PHYSICAL REVIEW B VOLUME 6, NUMBER 4 15 AUGUST 1972

Homogeneous Dynamical Conductivity of Simple Metals*

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(Received 11 January 1972)

Within the jellium model the zero wave vector, frequency-dependent conductivity is expressed in terms of a regular memory function. This quantity is calculated in lowest order in the impurity concentration and the electron-phonon coupling, thus yielding a reasonable approximation for the conductivity valid in the complete frequency regime. The standard results for the static conductivity including vertex corrections are reproduced. Deviations from Drude's formula because of spin-flip scattering in a magnetic field, because of resonance scattering, because of phonon creation at low temperatures, and because of breaking of the screening cloud attached to charged impurities are discussed.

I. INTRODUCTION

Recently a technique has been worked out[1] to calculate approximately certain very simple response functions of many-particle systems without being restricted either to the hydrodynamic regime or to the regime of high frequencies. In this paper we want to apply this technique to the familiar problem of determining the homogeneous dynamical conductivity of metals. To describe the metal we will use the oversimplified jellium model.

Using a standard Boltzmann equation and approximating the collision integral by a single collision frequency $(1/\tau)$ one arrives[2,3] at the classical Drude formula for the dynamical conductivity $\sigma(z)$. These approximations are impossible if the effective relaxation time τ becomes frequency dependent or if the frequencies are too large.

In the low-frequency limit the conductivity has been calculated from first principles by summing up infinite sets of diagrams for the current correlation function[4,5] or by truncating the hierarchy of equations of motion for the relevant Green's function.[6-9] The difficulties in a calculation of $\sigma(z)$ are caused by its resonance structure. The existence of a pole in $\sigma(z)$ near $z=0$ does exclude a finite-order-perturbation expansion. To overcome these difficulties one can introduce the ratio of external frequency z to the nonsecular frequencies of the system as a small parameter; this assumption, originally due to Bogoliubov,[10] excludes an extension of the results to higher frequencies.

At high frequencies $\sigma(z)$ is regular and can be obtained by perturbation theory. Much work has been done in this direction in connection with discussions of light absorption or plasmon damping. Yamada[6] and Plakida[9] have derived equations which yield the correct resonance structure for small frequencies and the correct perturbation results for large frequencies. But a solution of their equations in the complete frequency range has not been achieved.

We proceed by exactly expressing the response function in terms of a holomorphic memory function. This has been suggested in another context[1,11] and is quite similar to expressing particle propagators in terms of a self-energy. The memory function is frequency independent in the hydrodynamical regime and in first approximation can be evaluated by perturbation expansion with respect to small parameters (concentration of impurities, coupling constant, phonon density). Again this is similar to approximating self-energies in order to get quasiparticle energy and damping. Obviously, there is no difference in principle between a resonance of a one-particle Green's function (particle lifetime) and a resonance of $\sigma(\omega)$ (current lifetime). As a result we obtain our approximation for the conductivity valid in the whole frequency regime (Sec. III).

The general formulas will be studied under various additional simplifying assumptions. First (Sec. IV A) the electron-impurity scattering is treated in Born approximation. Drude's formula turns out to be valid for frequencies ω smaller than the Fermi energy ϵ_F and the relaxation time τ is given by the usual Boltzmann-equation expression. Then (Sec. IV B) spin-flip scattering is discussed in lowest order within the s-d model. It turns out that strong frequency dependence of the relaxation can be produced by external magnetic fields. The conditions under which remarkable deviations from Drude's formula can be expected will be given. In Sec. IV C the potential scattering of electrons is treated to first order in the impurity concentration.

Drude's formula is valid provided that the energy dependence of the electron-impurity-scattering cross section can be neglected. Generally, the conductivity is expressed in terms of the scattering or t matrix. For the special case of a simple scattering resonance on the Fermi surface explicit results for the deviations from Drude's formula are given. Then (Sec. IV D) the electron-phonon conductivity is discussed in lowest order of the electron-phonon coupling. At zero frequency Bloch's formula[2] is recovered. At low temperatures the effective relaxation time acquires a pronounced frequency dependence, as predicted by Holstein,[12] due to phonon-creation processes. Finally (Sec. IV E), the problem of dynamical impurity screening is discussed by treating the electron-electron interaction in the random-phase approximation (RPA) and the electron-impurity scattering in lowest order. For frequencies below the plasmon resonance ω_p the deviations from Drude's formula are small and the relaxation time τ is given by the Mott-Jones[2] expression. For frequencies above ω_p the conductivity is substantially larger than one would expect from Drude's formula because screening of the impurities cannot be achieved any more. For still higher frequencies σ drops below the classical value.

II. MODEL

We choose a description of metals known as the "jellium" model, in which the conduction electrons are assumed to move against a uniform positively charged medium. The Hamiltonian of the system reads

$$H = H_s + H_c + H' + H_0 \,. \tag{1}$$

H_s represents the free-band Hamiltonian of the conduction electrons,

$$H_s = \sum_p \epsilon(p) c_p^\dagger c_p \,, \tag{2}$$

where $c_p^\dagger$, c_p are the electron-creation and -annihilation operators characterized by quantum numbers $p = (\vec{p}, \sigma)$ ($\sigma = \pm\frac{1}{2}$ and $\vec{p}$ is a vector of the first Brillouin zone), obeying the usual anticommutation relations. We assume that an external static magnetic field B is applied in the z direction, so that the electron one-particle energies are split according to the Zeeman effect, $\epsilon(\vec{p}\sigma) = \epsilon_p - \sigma h_s$, where ϵ_p is the electron-band energy and $h_s = g_s \mu_B B$. The coupling of the electron orbital motion to the magnetic field is considered to be negligible and will not be discussed in the following. H_c describes the Coulomb interaction of the electrons

$$H_c = \tfrac{1}{2} \sum V(\vec{k}) c^\dagger_{\vec{p}+\vec{k}\sigma} c^\dagger_{\vec{p}'-\vec{k}\sigma'} c_{\vec{p}'\sigma'} c_{\vec{p}\sigma} \,, \tag{3a}$$

with

$$V(\vec{k}) = (4\pi e^2/k^2)(1 - \delta_{\vec{k},0}) \,, \tag{3b}$$

where the interaction with the uniform positively charged jellium has been taken into account. The term H' in the Hamiltonian is due to interaction of the electrons with deviations from uniformity, such as impurities and phonons,

$$H' = H_1 + H_2 + H_3 \,, \tag{4a}$$

$$H_1 = N^{-1} \sum_j \langle \vec{k} | U_1^j | \vec{k}' \rangle c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma} \,, \tag{4b}$$

$$H_2 = N^{-1} \sum_j \langle \vec{k} | U_2^j | \vec{k}' \rangle S_j^i s^i_{\sigma\sigma'} c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma'} \,. \tag{4c}$$

Here U_1^j and U_2^j denote the pseudopotential for spin-nonflip and spin-flip scattering, respectively, by the impurity at position $\vec{r}_j$,

$$\langle \vec{k} | U_\alpha^j | \vec{k}' \rangle = e^{i\vec{r}_j(\vec{k}-\vec{k}')} \langle \vec{k} | U_\alpha | \vec{k}' \rangle \,. \tag{4d}$$

$S_j^0 = S_j^z$ and $S_j^\pm = (S_j^x \pm i S_j^y)/\sqrt{2}$ are the spin operators of the impurity at $\vec{r}_j$ obeying the usual commutation relations. The sums on j run over N_i impurity sites and $N_i/N = c$ is the impurity concentration (N is the number of lattice cells). Since the impurities are considered to be randomly distributed, their positions will be averaged over in all physical quantities. A generalization to several types of impurities is straightforward.

In H_3 we shall incorporate the electron-phonon interaction

$$H_3 = \sum [D(\vec{k} - \vec{k}') c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma} b_{\vec{k}-\vec{k}'} + \text{H. c.}] \,, \tag{4e}$$

where $b^\dagger_{\vec{q}}$, $b_{\vec{q}}$ are creation and annihilation operators for phonons of momentum $\vec{q}$. For simplicity we consider only phonons of one polarization, say, longitudinal. Then the electron-phonon matrix element D may be specified further as[2]

$$D(\vec{q}) = (2 m_i N \omega_q)^{-1/2} q\, C(q) \,, \quad q = |\vec{q}| \tag{4f}$$

where m_i is the ionic mass, ω_q is a phonon frequency, and C is a slowly varying function of q. Having described by Eqs. (4c) and (4e) the coupling of electrons to time-dependent systems we have to add to the Hamiltonian the appropriate terms. Thus

$$H_0 = H_d + H_{\text{ph}} \,, \tag{5a}$$

where

$$H_d = h \sum_j S_j^0 \,, \quad h = \mu_B g_d B \tag{5b}$$

accounts for the time development of the impurity spins in the external magnetic field B and

$$H_{\text{ph}} = \sum \omega_q (b_q^\dagger b_q + \tfrac{1}{2}) \tag{5c}$$

represents the Hamiltonian of the phonons.

