$  as long as we thoroughly renormalize every self-energy part which occurs. The shift from  $\omega$  to  $\omega'$  merely produces a factor  $\exp(i\delta\mu t)$  in the Fourier transform of  $S'$ . Since, ultimately, we shall

work only with closed-loop diagrams, this factor will disappear.

Although the renormalization procedure is the one which eventually must be used in actual computations, it is not necessarily most convenient for formal manipulations. A simpler set of rules for graphical analysis may be found in the results of Luttinger and Ward. Suppose we expand the propagator  $S_\mu(\mathbf{k}, \omega)$  [Eq. (5-4)] in powers of  $\delta\mu$ ; i.e.,

$$S_\mu(\mathbf{k}, \omega) = \frac{1}{\epsilon_k - \omega} - \frac{1}{\epsilon_k - \omega} \delta\mu \frac{1}{\epsilon_k - \omega} + \dots \quad (5-9)$$

Luttinger and Ward point out that these factors  $\delta\mu$  just cancel those which were made to occur as interactions and which had the effect of removing anomalous contributions. Thus we may use the usual free-electron propagator and the contour method if we choose the branch point at  $\mu$  and do include anomalous graphs. The graphical analysis throughout the rest of the paper may be interpreted in this manner.

## VI. THE CONFIGURATION AVERAGE

The procedure of averaging over impurity configurations has been investigated in detail by Kohn and Luttinger<sup>4</sup> and used effectively by Edwards<sup>3</sup> in evaluating (4-18) for independent electrons. In this section we shall review Edwards' technique briefly, translating it into the language of the many-body formalism, and maintaining as much generality as we know how.

The interaction between electrons and impurities appears in the Hamiltonian in the form:

$$V_{\text{imp}} = \frac{1}{\Omega} \sum_{\mathbf{k}, \mathbf{q}} v(\mathbf{q}) \rho(\mathbf{q}) a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}}, \quad (6-1)$$

where

$$v(\mathbf{q}) = \int d^3\mathbf{x} e^{-i\mathbf{q} \cdot \mathbf{x}} v(\mathbf{x}), \quad (6-2)$$

$v(\mathbf{x} - \mathbf{r}_s)$  being the potential due to a scattering center at  $\mathbf{r}_s$ .  $\rho(\mathbf{q})$  is defined by:

$$\rho(\mathbf{q}) = \sum_s e^{-i\mathbf{q} \cdot \mathbf{r}_s}. \quad (6-3)$$

Here the sum is performed over all the impurity positions  $\mathbf{r}_s$  in the particular configuration.

Following Edwards, let us first examine the configuration average of the propagator  $S(\mathbf{k}, \mathbf{k}', \omega)$ . This function is defined by Eqs. (4-2) and (4-3), and may be expanded in a sum of graphs in the usual manner. Any particular graph contains the interaction  $V_{\text{imp}}$  a certain number of times, say  $m$ . Thus the contribution of such a graph to  $S$  contains the product  $\rho(\mathbf{q}_1)\rho(\mathbf{q}_2)\dots\rho(\mathbf{q}_m)$ , which may be brought out of the matrix element and averaged before performing the momentum and energy integrations.

If the impurities are distributed in a purely random fashion, the configuration average of a function  $F$  of

the  $N_i$  impurity positions,  $\mathbf{r}_1, \dots, \mathbf{r}_{N_i}$ , may be taken to be:

$$\bar{F} = \frac{1}{\Omega^{N_i}} \int d^3\mathbf{r}_1 \dots \int d^3\mathbf{r}_{N_i} F(\mathbf{r}_1, \dots, \mathbf{r}_{N_i}). \quad (6-4)$$

Performing this operation on the product of  $\rho$ 's, we find:

$$\begin{aligned} \langle \rho(\mathbf{q}_1) \dots \rho(\mathbf{q}_m) \rangle_{\text{av}} &= \frac{(2\pi)^3 N_i}{\Omega} \delta(\mathbf{q}_1 + \dots + \mathbf{q}_m) \\ &+ \frac{(2\pi)^6 N_i^2}{\Omega^2} \sum^{(2)} \delta(\mathbf{q}_1 + \dots) \delta(\mathbf{q}_s + \dots) \\ &+ \frac{(2\pi)^9 N_i^3}{\Omega^3} \sum^{(3)} \dots, \end{aligned} \quad (6-5)$$

neglecting terms which vanish when  $\Omega \rightarrow \infty$  but the density of impurities,  $n_i = N_i/\Omega$ , remains finite.  $\Sigma^{(2)}$  indicates a sum over all partitions of the  $\mathbf{q}$ 's into two groups;  $\Sigma^{(3)}$  sums three groups; and so on. Note that the first term in (6-5) corresponds to the case where all scattering events occur at the same impurity; the second term involves two different impurities, etc.