The linear response of an operator A due to a perturbation coupled to an operator B can be expressed in terms of the correlation function[11,13]

$$\chi_{AB}(z) = \langle\langle A ; B \rangle\rangle_z = -i \int_0^\infty e^{izt} \langle [A(t), B(0)] \rangle dt \,. \tag{6a}$$

These functions are holomorphic for all nonreal

z and decrease for large z like

$$\chi_{AB}(z) = \langle [A,B] \rangle / z \quad \text{for } |z| \to \infty \, . \tag{6b}$$

Furthermore, they obey the equations of motion

$$z \, \langle\langle A;B \rangle\rangle = \langle [A,B] \rangle + \langle\langle [A,H];B \rangle\rangle \tag{6c}$$

$$= \langle [A,B] \rangle - \langle\langle A\, ;\, [B,H] \rangle\rangle \, . \tag{6d}$$

In these equations $A(t)$ is the Heisenberg representation of operator A, $[A,B]$ denotes the commutator, and $\langle\;\rangle$ abbreviates the thermodynamical average at temperature T and the average over the random impurity positions. Units are chosen such that Planck's constant $\hbar$ and Boltzmann's constant k_B are equal to unity. $\chi(z)$ can be represented as a spectral integral

$$\chi(z) = (1/\pi) \int d\omega \, \chi''(\omega)/(\omega - z) \, , \tag{7a}$$

where the spectral function $\chi''(\omega)$ is given by the discontinuity across the real axis,

$$\chi(\omega \pm i_0) = \chi'(\omega) \pm i\chi''(\omega) \, . \tag{7b}$$

We want to discuss the dynamical homogeneous conductivity $\sigma(z)$ which is related to the current-current correlation function[3,14] $\chi(z)$ by

$$\sigma(z) = -i(e^2/z)\chi(z) + i\omega_p^2/(4\pi z) \, . \tag{8}$$

Here $\omega_p^2 = 4\pi e^2 N_e/m$ is the plasma frequency (N_e, m, e, are the electron density, mass, charge; we consider a system of unit volume). Furthermore,

$$-\langle\langle j_i\, ;\, j_j \rangle\rangle = \delta_{ij}\,\chi(z), \quad i,j = 1, 2, 3 \tag{9}$$

and

$$j_i = \sum v_i(\vec{k})\, c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \, , \tag{10}$$

with $v_i(\vec{k}) = \partial\epsilon_k/\partial k_i$, the ith component of the electron velocity. In the usual way[11] one verifies for the susceptibility (9)

$$\chi(z) = \chi(-z) \, , \tag{11a}$$

$$\chi^*(z) = \chi(z^*) \, . \tag{11b}$$

Thus χ' and χ'' in Eq. (7b) are real. Furthermore,[11]

$$\chi(z) = O(z^{-2}) \quad \text{for } |z| \to \infty \tag{11c}$$

and

$$\omega\chi''(\omega) \geq 0 \, . \tag{11d}$$

For all nonreal z one has the inequality[1,11]

$$\chi(z) \neq \chi_0 \, , \tag{12}$$

where χ_0 is the static limit of $\chi(z)$. Finally, we assume our system to be a normal conductor, i.e., the conductivity tends to a finite value as z approaches zero. Then we get from Eq. (8) for the static limit

$$\chi_0 = N_e/m \, . \tag{13}$$

III. MEMORY FUNCTION

We want to determine the dynamical conductivity by introducing first a representation of $\sigma(z)$ in terms of a relaxation or memory function $M(z)$. The procedure will be carried out in complete analogy to a recent calculation of the dynamical magnetic susceptibility in dilute magnetic alloys.[1] Let us consider the function

$$M(z) = z\chi(z)/[\chi_0 - \chi(z)] \, , \tag{14}$$

with χ_0 given by Eq. (13). Because of the inequality (12) $M(z)$ is a holomorphic function for all nonreal z. According to Eqs. (11a)–(11c), $M(z)$ decreases asymptotically like $1/z$ and obeys the symmetry relations $M^*(z) = M(z^*)$ and $M(z) = -M(-z)$. Consequently, $M(z)$ can be represented by a spectral integral

$$M(z) = (1/\pi) \int d\omega M''(\omega)/(\omega - z) \, , \tag{15a}$$

where

$$M(\omega \pm i0) = M'(\omega) \pm iM''(\omega) \tag{15b}$$

and M', M'' are real functions satisfying

$$M'(\omega) = -M'(-\omega) \, , \tag{16a}$$

$$M''(\omega) = M''(-\omega) \, . \tag{16b}$$

Solving Eq. (14) for χ one obtains the representation of the susceptibility in terms of the memory function M,

$$\chi(z) = \chi_0 M(z)/[z + M(z)] \, , \tag{17a}$$

and with Eqs. (8) and (13) one finds for the conductivity

$$\sigma(z) = (i/4\pi)\,\omega_p^2/[z + M(z)] \, . \tag{17b}$$

The completely general and correct equations (17) provide a useful starting point for actual calculations of χ and σ. As is well known, an evaluation of response functions like $\chi(z)$ by straightforward expansion in a small parameter like a coupling constant or density usually fails because of the singular character of these functions for small frequencies z. On the other hand, ordinary hydrodynamics yield a simple description of linear response for slowly varying disturbances and provides us with the resonance structure of the correlation functions in the low-frequency regime.[11] In microscopic theories the hydrodynamic resonances are usually generated by deriving and solving integral equations like Boltzmann's equation or vertex equations. In doing so one proves the validity of hydrodynamic equations. Here we adopt the view that occasionally one can avoid solving transport equations by starting from a correct representation of susceptibilities in terms of memory functions such that the resonance structure is already built in. Evaluation of the memory functions by expanding in a small parameter then yields a result for the susceptibility valid for all frequencies including the hydrodynamical ones. If the memory functions have been introduced in a proper way they should tend to constants in the hydrodynamic regime and vary moderately with frequency in the nonhydrodynamic regime. This requirement serves as a consistency test during the actual calculations.

From Eqs. (15b) and (17b), one obtains

$$\sigma(\omega \pm i_0) = (e^2 N_e/m)\{i[\omega + M'(\omega)] \pm M''(\omega)\}/ \{[\omega + M'(\omega)]^2 + M''(\omega)^2\} . \tag{18}$$

To get into contact with the ordinary theory let us perform a Taylor expansion of M for small frequencies,

$$M(\omega \pm i0) = \pm i M''(0) + \omega \left(\frac{\partial}{\partial \omega} M'(\omega) \right)_{\omega=0} + O(\omega^2) , \tag{19}$$

where M'' and M' are real according to the symmetry relations Eqs. (16). Substituting this into Eq. (18) one finds

$$\sigma(\omega \pm i0) = (e^2 n/m) a [i\omega \pm 1/\tau]/[\omega^2 + (1/\tau)^2] , \tag{20a}$$

with

$$a = \left(1 + \frac{\partial}{\partial \omega} M'(\omega) \bigg|_{\omega=0} \right)^{-1} , \tag{20b}$$

$$1/\tau = a M''(0) . \tag{20c}$$

Equation (20a) is the usual Drude formula for the dynamical conductivity[2,3] with τ being the relaxation time for charge transport and a denoting a charge renormalization constant of value close to unity. The classical result (20a) is thus valid, whenever expansion (19) makes sense and $[\partial M'(\omega)/\partial\omega]_0$ is small compared to unity. Trivially, Eq. (20a) does not yield the correct high-frequency behavior, since (19) is in contradiction to the $1/z$ decrease of $M(z)$ for large z. Thus independent of the specific nature of the relaxation mechanism which the electrons are subject to there exists a limiting frequency above which the Drude formula does not hold.

For vanishing impurity concentrations and electron-phonon coupling D the total current j is a constant of motion; thus $\chi(z)$ and $M(z)$ vanish in this case. Assuming a regular dependence of M on c and D one can expand Eq. (17a),

$$z\chi(z) = \chi_0 M(z) + O(c^2, D^3) . \tag{21}$$

On the other hand one finds from Eq. (6c),

$$z \langle\langle j_1 ; j_1 \rangle\rangle = \langle\langle A ; j_1 \rangle\rangle , \tag{22}$$

with

$$A = [j_1, H'] . \tag{23}$$

Furthermore, from Eq. (6d) one obtains

$$z \langle\langle A ; j_1 \rangle\rangle = \langle [A, j_1] \rangle - \langle\langle A ; A \rangle\rangle . \tag{24}$$

From Eqs. (22) and (24) at $z = 0$ and Eq. (13) we have the identity

$$\langle [A, j_1] \rangle = \langle\langle A ; A \rangle\rangle_{z=0} . \tag{25}$$

Taking together Eqs. (21), (22), (24), (25), and (9) one arrives at

$$\chi_0 M(z) + O(c^2, D^3) = [\langle\langle A ; A \rangle\rangle_z - \langle\langle A ; A \rangle\rangle_{z=0}]/z . \tag{26}$$

Thus evaluations of the correlation function $\langle\langle A ; A \rangle\rangle$ in lowest order of the impurity concentration and electron-phonon coupling yield $M(z)$ in lowest order. Inserting Eqs. (4) into Eq. (21) we decompose A as a sum of three operators in an obvious way,

$$A = \sum_{\alpha=1}^{3} A_\alpha , \tag{27a}$$

and define

$$\phi_{\alpha\beta}(z) = \langle\langle A_\alpha ; A_\beta \rangle\rangle_z , \tag{27b}$$

where

$$A_\alpha = [j_1, H_\alpha] . \tag{27c}$$

Explicitly

$$A_\alpha = \textstyle\sum_j A_\alpha^j , \quad \alpha = 1, 2 \tag{28a}$$

with

$$A_1^j = N^{-1} \sum \langle \vec{k} | U_1^j | \vec{k}' \rangle [v_1(\vec{k}) - v_1(\vec{k}')] c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma} , \tag{28b}$$

$$A_2^j = N^{-1} \sum \langle \vec{k} | U_2^j | \vec{k}' \rangle [v_1(\vec{k}) - v_1(\vec{k}')] S_j^i s^i_{\sigma\sigma'} c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma'} . \tag{28c}$$

Those contributions in $\sum_{i,j} \langle\langle A_\alpha^i ; A_\beta^j \rangle\rangle$ with $i \neq j$ are proportional to c^2 and can be neglected in first approximation. Trivially, in first order in the concentration there are no correlation effects involving two or more impurities and all correlation functions have to be evaluated for a system with just one impurity, say at the origin, which we denote by $\langle\langle\ \rangle\rangle^0$. Then one obtains

$$\phi_{\alpha\beta}(z) = cN \langle\langle A_\alpha^0 ; A_\beta^0 \rangle\rangle_z^0 , \quad \alpha = 1, 2. \tag{29}$$

For the phonon part of the operator A one finds

$$A_3 = \sum [v_1(\vec{k}) - v_1(\vec{k}')] \times [D(\vec{k} - \vec{k}') c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma} b_{\vec{k}-\vec{k}'} - \text{H. c.}]. \tag{28d}$$

In lowest order we can neglect nondiagonal elements of $\phi_{\alpha\beta}$, which are due to interference of the different scattering mechanisms. From Eq. (26) we then arrive at

$$M(z) = [\phi(z) - \phi(z = 0)]/(z\chi_0) + O(c^2, D^3) , \tag{30}$$

with

$$\phi(z)=\sum_{\alpha=1}^{3}\phi_{\alpha\alpha}(z)\ .$$

This is the general final result for the memory function.[15] The calculation of the conductivity of the model system under consideration has been reduced to the evaluation of correlation functions of the electron gas in the presence of one impurity or phonons. The achievement is that $M(z)$ contrary to $\sigma(z)$ can be expanded in powers of impurity concentration or coupling constants for $z\to 0$. Derivation of Eqs. (17) and (30) corresponds to an infinite partial summation of diagrams for the conductivity including self-energy and vertex corrections or to deriving and approximately solving a generalized Boltzmann equation.

IV. APPROXIMATIONS FOR MEMORY FUNCTION

Because of the Coulomb interaction and the impurity-spin dynamics as well as the phonon dynamics, evaluation of the memory function M is a many-body problem and can be carried out only approximately. The complications one has to face depend on how realistic a model one wants to discuss. Since we have neglected band-structure effects from the very beginning it does not seem worthwhile to work out all details of $\phi(z)$. We rather want to demonstrate how easy the known results are reproduced and to indicate in which respect our approach can yield some new results.

A. Free-Electron Gas with Lowest-Order Potential Scattering

To get a first impression of $M(z)$ let us evaluate Eq. (30) for a noninteracting electron gas scattered by weak spin-independent impurity potentials. Treating the electron-impurity interaction in the Born approximation one finds from Eqs. (4d), (28b), and (29),

$$\phi(z)=cN^{-1}\sum_{\vec{k}\vec{k}'\sigma}\ \sum_{\vec{p}\vec{p}'\tau}\langle\vec{k}|U_1|\vec{k}'\rangle[v_1(\vec{k})-v_1(\vec{k}')]\times\langle\vec{p}|U_1|\vec{p}'\rangle(v_1(\vec{p})-v_1(\vec{p}'))\times\langle\langle c^\dagger_{\vec{k}\sigma}c_{\vec{k}'\sigma};\,c^\dagger_{\vec{p}\tau}c_{\vec{p}'\tau}\rangle\rangle\ , \tag{31}$$

where the correlation function on the right-hand side can be determined for the free-electron gas. Thus,

$$\phi(z)=(2c/3m^2N)\sum_{\vec{k}\vec{k}'}|\langle\vec{k}|U_1|\vec{k}'\rangle|^2(\vec{k}-\vec{k}')^2\times[f(\epsilon_{\vec{k}'})-f(\epsilon_{\vec{k}})]/(z-\epsilon_{\vec{k}'}+\epsilon_{\vec{k}})\ , \tag{32}$$

where $f(\epsilon_{\vec{k}})$ denotes the Fermi function of energy $\epsilon_{\vec{k}}$. Substituting $\phi(z)$ into Eq. (30) one obtains for the absorptive part of the memory function

$$M''(\omega)=\tfrac{2}{3}\pi(N_i/N_e)m^{-1}N^{-2}\sum_{\vec{k}\vec{k}'}|\langle\vec{k}|U|\vec{k}'\rangle|^2\times(\vec{k}-\vec{k}')^2\,\delta(\omega-\epsilon_{\vec{k}'}+\epsilon_{\vec{k}})[f(\epsilon_{\vec{k}})-f(\epsilon_{\vec{k}'})]/\omega\ . \tag{33}$$

To simplify further we neglect the momentum dependence of U and evaluate (33) for frequencies ω less than the Fermi energy ϵ_F. Then M'' turns out to be frequency independent,

$$M''(\omega)=\tfrac{2}{3}\pi(N_i/N_e)(U\rho_F)^2\epsilon_F\ , \tag{34}$$

where ρ_F denotes the density of states per volume at the Fermi level. Thus the Drude formula Eq. (20a) works well in this crude picture at least for $\omega\ll\epsilon_F$. The energy dependence of the density of states and the momentum dependence of the pseudopotential will yield variations of M'' with ω, but these deviations from the Drude formula are so small that it does not seem feasible to detect them experimentally. Thus one can take $a=1$ in Eq. (20b) and use the zero-frequency limit of Eq. (33) to obtain

$$1/\tau=N_i v_F\int\!\!\int d\Omega\,\sigma_{\rm sc}(\Omega)(1-\cos\theta)\ , \tag{35a}$$

where v_F is the Fermi velocity $v_F=k_F/m$ and $\sigma_{\rm sc}(\Omega)$ is the differential scattering cross section in the Born approximation,

$$\sigma_{\rm sc}(\Omega)=(\pi k_F)^2|\rho_F U(\vec{k}_F-\vec{k}'_F)|^2\ . \tag{35b}$$

This is the well-known[2] formula for the electron-transport relaxation time τ due to impurity scattering. One realizes that our approach incorporates in a quite simple way what would be called self-energy and vertex corrections in a diagrammatic analysis of $\sigma(z)$.

B. Free-Electron Gas with Lowest-Order Spin-Flip Scattering

Let us proceed in this subsection with an analysis of pure-spin-flip scattering in much the same way as in Sec. IV A. In the absence of external magnetic fields one expects the frequency dependence of M to be the same as in the nonmagnetic case, at least to lowest order in the scattering potential. However, if a magnetic field is present, spin-flip scattering is an inelastic process and consequently at low temperatures the memory function develops a threshold at the Zeeman frequency of the impurity spins. We want to demonstrate how this threshold behavior leads to characteristic deviations from Drude's formula. Using Eqs. (28c) and (29), one finds

$$\phi(z)=cN^{-1}\sum_{\vec{k}\vec{k}'}\sum_{\vec{p}\vec{p}'}J_{\vec{k}\vec{k}'}[v_1(\vec{k})-v_1(\vec{k}')]J_{\vec{p}'\vec{p}}[v_1(\vec{p}')-v_1(\vec{p})]\times\langle\langle c^\dagger_{\vec{k}\sigma}s^i_{\sigma\sigma'}c_{\vec{k}'\sigma'}S^i;\,c^\dagger_{\vec{p}'\tau'}s^j_{\tau'\tau}c_{\vec{p}\tau}S^j\rangle\rangle\ , \tag{36}$$

where we changed to the conventional notation used in the context of the s-d model in denoting the spin-flip matrix element $\langle\vec{k}|U_2|\vec{k}'\rangle$ by $J_{\vec{k}\vec{k}'}$. To calculate ϕ in lowest order of J we have to evaluate the correlation function on the right-hand side of (36) for the noninteracting system, viz.,

$$\phi(z)=\phi_0(z)+\phi_+(z)+\phi_-(z)\ , \tag{37a}$$

$$\phi_0(z)=\frac{c}{3m^2N}\sum_{\vec{k}\vec{k}'}|J_{\vec{k}\vec{k}'}|^2(\vec{k}-\vec{k}')^2 s^0_{\sigma\sigma'}s^0_{\sigma'\sigma}\times\langle S^{02}\rangle\frac{f'-f}{[z-\epsilon'+\epsilon]}\ , \tag{37b}$$

$$\phi_\pm(z)=-\frac{c}{3m^2N}\sum_{\vec{k}\vec{k}'}|J_{\vec{k}\vec{k}'}|^2(\vec{k}-\vec{k}')^2 s^\mp_{\sigma\sigma'}s^\pm_{\sigma'\sigma}\times\frac{[\langle S^\pm S^\mp\rangle(f-f')\pm\langle S^0\rangle f'(1-f)]}{z-\epsilon'+\epsilon_\mp h}\ . \tag{37c}$$