It is apparent that the configuration average restores a sort of momentum conservation to the propagator. A slightly new kind of graph now may be drawn in which all the dotted lines associated with a particular scattering center are connected to the same point on the diagram. Equation (6-5) then tells us that the sum of the momenta of all lines leading into this point must vanish. Each such impurity point contributes a factor  $n_i$  to the graph. A graph of order  $n_i^3$  is drawn in Fig. 7. Remember that, since the impurities are fixed, each dotted line carries zero frequency.

The averaged propagator  $\bar{S}$  is a function only of  $k$  and  $\omega$ . It will be convenient to write it in the standard form:

$$\bar{S}(k, \omega) = \frac{1}{2\pi i} \frac{1}{\epsilon_k - \omega - \Sigma(k, \omega)}, \quad (6-6)$$

where  $\Sigma(k, \omega)$  is the proper self-energy part including the averaged impurity interactions.

In order to calculate  $\sigma$ , we must perform the configuration average on the product of two propagators, allowing for the possibility that the contractions indicated in (6-5) may connect interactions in different propagators and thus give rise to an effective exchange

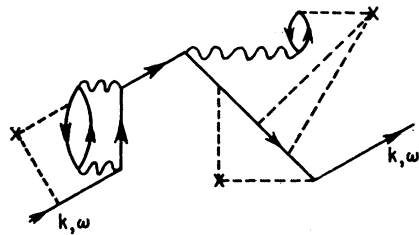


FIG. 7. A term in  $\bar{S}$  of order  $n_i^3$ .

of momentum between electron lines. In particular, let us define:

$$K(k, \omega_1, \omega_2) = \sum_{\mathbf{k}'} (\mathbf{k} \cdot \mathbf{k}') \langle S(\mathbf{k}, \mathbf{k}', \omega_1) S(\mathbf{k}', \mathbf{k}, \omega_2) \rangle_{\text{av}}. \quad (6-7)$$

The crucial trick in evaluating this quantity is to use the fact that

$$S(\mathbf{k}', \mathbf{k}, \omega) = S(-\mathbf{k}, -\mathbf{k}', \omega), \quad (6-8)$$

which follows in the usual way from time-reversal invariance. This step is actually rather significant. Our original formula (2-5) expresses  $\sigma$  as a matrix element; whereas we expect true probabilities, i.e., squared absolute values of transition amplitudes, to enter into a final expression for the conductivity. As we shall see, the time-reversal transformation introduces complex conjugates in just the right way to give us the sort of answer we expect.

We now insert (6-8) into (6-7) and arrive at a sum of all perturbation-theory terms with all possible contractions between the impurity interactions. Any one of these contributions to  $K$  may be represented by a diagram in which two electron lines of momenta  $\mathbf{k}'$  and  $-\mathbf{k}'$  enter at the bottom and leave at the top with momenta  $\mathbf{k}$  and  $-\mathbf{k}$ , respectively. A typical graph of this sort is drawn in Fig. 8. In order to sum these graphs, we use the idea of an "irreducible" interaction part. This is a diagram of the above kind which contains one or more impurity centers connected to *both* of the open electron lines, and which cannot be separated into two such diagrams by drawing a line which cuts each of the open electron lines only once and crosses no other lines of any sort. Figure 8, for example, contains two such irreducible interaction parts.

An important feature of these interaction parts is that the total incoming and outgoing momenta are always zero. Thus we may express any such part as a function only of the momentum exchanged between the external electron lines. Denoting the sum of all irreducible graphs by the symbol  $W$ , we may find the sum of all graphs by solving the integral equation:

$$\begin{aligned} \langle S(\mathbf{k}, \mathbf{k}', \omega_1) S(-\mathbf{k}, -\mathbf{k}', \omega_2) \rangle_{\text{av}} &= \bar{S}(k, \omega_1) \bar{S}(k, \omega_2) \delta_{\mathbf{k}, \mathbf{k}'} \\ &- \bar{S}(k, \omega_1) \bar{S}(k, \omega_2) \frac{1}{\Omega} \sum_{\mathbf{l}} W(\mathbf{k} - \mathbf{l}, \omega_1, \omega_2) \\ &\times \langle S(\mathbf{l}, \mathbf{k}', \omega_1) S(-\mathbf{l}, -\mathbf{k}', \omega_2) \rangle_{\text{av}}. \end{aligned} \quad (6-9)$$

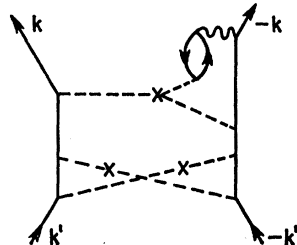


FIG. 8. A contribution to  $K$  containing two irreducible interaction parts.