Here $\epsilon=\epsilon_{\vec{k}\sigma}$, $\epsilon'=\epsilon_{\vec{k}'\sigma'}$, $f=f(\epsilon)$, $f'=f(\epsilon')$. Obviously, $\phi_\pm(\phi_0)$ describes spin- (non-) flip processes. Using Eq. (30) we find quantities M_0, $M_\pm$ by substituting expressions (37). Neglecting the momentum dependence of J as well as the variation of the density of states with energy and restricting ourselves to $\omega\ll\epsilon_F$, the integrals in Eq. (37) may be easily done. Thus for the imaginary part of the spin-nonflip contribution M_0'' one finds similar to the normal-scattering case,

$$M_0''(\omega)=C\,\langle S^{02}\rangle\ , \tag{38a}$$

$$C=\tfrac{1}{6}\pi\,(N_i/N_e)\,(J\rho_F)^2\,\epsilon_F\ , \tag{38b}$$

which is frequency independent, while spin-flip scattering gives rise to frequency-dependent components

$$M_\pm''(\omega)=\tfrac{1}{2}C\,[S(S+1)-\langle S^{02}\rangle\pm\langle S^0\rangle\coth(\omega\mp h)/2T](\omega\mp h)/\omega\ . \tag{38c}$$

Summarizing, the absorptive part of the memory function is given by

$$M''(\omega)=C\left[S(S+1)+\tfrac{1}{2}\langle S_0\rangle\left(\frac{\omega-h}{\omega}\coth\frac{\omega-h}{2T}-(h\to-h)\right)\right]. \tag{39}$$

$M(z)$ is defined by its spectral density M'' and dispersion relation Eq. (7a). The function $F(z)=2[M(z)/C-\langle S^{02}\rangle]$ appeared to determine the impurity-spin relaxation in a calculation of the dynamical impurity-spin susceptibility.[1,16] In Ref. 16, $F(z)$ has been given in closed form in terms of digamma functions, and $F'(\omega)$ as well as $F''(\omega)$ are plotted for various values of h and T as a function of frequency. Here we want to discuss $M(z)$ by considering various limiting cases. Since M'' (M') is an even (odd) function of frequency by virtue of Eqs. (16) and (39) we confine the discussion to positive frequencies. One observes that $M''(\omega)$ is a monotonically increasing function of minimum value

$$M''(\omega=0)=C\left[S(S+1)-\langle S^0\rangle\frac{\partial}{\partial h}\left(h\coth\frac{h}{2T}\right)\right] \tag{40a}$$

and saturation value

$$M''(\omega=\infty)=CS(S+1)\ . \tag{40b}$$

For small h/T, $M''(\omega)$ is practically constant,

$$M''(\omega)=CS(S+1)\quad\text{for } h/T\ll 1, \tag{40c}$$

i.e., the spin-flip-scattering threshold is washed out completely by the thermal motion. Accordingly the conductivity is given by Drude's formula with Eqs. (40c), (39a), and (38b) inserted in Eq. (18).

On the other hand, for large h/T, $M''(\omega)$ shows a frequency dependence

$$M''(\omega)=C\times\begin{cases}S^2 & \text{if } |\omega|<h\\ S(S+1)-Sh/|\omega| & \text{if } |\omega|>h\end{cases}\qquad\text{for } h/T\gg 1, \tag{40d}$$

which is quite in accordance with the threshold behavior one would expect for spin-flip scattering at $T=0$ on physical grounds. The pronounced variation of M'' induces a sizable real part M' via dispersion relation Eq. (15a),

$$M'(\omega)=C(S/\pi)\,[(1+h/\omega)\ln|1+\omega/h|-(1-h/\omega)\ln|1-\omega/h|\,]\ . \tag{40e}$$

Thus in the limit of high field and/or low temperature a Drude description of the conductivity is not valid and we have to resort to the general formula, Eq. (18). However, some features of the dynamical conductivity at low frequencies may be discussed by employing the renormalized Drude formula, Eq. (20a). From Eqs. (19), (39), and (40) we find

$$\left.\frac{\partial M'(\omega)}{\partial\omega}\right|_{\omega=0}=(S\pi\tau_0 h)^{-1}\quad\text{for } h/T\gg 1\ , \tag{41a}$$

where the bare relaxation time τ_0 is given by

$$1/\tau_0=M''(0)=CS^2\quad\text{for } h/T\gg 1\ . \tag{41b}$$

At low temperatures, $1/\tau_0\gg T$, and consequently there exists a regime of h values satisfying

$$T\ll h\ll 1/\tau_0\ ,$$

such that $[\partial M'(\omega)/\partial\omega]_{\omega=0}$ as given by Eq. (41a) is much larger than 1 and the renormalization constant as defined by Eq. (20b) is to a good approximation $a\cong S\pi\tau_0 h$. The renormalized relaxation time τ [Eq. (20c)] turns out to be independent of the coupling constant

$$1/\tau=\pi Sh\quad\text{for } T\ll h\ll 1/\tau_0\ . \tag{41c}$$

Thus the real part of the conductivity, which is predicted to be a Lorentzian of width $1/\tau_0$ by Drude's formula, shrinks drastically to a width $1/\tau$ independent of the coupling strength, if a sufficiently strong magnetic field is applied. Similarly, the slope of the imaginary part of the conductivity at the origin increases with decreasing magnetic field. In Figs. 1(a) and 1(b) the real and imaginary parts of the conductivity, normalized to the static value, are plotted as a function of $\omega\tau_0$ for two values of magnetic field, as calculated from Eq. (18), using M'' and M' given by Eqs. (40d) and (40e) and taking $S=\frac{1}{2}$. It is worth mentioning that the sum rule on the real part of the conductivity $\int d\omega\,\sigma'(\omega)=\frac{1}{2}\omega_p^2$ is exactly fulfilled by any solution of the form Eq. (18) following from the analyticity requirements on $\chi(z)$ and $M(z)$. All other sum rules are satisfied to lowest order.

For dilute alloys of Mn in Cu with concentrations of about 0.6 at.% one expects [using the unitarity limit for $(\rho_F J)$ and taking $S=\frac{1}{2}$] $1/\tau_0$ to be of the order of 40 °K. At temperatures well below 6 °K a magnetic field of 60 kG would produce a situation sketched in Fig. 1(c).

If in addition to spin-flip scattering there is potential scattering either by the same or by different impurities, one has to add to (38c) a contribution given by Eq. (33). Then the anomalies will be suppressed to some extent.

C. Free-Electron Gas with Resonance Scattering

From the work of Plakida[9] it is known that resonance scattering of electrons by localized phonons produces anomalies in the frequency dependence of the conductivity. Let us examine a similar problem within the framework of our approach and model. We consider a noninteracting electron gas scattered by nonmagnetic impurities of dilute concentration. Contrary to Sec. IV A we drop the restriction to weak scattering potentials, so that Born's approximation is no longer adequate and multiple scattering by a single impurity has to be taken into account. Then Eq. (31) is valid, but the correlation function appearing on the right-hand side of this equation has to be calculated for a system with one impurity located, say, at the origin. The evaluation of this function can be reduced to solving a one-electron scattering problem.

According to Eq. (6c) the correlation function

$$R_{\vec{k}\vec{k}',\vec{p}\vec{p}'}(z)=\langle\langle c^\dagger_{\vec{k}}c_{\vec{k}'}\,;\;c^\dagger_{\vec{p}'}c_{\vec{p}}\rangle\rangle_z \tag{42a}$$

is determined by solving the equation of motion

$$(z-\epsilon_{\vec{k}'}+\epsilon_{\vec{k}})R_{\vec{k}\vec{k}',\vec{p}\vec{p}'}(z)=\delta_{\vec{k}',\vec{p}}\,\langle c^\dagger_{\vec{k}}c_{\vec{p}}\rangle-\delta_{\vec{k}\vec{p}}\langle c^\dagger_{\vec{p}'}c_{\vec{k}'}\rangle$$
$$-\sum_{\vec{k}''}\langle\vec{\mathrm{k}}'|U|\vec{\mathrm{k}}''\rangle R_{\vec{k}\vec{k}'',\vec{p}\vec{p}'}+\sum_{\vec{k}}\langle\vec{\mathrm{k}}''|U|\vec{\mathrm{k}}\rangle R_{\vec{k}''\mathrm{k}\vec{p}\vec{p}}\,. \tag{42b}$$

On the other hand, the usual one-particle Green's functions

$$G_{\vec{k}\vec{k}'}(z)=\langle\langle c_{\vec{k}}\,;\,c^\dagger_{\vec{k}'}\rangle\rangle_+ \tag{43a}$$