Equation (6-9) is exactly the Bethe-Salpeter equation in a new context.

An expansion of each term in (6-9) in spherical harmonics makes it possible to perform the angular integration required in (6-7). After a few standard manipulations, we may arrive at the following integral equation for  $K$ :

$$\begin{aligned} K(k, \omega_1, \omega_2) &= k^2 \bar{S}(k, \omega_1) \bar{S}(k, \omega_2) \\ &- \int_0^\infty kl \bar{S}(k, \omega_1) \bar{S}(k, \omega_2) w(k, l, \omega_1, \omega_2) K(l, \omega_1, \omega_2) dl. \end{aligned} \quad (6-10)$$

The interaction term  $w$  is defined by:

$$w(k, l, \omega_1, \omega_2) = \frac{1}{4\pi^2} \int_0^\pi W(\mathbf{k} - \mathbf{l}, \omega_1, \omega_2) \sin\theta \cos\theta d\theta, \quad (6-11)$$

where  $\theta$  is the angle between  $\mathbf{k}$  and  $\mathbf{l}$ .

## VII. SOME PROPERTIES OF $\bar{S}$

In order to solve (6-10) and evaluate the conductivity, we must examine the propagator  $\bar{S}(k, \omega)$  in some detail.

From the spectral representation (4-3), it is apparent that:

$$S^*(\mathbf{k}, \mathbf{k}', \omega) = -S(\mathbf{k}', \mathbf{k}, \omega^*). \quad (7-1)$$

Thus, if we evaluate the proper self-energy part  $\Sigma(k, \omega)$  as  $\omega$  approaches the real axis and write it as the sum of its real and imaginary parts, it follows that:

$$\Sigma(k, \omega \pm i\epsilon) = \Delta(k, \omega) \pm i\Gamma(k, \omega). \quad (7-2)$$

That is, the imaginary part of the single-particle level shift changes sign across the cut.

The function  $\bar{S}(k, \omega)$  is completely determined according to (4-3) by its discontinuity at the cut, i.e., the spectral function. From (7-2) we have:

$$\begin{aligned} \bar{S}(k, \omega + i\epsilon) - \bar{S}(k, \omega - i\epsilon) \\ = \frac{\Gamma(k, \omega)}{\pi} \frac{1}{e(k, \omega)^2 + \Gamma(k, \omega)^2}, \end{aligned} \quad (7-3)$$

where

$$e(k, \omega) = \epsilon_k - \omega - \Delta(k, \omega). \quad (7-4)$$

If  $\Gamma$  is small and constant in the region near  $e(k, \omega) = 0$ , the expression in (7-3) has the familiar "Lorentz shape." In this case  $\Gamma$  is a measure of the width, i.e., the probability of decay, of the single-particle state.

Following the procedure developed in Chapter VI,  $\Sigma(k, \omega)$  may be expanded in powers of  $n_i$ , the density of impurities. The zeroth term in this expansion contains no interactions with impurities, and is just the ordinary electronic self-energy,  $\Sigma'(k, \omega)$ . We have previously assumed that the imaginary part of this self-energy vanishes when  $\omega$  is equal to the chemical potential of the system of interacting electrons without impurities. As mentioned in Chapter V, we shall neglect any change



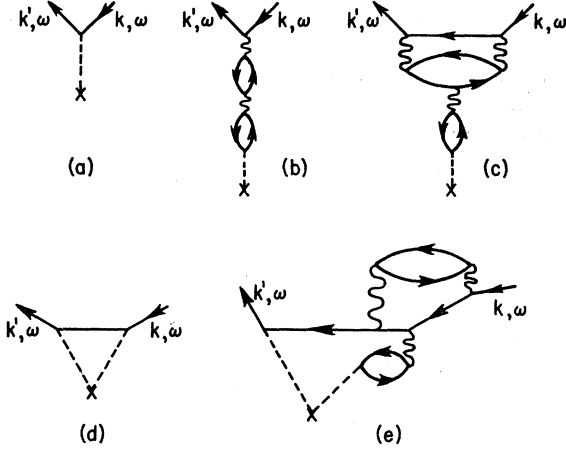


FIG. 9. Some contributions to  $t^+(\mathbf{k}', \mathbf{k}, \omega)$ . Graphs (a) and (b) are contained in  $v_s$ ; (c) is contained in  $\bar{v}$ . Graphs (d) and (e) contribute imaginary parts to  $t^+$  even when  $\omega = \mu$ .

in  $\mu$  due to the presence of the impurities. Thus we shall assume that the  $\mu$  which occurs here is the same number which appears in Eq. (4-15).<sup>12</sup> Therefore the leading term in  $\Gamma(k, \mu)$  is proportional to  $n_i$ . This is as it must be, since the decay probability which enters into the conductivity should be proportional to the impurity density.