[the subscript + indicates that the anticommutator has to be used in the defining equation (6a)] obey the equations

$$(z-\epsilon_{\vec{k}})G_{\vec{k}\vec{k}'}(z)+\sum_{\vec{k}''}\langle\vec{\mathrm{k}}|U|\vec{\mathrm{k}}''\rangle G_{\vec{k}''\mathrm{k}'}(z)=\delta_{\vec{k}\vec{k}'}\,, \tag{43b}$$

$$(z+\epsilon_{\vec{k}'})G_{\vec{k}\vec{k}'}(z)-\sum_{\vec{k}''}\langle\vec{\mathrm{k}}''|U|\vec{\mathrm{k}}\rangle G_{\vec{k}\vec{k}''}(z)=\delta_{\vec{k}\vec{k}'}\,. \tag{43c}$$

The absorptive part of $G(z)$, which is defined according to Eq. (7b), determines the thermal aver-

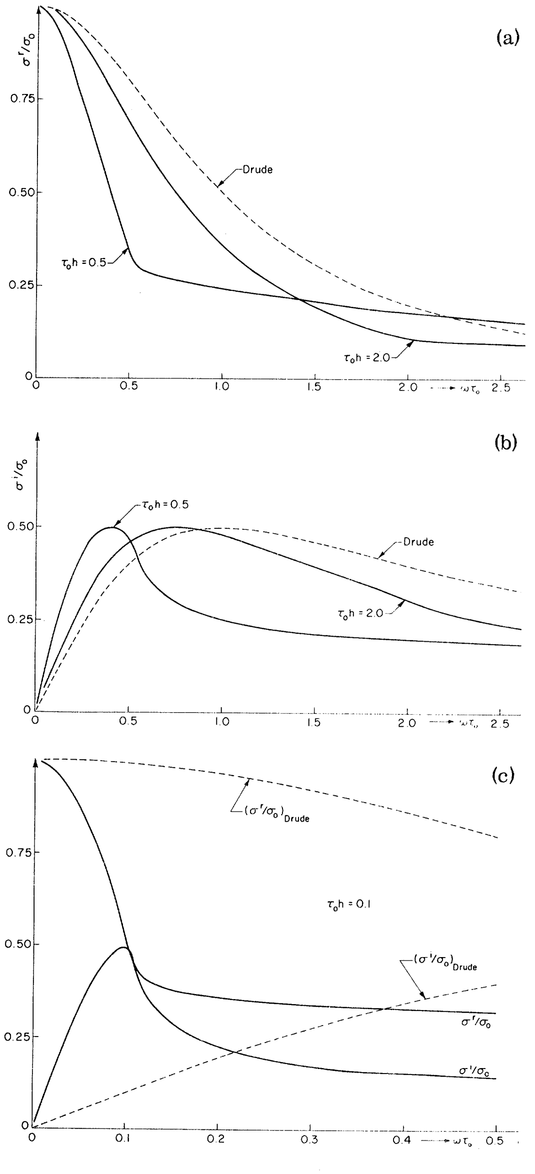

FIG. 1. Real part σ^r and imaginary part σ^i of the conductivity due to spin-flip scattering in a magnetic field [Eqs. (18), (40d), and (40e)], vs frequency, for low temperatures ($T \ll h$) and various values of magnetic field B. $1/\tau_0=M''(0)$ is the zero-frequency relaxation rate, σ_0 is the dc conductivity, and $h=g\mu_B B$ is the impurity Zeeman energy. The dashed curves are according to Drude's formula.

ages on the right-hand side of Eq. (42b) by

$$(-1/\pi)\int d\omega\, G''_{\vec{k}\vec{k}'}(\omega)f(\omega)=\langle c^{\dagger}_{\vec{k}'}c_{\vec{k}}\rangle\ . \tag{43d}$$

Furthermore,

$$(-1/\pi)\int d\omega\, G''_{\vec{k}\vec{k}'}(\omega)=\delta_{\vec{k}\vec{k}'}\ . \tag{43e}$$

Using Eqs. (43a)–(43e) one verifies that the solution of Eq. (42b) is given by

$$R_{\vec{k}\vec{k}',\vec{p}\vec{p}'}(z)=(1/\pi)^2\int d\epsilon'\, d\epsilon\, G''_{\vec{k}'\vec{p}'}(\epsilon')G''_{\vec{p}\vec{k}}(\epsilon)\times[f(\epsilon)-f(\epsilon')]/[z-\epsilon'+\epsilon]\ . \tag{44}$$

Hence R is expressed by one-electron propagators. We want to eliminate the bare interactions everywhere by introducing the scattering matrix t, which is defined in a standard fashion by

$$\langle\vec{k}|t(z)|\vec{k}'\rangle=\langle\vec{k}|U|\vec{k}'\rangle+\sum_{\vec{k}\vec{k}_1'}\langle\vec{k}|U|\vec{k}_1'\rangle g_{\vec{k}_1'\vec{k}_1}(z)\times\langle\vec{k}_1|t(z)|\vec{k}'\rangle\ , \tag{45a}$$

where g abbreviates the free propagator

$$g_{\vec{k}\vec{k}'}(z)=\delta_{\vec{k}\vec{k}'}/(z-\epsilon_{\vec{k}})\ . \tag{45b}$$

The renormalized Green's function is then given by

$$G_{\vec{k}\vec{k}'}(z)=g_{\vec{k}\vec{k}'}(z)+\sum_{\vec{k}_1\vec{k}_1'}g_{\vec{k}\vec{k}_1}(z)\langle\vec{k}_1|t(z)|\vec{k}_1'\rangle g_{\vec{k}_1'\vec{k}'}(z)\ . \tag{45c}$$

Substitution of Eqs. (44) and (45) into (31) yields

$$\phi(z)=cN\pi^{-2}\int d\epsilon'\, d\epsilon\, Y(\epsilon,\epsilon')\times[f(\epsilon)-f(\epsilon')]/[z-\epsilon'+\epsilon]\ , \tag{46a}$$

$$\begin{aligned}Y(\epsilon,\epsilon')=\tfrac{2}{3}(Nm)^{-2}\Big[&\sum_{\vec{k}\vec{p}}\langle\vec{k}|t''(\epsilon')|\vec{p}\rangle G''_{\vec{p}\vec{k}}(\epsilon)\vec{k}\cdot\vec{p}\\&-\sum_{\vec{k}\vec{p}'}\langle\vec{k}|(tg)''(\epsilon')|\vec{p}'\rangle\langle\vec{p}'|(tg)''(\epsilon)|\vec{k}\rangle\vec{k}\cdot\vec{p}'\\&-\sum_{\vec{k}'\mathrm{p}}\langle\vec{k}'|(gt)''(\epsilon')|\vec{p}\rangle\langle\vec{p}|(gt)''(\epsilon)|\vec{k}'\rangle\vec{k}'\cdot\vec{p}\\&+\sum_{\vec{k}'\vec{p}'}G''_{\vec{k}'\vec{p}'}(\epsilon')\langle\vec{p}'|t''(\epsilon)|\vec{k}'\rangle\vec{k}'\cdot\vec{p}'\Big]\ .\end{aligned} \tag{46b}$$

Here the factor of 2 is due to a sum on spins and an obvious matrix notation has been used. Let us evaluate some of the discontinuities in Eq. (46b):

$$Y(\epsilon,\epsilon')=Y_1(\epsilon,\epsilon')+Y_2(\epsilon,\epsilon')\ , \tag{47a}$$

$$\begin{aligned}Y_1(\epsilon,\epsilon')=-\tfrac{2}{3}\pi(Nm)^{-2}\Big[&\sum_{\vec{k}}\langle\vec{k}|t''(\epsilon')|\vec{k}\rangle\delta(\epsilon-\epsilon_{\vec{k}})\vec{k}^2+\sum_{\vec{k}'}\delta(\epsilon'-\epsilon_{\vec{k}'})\langle\vec{k}'|t''(\epsilon)|\vec{k}'\rangle\vec{k}'^2+\pi\sum_{\vec{k}\vec{p}'}\langle\vec{k}|t(\epsilon_+')|\vec{p}'\rangle\langle\vec{p}'|t(\epsilon_-)|\vec{k}\rangle\\&\times\delta(\epsilon'-\epsilon_{\vec{p}'})\delta(\epsilon-\epsilon_{\vec{k}})\vec{k}\cdot\vec{p}'+\pi\sum_{\vec{k}'\vec{p}}\langle\vec{k}'|t(\epsilon_-')|\vec{p}\rangle\langle\vec{p}|t(\epsilon_+)|\vec{k}'\rangle\delta(\epsilon'-\epsilon_{\vec{k}'})\delta(\epsilon-\epsilon_{\vec{p}})\vec{k}'\cdot\vec{p}\Big]\ ,\end{aligned} \tag{47b}$$

$$\begin{aligned}Y_2(\epsilon,\epsilon')=\tfrac{2}{3}(Nm)^{-2}\Big\{&\sum_{\vec{k}\vec{p}}\vec{k}\cdot\vec{p}\,\langle\vec{k}|t''(\epsilon')|\vec{p}\rangle\langle\vec{p}|(gtg)''(\epsilon)|\vec{k}\rangle+\sum_{\vec{k}'\vec{p}'}\vec{k}'\cdot\vec{p}'\,\langle\vec{k}'|(gtg)''(\epsilon')|\vec{p}'\rangle\langle\vec{p}'|t''(\epsilon)|\vec{k}'\rangle\\&-\sum_{\vec{k}\vec{p}'}\vec{k}\cdot\vec{p}'\big[\langle\vec{k}|t''(\epsilon')g(\epsilon_-')|\vec{p}'\rangle\langle\vec{p}'|(tg)''(\epsilon)|\vec{k}\rangle+\langle\vec{k}|t(\epsilon_+')g''(\epsilon')|\vec{p}'\rangle\langle\vec{p}'|t''(\epsilon)g(\epsilon_+)|\vec{k}\rangle\big]\\&-\sum_{\vec{k}'\vec{p}}\vec{k}'\cdot\vec{p}\big[\langle\vec{k}'|(gt)''(\epsilon')|\vec{p}\rangle\langle\vec{p}|g(\epsilon_-)t''(\epsilon)|\vec{k}'\rangle+\langle\vec{k}'|g(\epsilon_+')t''(\epsilon')|\vec{p}\rangle\langle\vec{p}|g''(\epsilon)t(\epsilon_+)|\vec{k}'\rangle\big]\Big\}\ .\end{aligned} \tag{47c}$$