The contribution to  $\Sigma(k, \omega)$  which is linear in  $n_i$  is the diagonal element of the matrix  $t^+(\mathbf{k}', \mathbf{k}, \omega)$  which describes the scattering of an electron by a single screened impurity center. This matrix is defined according to Chapter VI by a series of graphs, some of which are illustrated in Fig. 9. The superscript “+” indicates that  $t^+$  is to be evaluated for  $\omega$  just above the real axis, consistent with the choice of sign of  $\Gamma$  in (7-2). We then have:

$$\Gamma(k, \mu) = n_i \text{Im} t^+(\mathbf{k}, \mathbf{k}, \mu). \quad (7-5)$$

The terms in  $\Sigma$  proportional to higher powers of  $n_i$  are given by the coherent forward scattering amplitudes for an electron in interaction with two or more impurity centers. As long as the average spacing between impurities is large compared with the wavelength of an electron at the Fermi surface, we may expect such corrections to  $\Sigma$  to be negligible.

The form of Eq. (7-5) strongly suggests that  $\Gamma(k, \mu)$  may conveniently be rewritten by means of an optical theorem. In fact, for noninteracting electrons,  $t^+(\mathbf{k}, \mathbf{k}, \mu)$  is just the forward scattering part of the standard  $t$  matrix, and we may write immediately:

$$\Gamma(k_F, \mu) = \frac{1}{2} n_i (k_F/m) \sigma_T(k_F), \quad (7-6)$$

where  $\sigma_T(k_F)$  is the total cross-section for scattering of

<sup>12</sup> In any case, the same perturbation theoretic analysis which indicates that  $\Sigma'$  is real at  $\omega = \mu$  also tells us that the imaginary part of  $\Sigma'$  goes as  $(\omega - \mu)^2$  near  $\omega = \mu$ . Since any shift in  $\mu$  due to the impurities will be of order  $n_i$ , the error made in neglecting this shift is of order  $n_i^2$ ; so it can have no effect on the present calculation.

a free electron moving with the Fermi momentum  $k_F$ . A similar theorem now will be proven for the general case.

Starting from the assumption that  $\Sigma'(k, \mu)$  is real, we may construct a series of contributions to the scattering matrix  $t^+(\mathbf{k}', \mathbf{k}, \omega)$  which are also real at  $\omega = \mu$ . Consider first the screened impurity potential which is the sum of all graphs of the form shown in Figs. 9(a) and (b). This function, which we shall denote by  $v_s(\mathbf{k}', \mathbf{k})$ , is real and independent of  $\omega$ . Its explicit form is given in reference 7. Then suppose we take any proper electronic self-energy part and insert an arbitrary number of interactions with the screened impurity into its internal lines. Summing all possible diagrams of this sort must be the same as replacing every internal line in  $\Sigma'$  by the propagator for a single electron moving in the potential  $v_s$ . Call this modified self-energy part  $\Sigma_s(\mathbf{k}', \mathbf{k}, \omega)$ . The desired contribution to the scattering matrix is then:

$$\bar{v}(\mathbf{k}', \mathbf{k}) = v_s(\mathbf{k}', \mathbf{k}) + \Sigma_s(\mathbf{k}', \mathbf{k}, \mu) - \Sigma'(\mathbf{k}, \mu) \delta_{\mathbf{k}, \mathbf{k}'}. \quad (7-7)$$

Note that we have subtracted out the diagonal part of  $\Sigma_s$  which contains no impurity interaction.

Being a localized and well-behaved potential,  $v_s$  cannot shift the bottom of the continuum of the free-electron spectrum. Thus  $\Sigma_s$  should be real whenever  $\Sigma'$  is, which implies that  $\bar{v}$  as defined by (7-7) must be real also.

In terms of  $\bar{v}$  we have:

$$t^+(\mathbf{k}', \mathbf{k}, \mu) = \bar{v}(\mathbf{k}', \mathbf{k}) - \frac{2\pi i}{\Omega} \sum_{\mathbf{l}} \bar{v}(\mathbf{k}, \mathbf{l}) \times S'(\mathbf{l}, \mu + i\epsilon) t^+(\mathbf{l}, \mathbf{k}, \mu), \quad (7-8)$$

where  $S'$ , the true one-electron propagator without impurity interactions, may be written:

$$2\pi i S'(\mathbf{k}, \mu + i\epsilon) = \frac{1}{\epsilon_k - \mu - \Sigma'(k, \mu) - i\epsilon} = \frac{1}{E_k - \mu - i\epsilon}, \quad (7-9)$$

where

$$\Sigma'(k, \mu) = \Delta'(k, \mu)$$

is real and

$$E_k \equiv \epsilon_k - \Delta'(k, \mu).$$

The problem of calculating  $t^+(\mathbf{k}', \mathbf{k}, \mu)$  is hereby reduced to that of calculating the scattering of a free particle of energy  $\mu$  by the real potential  $\bar{v}$  as described by the Hamiltonian:

$$(\tilde{H})_{\mathbf{k}', \mathbf{k}} = E_k \delta_{\mathbf{k}', \mathbf{k}} + (1/\Omega) \bar{v}(\mathbf{k}', \mathbf{k}). \quad (7-10)$$

$\tilde{H}$  is Hermitian, and  $\bar{v}$ , like  $v_s$ , will not shift the continuum part of the spectrum of  $\tilde{H}$ . Iteration of Eq. (7-8) simply generates the Born expansion for the scattering matrix  $t^+$ . The usual theorems based on

completeness are now applicable; and in particular<sup>13</sup>:

$$\text{Im}t^+(\mathbf{k}, \mathbf{k}, \mu) = \frac{\pi}{\Omega} \sum_1 |t^+(\mathbf{k}, \mathbf{l}, \mu)|^2 \delta(E_l - \mu). \quad (7-11)$$

This is the most general form of the desired theorem.

From (7-5), (7-11), and the definition of  $E_l$ , we have:

$$\Gamma(k, \mu) = \frac{n_i k_F^2}{4\pi(k_F/m - \partial\Delta'/\partial k_F)} \int_0^\pi |t^+(\mathbf{k}, \mathbf{k}_F, \mu)|^2 \times \sin\theta d\theta, \quad (7-12)$$

where  $k_F$  is the solution of:

$$k_F^2/2m - \mu - \Delta'(k_F, \mu) = 0, \quad (7-13)$$

[see Eq. (5-4)], and  $\theta$  is the angle between  $\mathbf{k}$  and  $\mathbf{k}_F$ . The term  $k_F/m - \partial\Delta'/\partial k_F$  may be rewritten somewhat more physically in terms of the group velocity of a single-particle-like excitation at the Fermi surface. When  $\Sigma'(k, \omega)$  is real, the frequency  $\omega(k)$  is determined by:

$$k^2/2m - \omega - \Delta'(k, \omega) = 0. \quad (7-14)$$

Solving for the group velocity, we find:

$$u_{\text{group}} = \frac{d\omega}{dk} = N_k \left( \frac{k}{m} - \frac{\partial\Delta'}{\partial k} \right). \quad (7-15)$$

The number  $N_k$ , defined by:

$$N_k^{-1} = 1 + \frac{\partial\Delta'}{\partial\omega} \bigg|_{\omega=\omega(k)}, \quad (7-16)$$

is a normalization constant which tells the probability of finding the "bare" electron  $\mathbf{k}$  in the true state of that wave number. Note also that  $N_k$  is the residue of  $S'(k, \omega)$  at its pole.<sup>14</sup> In terms of the group velocity  $u_F$  at  $k = k_F$ , we have:

$$\Gamma(k, \mu) = \frac{n_i k_F^2 N_{k_F}}{4\pi u_F} \int_0^\pi |t^+(\mathbf{k}, \mathbf{k}_F, \mu)|^2 \sin\theta d\theta. \quad (7-17)$$

It is easily seen that (7-17) reduces to (7-6) when  $u_F = k_F/m$ , and  $N_{k_F} = 1$ .

In order to estimate the magnitude and  $k$  dependence of  $\Gamma$ , let us approximate  $t^+$  in (7-17) by:

$$t^+(\mathbf{k} + \mathbf{q}, \mathbf{k}) = t^+(q) \cong v_s(q) \cong \frac{4\pi e^2 Z}{q^2 + \kappa^2}, \quad (7-18)$$

where

$$\kappa^2 = \frac{4me^2 k_F}{\pi} = \xi r_s k_F^2, \quad \xi = -\left(\frac{2\pi}{3}\right)^{\frac{1}{3}} \cong 0.65.$$

For independent electrons ( $u_F = k_F/m$ , etc.):

$$\Gamma(k, \epsilon_F) \cong \frac{4n_i Z^2}{3n_e} \frac{1}{[(k/k_F + 1)^2 + \xi r_s][(k/k_F - 1)^2 + \xi r_s]} \text{ry.} \quad (7-19)$$

This function has a maximum at  $k = k_F$  and a width of about  $k_F \kappa/m = 6/r_s^{\frac{1}{3}}$  ry. The magnitude of  $\Gamma$  at its peak is about  $n_i/3\xi n_e r_s = 0.51 n_i/n_e r_s$  ry.