The discontinuity of the t matrix can be expressed by means of the optical theorem

$$\begin{aligned}\langle\vec{k}|t''(\epsilon)|\vec{k}'\rangle&=\langle\vec{k}|t(\epsilon_+)g''(\epsilon)t(\epsilon_-)|\vec{k}'\rangle\\&=\langle\vec{k}|t(\epsilon_-)g''(\epsilon)t(\epsilon_+)|\vec{k}'\rangle\ .\end{aligned} \tag{47d}$$

Here $\epsilon_\pm$ indicates that the upper or lower boundary value of the t matrix in the complex energy plane has to be taken.

Substitution of Eq. (46a) into Eq. (30) yields for the absorptive part of the memory function

$$M''(\omega)=(N_i/N_e)m(1/\pi)\int d\epsilon'\, d\epsilon\, Y(\epsilon,\epsilon')\times\delta(\omega+\epsilon-\epsilon')[f(\epsilon)-f(\epsilon')]/\omega\ . \tag{47e}$$

For a noninteracting-electron gas Eqs. (47a)–(47e) are the exact linear in c expression for $M''(\omega)$. The calculation of the dynamical conductivity has been reduced to the evaluation of some integrals over products of the electron-impurity scattering matrix.

Equations (47a)–(47e) are not very transparent and therefore we consider two special cases in the following. First, we evaluate the static limit for zero temperature. Observing that

$$Y_2(0,0)=0 \tag{48a}$$

and using Eq. (47d), one arrives at

$$M''(0)=1/\tau_0=(N_i/N_e)(m/\pi)Y_1(0,0)\ , \tag{48b}$$

$$Y_1(0,0)=\tfrac{2}{3}\pi^2(Nm)^{-2}\sum_{\vec{k}\vec{k}'}|\langle\vec{k}|t(0_+)|\vec{k}'\rangle|^2\times(\vec{k}-\vec{k}')^2\delta(\epsilon_{\vec{k}})\delta(\epsilon_{\vec{k}'})\ . \tag{48c}$$

Comparing Eqs. (48) with Eq. (33) we notice that the bare interaction matrix element has been replaced by the scattering matrix at the Fermi energy. Thus Eq. (35) holds, where σ_{sc} now denotes the correct electron-impurity cross section.

Second, let us assume a scattering resonance for a certain angular momentum, which we want to describe by a Breit-Wigner formula. The momentum dependence of the scattering matrix does not seem to be important in this case and as a first approximation we neglect it completely. Then the first two terms of Eq. (47b) are the only contributions to $Y(\epsilon, \epsilon')$. Again employing Eq. (47d), one finds

$$Y(\epsilon, \epsilon') = (\pi^2/3m)\left[(\epsilon+\epsilon_F)\left|\rho_F t(\epsilon')\right|^2 + (\epsilon'+\epsilon_F)\left|\rho_F t(\epsilon)\right|^2\right]. \tag{49a}$$

and

$$\rho_F t(\epsilon_\pm) = (1/\pi)\,\Gamma/(\epsilon-\epsilon_0 \pm i\Gamma)\ . \tag{49b}$$

Here ϵ_0 and Γ denote position and width of the resonance. Substituting these expressions into Eq. (47e) one finds for low temperatures ($T \ll \Gamma$)

$$M''(\omega) = \frac{1}{3\pi}\,\frac{N_i}{N_e}\,\Gamma^2\left(\frac{1}{2\omega}\ln\frac{(\omega-\epsilon_0)^2+\Gamma^2}{(\omega+\epsilon_0)^2+\Gamma^2} - \frac{2}{\Gamma}\tan^{-1}\frac{\epsilon_0}{\Gamma} + \frac{\epsilon_F+\epsilon_0+\omega}{\omega\Gamma}\tan^{-1}\frac{\epsilon_0+\omega}{\Gamma} - \frac{\epsilon_F+\epsilon_0-\omega}{\omega\Gamma}\tan^{-1}\frac{\epsilon_0-\omega}{\Gamma}\right)\ . \tag{49c}$$

The real part is determined by the dispersion relation Eq. (15a). There are anomalies near the resonance energy ϵ_0.

To simplify the discussion let us specialize Eq. (49b) by assuming the resonance to occur at the Fermi energy. Then

$$M''(\omega) = (2/3\pi)\,(N_i/N_e)\,\epsilon_F(\Gamma/\omega)\tan^{-1}(\omega/\Gamma)\ . \tag{50}$$

Since Eq. (49b) cannot be taken literally anyway, we replace M'' by a more convenient function of a similar ω dependence and write

$$M(\omega \pm i0) = -(2/3\pi)\,(N_i/N_e)\,\epsilon_F\,\delta/(\omega \pm i\delta)\ , \tag{51}$$

where δ is close to Γ.

If the resonance width δ is large compared to the zero-frequency relaxation rate $M''(0) = 1/\tau_0$, the conductivity due to Eqs. (51) and (17b) agrees well with Drude's formula. If, however, $\tau_0\delta$ is of order one the real part of the conductivity is larger than one would find from Drude's result [see Fig. 2(a)]; the imaginary part is suppressed and can be negative [see Fig. 2(b)]. For simple metals with normal impurities one can hardly expect resonances sharp enough to test our results. However, Eq. (51) might be an approximation for dilute magnetic alloys under conditions where the Kondo effect is present. In this case δ will approximately be given by the Kondo temperature and situations with $\tau_0\delta < 1$ can be realized. Indeed, results for the dynamical conductivity similar to Figs. 2(a) and 2(b) have been found in Ref. 17. There the Bloomfield-Hamann expression for the t matrix in the s-d model has been used to calculate $\sigma(\omega)$ by standard methods. Anomalies of this kind have been observed recently in the far-infrared surface resistance of *Cu*Fe.[18]

D. Free-Electron Gas with Phonon Scattering

It is well known from the work of Holstein[12] that an ideally pure metal at zero temperature, although possessing vanishing electrical resistance in the static limit, shows some finite resistance for finite frequencies. This is attributed to electron-phonon scattering processes in the bulk, in which phonons are created. (There is also a contribution from surface scattering which we wish to discard here.) Thus one may expect a strongly frequency-dependent memory function in this case and our approach proves to be very useful. Treating the electron-phonon interaction in the Born approximation, we find from Eqs. (27b) and (28d)

$$\phi(z) = -\sum_{\vec{k}\vec{k}'\vec{p}\vec{p}'}[v_1(\vec{k})-v_1(\vec{k}')][v_1(\vec{p})-v_1(\vec{p}')] \times [D(\vec{k}-\vec{k}')D^*(\vec{p}-\vec{p}') \times \langle\langle c^\dagger_{\vec{k}\sigma}c_{\vec{k}'\sigma}b_{\vec{k}-\vec{k}'}\,;\,c^\dagger_{\vec{p}\tau}c_{\vec{p}'\tau}b^\dagger_{\vec{p}-\vec{p}'}\rangle\rangle + \text{c. c.}\,]\ . \tag{52}$$

In Eq. (52) the correlation function on the right-hand side has to be evaluated in the absence of electron-phonon interaction. Simplifying further we drop the electron-electron interaction, too, and using the equation of motion Eq. (6c), we obtain

$$\phi(z) = -\tfrac{2}{3}m^{-2}\sum_{\vec{k}\vec{k}'}\left|D(\vec{k}-\vec{k}')\right|^2(\vec{k}-\vec{k}')^2 \times [f(1-f')(1+n)-(1-f)f'n] \times [(\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}-\omega_{\vec{k}-\vec{k}'}+z)^{-1}+(\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}-\omega_{\vec{k}-\vec{k}'}-z)^{-1}]\ , \tag{53a}$$

where f, f', (n) denotes the Fermi (Bose) function of argument $\epsilon_{\vec{k}}$, $\epsilon_{\vec{k}'}$, ($\omega_{\vec{k}-\vec{k}'}$). Substituting Eq. (53a) into Eq. (30) one finds for the absorptive part of the memory function

$$M''(\omega) = \tfrac{2}{3}\pi\,(mN_e)^{-1}\sum_{\vec{k}\vec{k}'}\left|D(\vec{k}-\vec{k}')\right|^2(\vec{k}-\vec{k}')^2 \times (1-f)f'n[\omega^{-1}(e^{\omega/T}-1)\,\delta\,(\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}-\omega_{\vec{k}-\vec{k}'}+\omega) + (\text{terms with } \omega \rightarrow -\omega)]\ . \tag{53b}$$