### VIII. EVALUATION OF THE CONDUCTIVITY

Returning now to the expression for  $\sigma$  given in (4-15) and using the definition of  $K$  in (6-7), we have:

$$\sigma = \frac{2\pi e^2}{3m^2 \Omega} \sum_{\mathbf{k}} \lim_{\epsilon \rightarrow +0} \{ 2 \text{Re} K(k, \mu + i\epsilon, \mu + i\epsilon) - 2K(k, \mu + i\epsilon, \mu - i\epsilon) \}. \quad (8-1)$$

Here the expression (4-11) for  $\mathcal{G}(\omega_1, \omega_2)$  has been simplified a bit by use of Eq. (7-1), which describes the behavior of  $S$  under complex conjugation.

First, let us examine the second term in brackets in (8-1). The integral equation (6-10) for this function, which we shall denote by  $K_{+-}$ , is:

$$K_{+-}(k) = -\frac{1}{4\pi^2} \frac{1}{e(k)^2 + \Gamma(k)^2} \times \left\{ k^2 - \int_0^\infty kl w_{+-}(k, l) K_{+-}(l) dl \right\}. \quad (8-2)$$

(From now on, functions like  $e$  and  $\Gamma$  always will be understood to be evaluated at  $\omega = \mu$ .) The interaction term  $W_{+-}$  which determines  $w_{+-}$  according to (6-11) is given to first order in  $n_i$  by:

$$W_{+-}(\mathbf{k}, \mathbf{l}) = 4\pi^2 n_i t^+(\mathbf{k}, \mathbf{l}) t^-(\mathbf{k}, -\mathbf{l}) = 4\pi^2 n_i |t^+(\mathbf{k}, \mathbf{l})|^2, \quad (8-3)$$

which follows from the graphical analysis of Sec. VI. Thus

$$w_{+-}(k, l) = n_i \int_0^\pi |t^+(k, l, \theta)|^2 \sin\theta \cos\theta d\theta. \quad (8.4)$$

Apart from the factor  $\cos\theta$ , this expression is very similar to that which appears in Eq. (7-17) for  $\Gamma(k)$ .  $w_{+-}(k, l)$  has a maximum at  $k = l$ , and has the same width as  $\Gamma(k)$ .

It is apparent from the form of Eq. (8-2) that  $K_{+-}(k)$  is sharply peaked near values of  $k$  which satisfy  $e(k) = 0$ . The solution of this equation is not exactly  $k_F$  according to Eq. (7-13), since the  $\Delta(k)$  which appears in  $e(k)$  contains the impurity interactions. On the other hand, the correction to  $k_F$  due to these interactions is of order  $n_i$ , and it is consistent with our model of rare impurities to neglect it. In other words, we assume that the single-electron-like excitation is sufficiently well localized

<sup>13</sup> For example, see M. Gell-Mann and M. L. Goldberger, Phys. Rev. 91, 398 (1953).

<sup>14</sup> This point is discussed in detail by L. Van Hove, Physica 21, 901 (1955), and Physica 22, 343 (1956); and by N. M. Hugenholtz, Physica 23, 481 (1957). Note, however, that their propagator is not quite the same as ours.

between scattering events that it propagates as if there were no impurities present at all.

In the neighborhood of  $k=k_F$ , we may solve (8-2) by evaluating:

$$M = \int_0^\infty l w_{+-}(k_F, l) K_{+-}(l) dl$$

$$= -\frac{1}{4\pi^2} \int_0^\infty \frac{l^2 w_{+-}(k_F, l) dl}{e(l)^2 + \Gamma(l)^2} + \frac{1}{4\pi^2} \int_0^\infty \frac{l^2 w_{+-}(k_F, l) dl}{e(l)^2 + \Gamma(l)^2}$$

$$\times \int_0^\infty l' w_{+-}(l, l') K_{+-}(l') dl'. \quad (8-5)$$

The expression  $w_{+-}(k_F, l)[e(l)^2 + \Gamma(l)^2]^{-1}$  here plays the role of a delta function for sufficiently small  $n_i$ . Its normalization is

$$\frac{1}{4\pi^2} \int_0^\infty \frac{w_{+-}(k_F, l) dl}{e(l)^2 + \Gamma(l)^2} = \frac{N_{k_F} w_{+-}(k_F, k_F)}{4\pi u_F \Gamma(k_F)} + O\left(\frac{\Gamma}{\epsilon_F}\right). \quad (8-6)$$