For $\omega \ll \epsilon_F$ we can carry out the $\vec{k}$, $\vec{k}'$ sums in standard fashion. Inserting expression (4f) for D and observing that $|\vec{k}|$ and $|\vec{k}'|$ are pinned to the Fermi surface due to the presence of the Fermi factors we do the $\epsilon_{\vec{k}}$, $\epsilon_{\vec{k}'}$ integrations first. The remaining angular integration is conventionally formulated in terms of the phonon wave vector

$\vec{q}[\,q^2=(\vec{k}-\vec{k}')^2\sim 2k_F^2(1-\cos\theta)]$:

$$M''(\omega)=\tfrac{1}{8}\pi^3(mm_i Nk_f^5)^{-1}\rho_F^2\int_0^{q_D} dq\, q^5|C(q)|^2\omega_q^{-1}$$

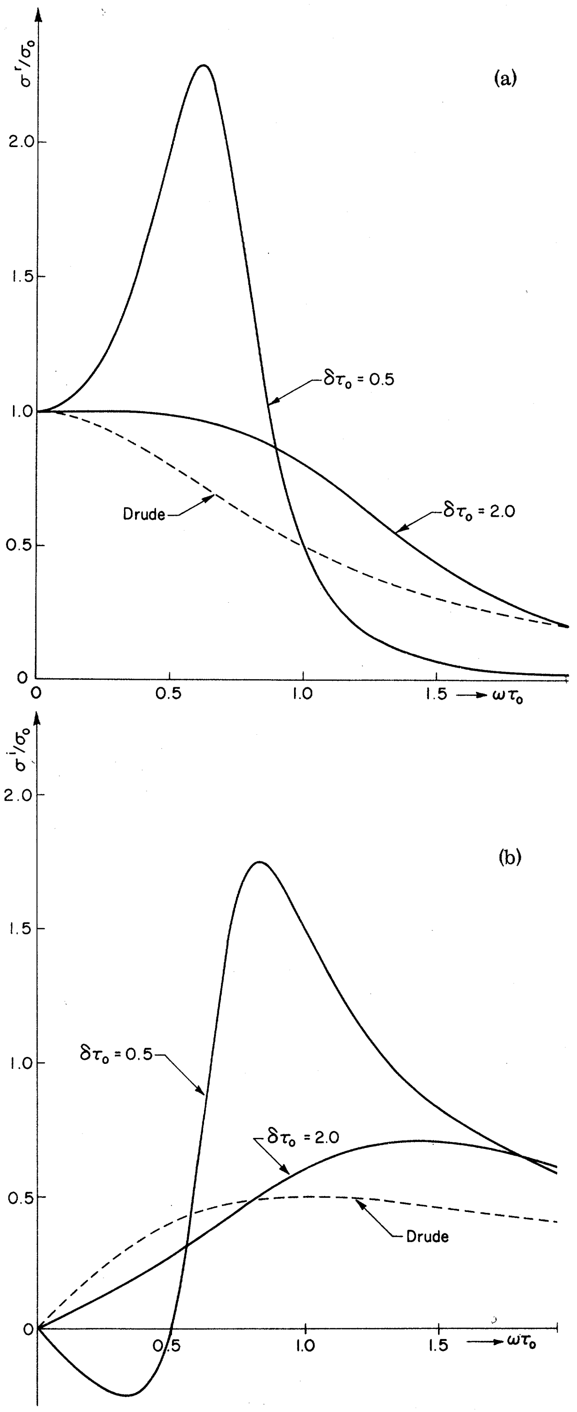

FIG. 2. Real part (a) and imaginary part (b) of the conductivity due to impurity-resonance scattering [Eqs. (18) and (51)], vs frequency. $1/\tau_0$ is the zero-frequency relaxation rate, σ_0 is the dc conductivity, and δ denotes the resonance width. The dashed curves are according to Drude's formula.

$$\times(e^{\omega_q/T}-1)^{-1}\{(1-\omega_q/\omega)(e^{\omega/T}-1)/[e^{(\omega-\omega_q)/T}-1]$$
$$+\text{(terms with } \omega\to-\omega)\}\,. \qquad (54a)$$

Here q_D is the Debye wave vector.

To discuss Eq. (54a) further we neglect phonon dispersion assuming a Debye spectrum $\omega_q=cq$ and take $C(q)$ to be constant $C(q)=1/\rho_F$.[2] Then one finds for the zero-frequency limit of Eq. (54a),

$$M''(0)=(\tfrac{1}{4}\pi^3)(q_D^6/mm_i Nk_F^5\Theta_D)(T/\Theta_D)^5 J_5(\Theta_D/T)\,, \qquad (54b)$$

where

$$J_5(y)=\int_0^y dx\, x^5 e^x/(e^x-1)^2$$
$$=\begin{cases}\tfrac{1}{4}y^4 & \text{for } y\to 0\\ 5\,!\,\zeta(5)\simeq 124.4 & \text{for } y\to\infty\end{cases}$$

is a Debye integral ($\Theta_D=cq_D$ is the Debye temperature). The result (54b), when substituted into Eq. (18), leads to the well-known Bloch formula for the electron-phonon conductivity.[2] Thus our approach enables one to obtain this important result of the transport theory of metals without invoking Boltzmann's equation and a variational principle to solve it approximately.

We proceed with evaluating Eq. (54a) in the high-frequency limit $\omega\gg\Theta_D$, T using again the approximation which led to Eq. (54b). The result is

$$M''(\omega)=(\tfrac{1}{4}\pi^3)(q_D^6/mm_i Nk_F^5\Theta_D)(T/\Theta_D)^5 J(\Theta_D/T)$$
$$\text{for } \omega\gg\Theta_D,\ T\,, \qquad (54c)$$
$$J(y)=\frac{1}{2}\int_0^y dx\, x^4\coth\tfrac{1}{2}x=\begin{cases}\tfrac{1}{10}y^5 & \text{for } y\to\infty\\ \tfrac{1}{4}y^4 & \text{for } y\to 0\,.\end{cases}$$

Comparing Eq. (54c) with (54b) one notices that at high temperatures ($T\gg\Theta_D$) the high-frequency value of M'' coincides with its static limit. Indeed, a high-temperature expansion of (54a) yields a frequency-independent M''. At low temperatures, however, we find the behavior predicted by Holstein. While $M''(0)$ vanishes as T^5, $M''(\omega)$ attains a temperature-independent value for frequencies large compared to the Debye frequency.

To show the frequency dependence of $M''(\omega)$ at low temperatures more explicitly, we evaluate Eq. (54a) at zero temperature within the simple Debye model,

$$M''(\omega)=(\pi^3 q_D^6/240mm_i Nk_F^5\Theta_D)$$
$$\times\begin{cases}(\omega/\Theta_D)^5 & \text{for } |\omega|<\Theta_D\\ 6-5\omega_D/\omega) & \text{for } |\omega|>\Theta_D\,.\end{cases} \qquad (54d)$$

The real part may be obtained via dispersion relation Eq. (15a).

It is clear that $M''(\omega)$ as given by Eq. (54d), if substituted into Eq. (18), gives rise to strong deviations from the Drude behavior of the conductivity. These deviations have been detected experimentally in the far-infrared absorptivity of lead.[19,20] A theoretical explanation of these experiments based on Holstein's electron-phonon Boltzmann equation has been given.[21,22] The results of Ref. 22 reduce to ours in the weak-coupling limit and for $q=0$. In Ref. 23 a discussion of the frequency-dependent conductivity of electron-phonon systems is given, which appears to be very similar to ours. However, due to the fact that the quantity $1/\tau(\omega)$ in Ref. 23, which corresponds to $M(z)$ in this paper, is taken to be real, the resulting expression for $\sigma(\omega)$ fails to satisfy analyticity requirements, as was pointed out in Ref. 24.