In deriving this result we require that  $\Gamma(k)$  be constant in the region of width  $\Gamma$  about  $k=k_F$ . From the estimates at the end of Sec. VII, we see that this condition is  $\Gamma(k_F)m/k_F \cong n_F s^{\frac{1}{2}}/12n_e \ll 1$ , which is easily satisfied for rare impurities and dense electrons. We also assume that  $\Delta(k)$  is a well-behaved function in this region. Defining in analogy to (7-17):

$$\Gamma'(k) = \frac{k_F^2 N_{k_F} w_{+-}(k, k_F)}{4\pi u_F}$$

$$= \frac{N_{k_F} n_i k_F^2}{4\pi u_F} \int_0^\pi |t^+(k, k_F, \theta)|^2 \sin\theta \cos\theta d\theta, \quad (8-7)$$

we have

$$\frac{1}{4\pi^2} \frac{w_{+-}(k_F, l)}{e(l)^2 + \Gamma(l)^2} \cong \frac{\Gamma'(k_F)}{k_F^2 \Gamma(k_F)} \delta(k - k_F), \quad (8-8)$$

to order  $\Gamma/\epsilon_F$ . Note that this equation is valid only when the expression appears in a convergent integral along with other functions which are slowly varying near  $k=k_F$ .

Substituting (8-8) into (8-5), we see that  $M$  reappears as the integral over  $l'$ , and we can solve the equation to find:

$$M = -\frac{k_F \Gamma'(k_F)}{\Gamma(k_F) - \Gamma'(k_F)}. \quad (8-9)$$

Thus, for  $k$  near  $k_F$ :

$$K_{+-}(k) = -\frac{k_F^2}{4\pi^2} \frac{\Gamma(k_F)}{\Gamma(k_F) - \Gamma'(k_F)} \frac{1}{e(k)^2 + \Gamma(k)^2}$$

$$\cong -\frac{k_F^2 N_{k_F} \delta(k - k_F)}{4\pi u_F (\Gamma(k_F) - \Gamma'(k_F))} + O\left(\frac{\Gamma}{\epsilon_F}\right). \quad (8-10)$$

Equation (8-10) is not a solution of (8-2) for values of  $k$  far away from  $k_F$ , since  $w_{+-}(k, l)$  becomes small for  $k \neq l$ . [For Coulomb interactions,  $\Gamma(k) \sim k^{-4}$  and  $\Gamma'(k) \sim k^{-5}$  for  $k \gg k_F$ .] The dominant contribution to the integral over  $l$  in (8-2), however, still comes from the region near  $l=k_F$ , where  $K_{+-}$  is well approximated by (8-10). Evaluating (8-2) in this manner, we find:

$$K_{+-}(k) = -\frac{1}{4\pi^2} \frac{1}{e(k)^2 + \Gamma(k)^2} \left\{ k^2 + \frac{k k_F \Gamma'(k)}{\Gamma(k_F) - \Gamma'(k_F)} \right\}. \quad (8-11)$$

For  $k$  near  $k_F$ , (8-11) reduces to (8-10), thus checking the consistency of the solution. As  $k$  becomes much larger than  $k_F$ , the second term in brackets vanishes as  $k^{-4}$ .

As it stands, (8-11) cannot be used to evaluate  $\sigma$  in (8-1) because the sum over  $k$  diverges at large  $k$ . To achieve convergence, we must include the contribution from  $K_{++}(k)$  as indicated in (8-1). The inhomogeneous term in the integral equation (6-10) for  $K_{++}$  is:

$$k^2 \text{Re}(\bar{S}(k, \mu + i\epsilon))^2 = \frac{k^2}{4\pi^2} \frac{\Gamma(k)^2 - e(k)^2}{[e(k)^2 + \Gamma(k)^2]^2}. \quad (8-12)$$

As before, (8-12) is sharply peaked near  $k=k_F$ . Unlike (8-6), however, the analogous normalization integral vanishes to order  $\Gamma/\epsilon_F$ . Thus iteration of the integral equation yields corrections of order  $\Gamma/\epsilon_F$ , which we neglect. In this approximation we have simply:

$$\text{Re} K_{++}(k) \cong \frac{k^2}{4\pi^2} \frac{\Gamma(k)^2 - e(k)^2}{[e(k)^2 + \Gamma(k)^2]^2}. \quad (8-13)$$

For large  $k$ , then:

$$2 \text{Re} K_{++}(k) - 2 K_{+-}(k) \cong -\frac{k^2}{\pi^2} \frac{\Gamma^2(k)}{[e(k)^2 + \Gamma(k)^2]^2}, \quad k \gg k_F, \quad (8-14)$$

which assures convergence in (7-1).