E. Weak-Potential Scattering and Interacting-Electron Gas

As final example we consider potential scattering of the interacting-electron gas by a small local pseudopotential $U(\vec{q})$. From Eqs. (28b) and (29), one obtains

$$\phi(z)=-2\sum_{\vec{q}}(\vec{q}^{\,2}/3m^2)\,|\,U(\vec{q})\,|^2\chi_{\rho\rho}(\vec{q},z)\,, \tag{55a}$$

where

$$\chi_{\rho\rho}(\vec{q},z)=\langle\langle\rho_{\vec{q}}\,;\ \rho^{*}_{\vec{q}}\rangle\rangle\,, \tag{55b}$$

$$\rho_{\vec{q}}=\sum_{\vec{p}}c^{\dagger}_{\vec{p}+\vec{q}}c_{\vec{p}}\,. \tag{55c}$$

$\chi_{\rho\rho}$ denotes the density-density correlation function of the interacting-electron gas without impurities. $\chi_{\rho\rho}$ is related to the longitudinal dielectric constant[3] by

$$\epsilon^{-1}(q,z)=1+(4\pi e^2/q^2)\,\chi_{\rho\rho}(q,z)\,. \tag{55d}$$

Substituting these results into Eq. (30) one arrives at a formula for the memory function M,

$$M(z)=\frac{2}{3}\,\frac{N_i}{N_e^2}\,\omega_p^2\int\frac{d^3q}{(2\pi)^3}\,|\,Q(q)\,|^2\times\frac{\epsilon^{-1}(q,0)-\epsilon^{-1}(q,z)}{z}\,. \tag{55e}$$

A formula of this type for the high-frequency relaxation has been obtained earlier in another context.[25,26] In (55e) Q abbreviates the quotient of the pseudopotential U and the Coulomb potential

$$Q(q)=U(q)\,q^2/4\pi e^2\,. \tag{55f}$$

The zero-frequency limit of $M(z)$ is found by exploiting the expansion of ϵ for small ω[3]

$$\epsilon(q,\omega\pm i0)=1+\frac{q_s^2}{q^2}\pm\frac{i\frac{1}{2}\pi\,(q_s^2/q^2)\omega}{(qv_F)}+\cdots\,, \tag{56a}$$

where $v_F=k_F/m$ denotes the Fermi velocity and q_s is the screening wave vector. Hence,

$$M(\pm i0)=\pm i\,\tfrac{3}{16}\pi(N_i/N_e)(q_s^2v_F^2/3\omega_p^2)\,(\omega_p^4/\epsilon_F^3)\times\int_0^{2k_F}dq\,q^3\,|\,Q(q)\,|^2/(q^2+q_s^2)^2\,. \tag{56b}$$

In the Thomas-Fermi approximation for the screening wave vector, $q_s^2=3\omega_p^2/v_F^2$ and replacing $U(q)$ by the bare Coulomb potential for charge Z (i.e., $Q=Z$) in Eq. (55e) one recovers the Mott-Jones formula[2] for the electron-relaxation frequency $1/\tau$.

To discuss the frequency dependence of $M(z)$ in detail, we set $Q=1$ and use the RPA expression for $\epsilon^{-1}(q,z)$ in the right-hand side of Eq. (55e), viz.,

$$\epsilon^{-1}(q,z)-1=\frac{(4\pi e^2/q^2)\chi^0_{\rho\rho}(q,z)}{1-(4\pi e^2/q^2)\chi^0_{\rho\rho}(q,z)}\,, \tag{57a}$$

with $\chi^0_{\rho\rho}$ abbreviating the density correlation function for the noninteracting-electron gas. Then one finds at zero temperature

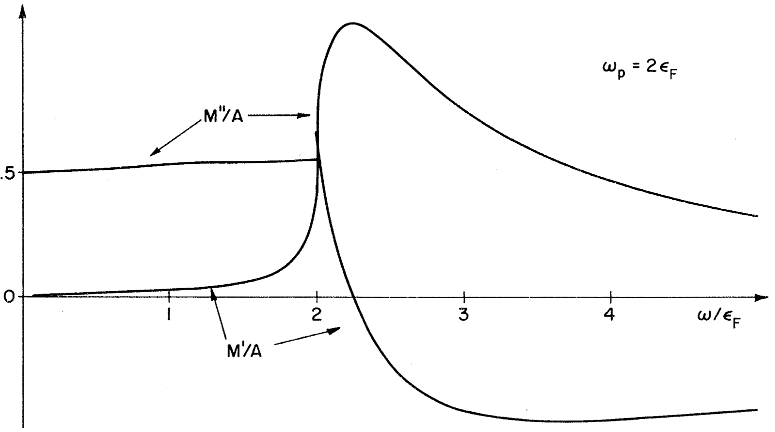

FIG. 3. Real part M' and imaginary part M'' of the relaxation function in RPA [Eqs. (57)], normalized to $A=2M''(0)$, vs frequency. ϵ_F denotes the Fermi energy, and the electron-gas density has been chosen such that the plasmon resonance ω_p occurs at $2\epsilon_F$.

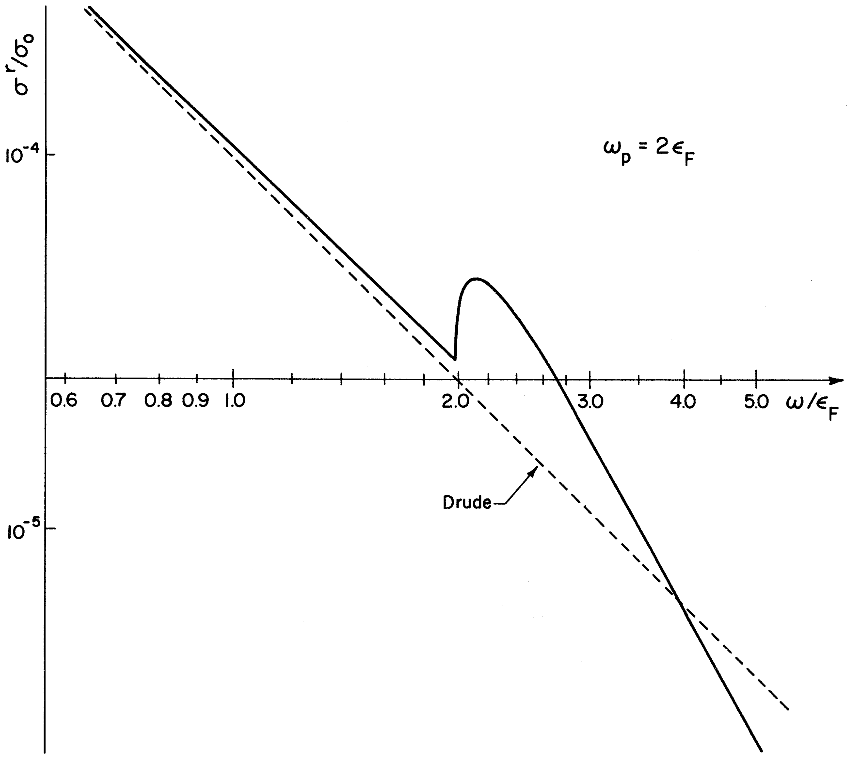

FIG. 4. Real part of the conductivity with relaxation function in RPA. Parameters as in Fig. 3. σ_0 denotes the dc conductivity and the dashed curve represents Drude's formula.

$$M(z) = \frac{A[F(z/\epsilon_F) - F(0)]}{z/\epsilon_f}, \tag{57b}$$

$$F(y) = \int dx\, x^2 f(x, y)/[x^2 + f(x, y)], \tag{57c}$$

with $f(x, y)$ denoting the Lindhard function

$$f(x, y) = \tfrac{1}{2}x_0^2 (1 + (2x)^{-3}\{[(y + x^2)^2 - (2x)^2] \times \ln[(y + x^2 - 2x)/(y + x^2 + 2x)] + [\text{terms with } y \rightarrow -y]\}) \tag{57d}$$

and

$$x_0 = q_s/k_F = (\omega_p/\epsilon_F)(\tfrac{3}{4})^{1/2},$$

$$A = (\tfrac{4}{3})(N_i/N_e)x_0^2 \epsilon_F .$$

The integrand in Eq. (57c) exhibits a pole at the plasmon frequency, giving rise to a square-root-type singularity of $F(y)$. Using the asymptotic expansion[3] of $f(x, y)$ for $x/y \ll 1$, one finds for z close to ω_p

$$[M(z) - M(\omega_p)] = -\tfrac{1}{4}\pi A(5\omega_p/6\epsilon_F)^{3/2}[(\omega_p - z)/\epsilon_F]^{1/2}. \tag{57e}$$

In Fig. 3 the real and imaginary parts of the memory function M are plotted as calculated from Eqs. (57a)-(57e). For frequencies below ω_p the absorptive part M'' increases very slowly only. At the plasma resonance the screening breaks down, the electrons feel the bare Coulomb potential and M'' increases by a factor of 2. For very large frequencies M'' tends to zero as $1/\omega^2$. The real part M' shows a peak near ω_p. The conductivity according to Eq. (18) is plotted in Fig. 4. For frequencies below ϵ_F (or ω_p) deviations from Drude's formula are not larger than 5-10%. At ω_p, however, the breakdown of the screening of the charged impurities affects the real part of the conductivity quite drastically. Indeed, as may be seen from Fig. 4, σ^r increases by 70% in the vicinity of ω_p and falls off as $1/\omega^4$ for increasing ω. Since M''/ϵ_F is a small quantity, the imaginary part σ^i is not much influenced. We suggest to investigate these predicted anomalies by measuring the light absorption of thin films of metals with charged impurities for frequencies above ω_p. Since ω_p is always very much larger than $1/\tau$, the anomalies described above can be obtained by applying standard perturbation theory.[25-27]

ACKNOWLEDGMENTS

We gratefully acknowledge discussions with Professor W. Brenig, Professor J. W. Wilkins, and Dr. G. Brändli.

*Work supported [illegible] part by the U. S. Office of Naval Research under Contract No. N00014-67-A-0077-0010, Technical Report No. 20, and by the Max-Planck-Gesellschaft zur Förderung der Wissenschaften.

†On leave from Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany.

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