Having achieved convergence, we may evaluate (8-1) using only the contribution near  $k=k_F$ . According to the last paragraph's discussion,  $K_{++}$  will not contribute to lowest order in  $\Gamma/\epsilon_F$ ; thus we need only  $K_{+-}$  as given by (8-10). We have:

$$\sigma = \frac{e^2 k_F^4 N_{k_F}}{6m^2 \pi^2 u_F} [\Gamma(k_F) - \Gamma'(k_F)]^{-1}$$

$$= \frac{2e^2 k_F^2}{3\pi m^2 n_i} \left[ \int_0^\pi |t(k_F, k_F, \theta)|^2 (1 - \cos\theta) \sin\theta d\theta \right]^{-1}. \quad (8-15)$$

This expression for  $\sigma$  reduces to a more familiar form in the case of independent electrons. Taking  $N_{k_F} = 1$

and  $u_F = k_F/m$ , we have:

$$\sigma = (n_e e^2 / m) \tau \quad (8-16)$$

where,

$$\frac{1}{\tau} = 2[\Gamma(k_F) - \Gamma'(k_F)] = 2\pi n_i \frac{k_F}{m} \int_0^\pi \sigma(\theta) \times (1 - \cos\theta) \sin\theta d\theta, \quad (8-17)$$

and  $\sigma(\theta)$  is the differential scattering cross section for an electron of momentum  $k_F$ .

Equation (8-16) is the standard classical expression for the conductivity.  $\Gamma$ , the decay rate for the single-particle state, is the usual "scattering-out" probability; and  $\Gamma'$  turns out to be the "scattering-in" term. Note that there is no effect of the exclusion principle remaining even in the calculation of  $\sigma(\theta)$  in (8-17).  $\sigma(\theta)$

is the exact cross section for a free electron scattered by an isolated impurity center. This happened mathematically because we defined the poles in  $t^+$  by keeping  $\omega$  always just above the real axis.

In similar fashion, it should be possible to rewrite (8-15) in terms of a scattering cross section for effective electrons scattered by shielded impurities. This would involve finding the correct normalization for these scattering states (see Van Hove<sup>14</sup>), and it seems simplest, even if a bit less physical, to keep (8-15) in its present form.

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### Electro-Optic Kerr Effect and Polarization Reversal in Deuterium-Doped Rochelle Salt

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Polarization reversal as a function of nucleation and growth of domains in ferroelectric deuterium-doped Rochelle salt was investigated by means of the electro-optic Kerr effect. The results indicate that a phenomenological model based on statistical nucleation of domains in a plane including the ferroelectric axis followed by a two-dimensional sidewise expansion of the domains, will adequately account for the experimental observations for fields larger than 50 volts/cm. For lower fields, the process is controlled primarily by the nucleation of new domains due to localized stresses which hinder the displacement of domain walls.

#### 1. INTRODUCTION

A STUDY of the polarization process in Rochelle salt (RS) was undertaken for a dual purpose. First, some features of polarization reversal interpreted as the nucleation and motion of antiparallel domains have only been partially investigated. Second, the validity of a phenomenological model for the reversal mechanism was to be tested on a ferroelectric crystal in which domain dynamics could be discerned optically, under polarized light, as well as electrically, from a study of the displacement current transients.

The displacement current parameters predicted from this model were shown to be in excellent agreement with experiment in the case of colemanite.<sup>1</sup> No direct visual observations could be made however, which might provide additional justification for the choice of a reversal mechanism based only on nucleation and subsequent sidewise expansion of domains. Two-dimensional wall displacement was observed in barium

titanate<sup>2-4</sup> under restricted experimental conditions and some features of the above model were confirmed. Rochelle salt, however, offers because of its large electro-optic effects, the advantage of unrestricted observations of electrical and optical features of the polarization reversal process.

Mitsui and Furuichi<sup>5</sup> studied the domain structure and domain dynamics of Rochelle salt showing that the spontaneous shear deformation between neighboring domains causes the optical indicatrix to turn in opposite directions about the  $a$  axis leading to a difference in extinction positions between adjacent domains. Indenbom and Chernysheva<sup>6</sup> discussed the monoclinicity of Rochelle salt using quantitative measurements of the turning angle of the optical indicatrix to define a thermodynamic potential theory analogous

<sup>2</sup> R. C. Miller, Phys. Rev. **111**, 736 (1958).

<sup>3</sup> R. C. Miller and A. Savage, Phys. Rev. **112**, 755 (1958).

<sup>4</sup> R. C. Miller and A. Savage, Phys. Rev. **115**, 1176 (1959).

<sup>5</sup> T. Mitsui and J. Furuichi, Phys. Rev. **90**, 193 (1953).

<sup>6</sup> V. L. Indenbom and M. A. Chernysheva, Kristallografiya **2** (1957) [translation: Soviet Phys.-Cryst. **2**, 522 (1957)].

<sup>1</sup> H. H. Wieder, J. Appl. Phys. **31**, 180 (1960).