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Spin-fluctuation contribution to the high-frequency electrical conductivity of nearly magnetic transition metals

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The high-frequency limit of the electrical conductivity of nonmagnetic transition metals is calculated. The conduction electrons are assumed to be scattered by the spin fluctuations in the partially filled d bands. The frequency-dependent conductivity has a Drude-type form, in which the scattering rate is itself frequency dependent. The scattering rate is increased as the magnetic susceptibility is enhanced by the spin fluctuations. The scattering rate exhibits a complicated frequency and temperature dependence. However, in the dc limit it does follow the low-temperature T^2 law of electron-electron collisions followed at higher temperatures by a linear dependence on T. On the other hand, at $T=0$, the scattering rate is proportional to ω^2 for low frequency.

I. INTRODUCTION

The properties of transition metals have been the subject of extensive research. As with most metals, many of them undergo transitions, either to a magnetically ordered phase or to a superconducting phase. Except in rare cases, the magnetic ordering precludes further transitions to a superconducting phase. There is a small, but important, class of transition metals and alloys which remain paramagnetic and nonsuperconducting down to the lowest measured temperatures. In these systems it is believed that the interaction responsible for magnetic ordering is just too feeble to produce a phase transition, but strong enough to produce low-frequency spin fluctuations. These spin fluctuations are local regions in which there is magnetic order, but they are formed and decay over long periods of time. At low temperatures these collective excitations are good bosonlike elementary excitations of the system. These spin fluctuations are held as being responsible for suppressing s-wave superconductivity in these systems (Berk and Schrieffer[1]).

The spin fluctuations are also expected to manifest themselves in other properties: The dynamic susceptibility should be peaked at low frequencies (Izuyama, Kim, and Kubo[2] and Doniach[3]) and the specific heat should exhibit a large-γ T term (Berk and Schrieffer[1] and Doniach and Engelsberg[4]). The spin-fluctuation contribution to the electrical dc conductivity (Lederer and Mills,[5,6] Rice,[7] and Kaiser and Doniach[8]) should give rise to a T^2 law characteristic of electron-electron scattering. This is in quantitative agreement with the experimentally measured low-temperature dc conductivity (Schindler and Coles[9]).

In this paper we calculate the high-frequency electrical conductivity for these materials. The ac conductivity can be observed from optical-absorption measurements at the infrared end of the spectrum. Our results can be expressed in the form of an intraband Drude conductivity. The scattering time, however, is different from the scattering time which enters the expression for the dc conductivity in that it is frequency dependent. In general, the ac scattering rate is larger than the dc scattering rate and can have different temperature dependencies. The scattering rate does reduce, in the limit of zero frequency, to the usual T^2 dependence characteristic of the phase space available for electron-electron scattering, followed at higher temperatures by a linear dependence on T.

In Sec. II we shall introduce the model of the system and summarize some relevant features of the spin fluctuations. The high-frequency limit of the electrical conductivity is calculated in Sec. III. The calculation proceeds within the framework in which the spin fluctuations are treated by the random-phase approximation (RPA). It is established that it is not sufficient to calculate the transport scattering weight, due to emission or absorption of spin waves, utilizing the Fermi golden rule. It is shown that, in a conserving approximation, other processes representing the scattering of the spin fluctuations can combine and cancel with the terms calculated from the Fermi golden rule, in the absence of umklapp scattering. Physically, this means that in the steady state both the spin fluctuations and the electrons are dragged out of equilibrium by the electric field. The spin fluctuations do not act as a momentum sink as implied in the Fermi golden-rule calculation. In the presence of umklapp scattering processes, the crystal as a whole is able to absorb momentum and a finite transport scattering rate results. In Sec. IV the results of the calculation and its implications are discussed. We examine some special limits of the ac scattering rate and compare the results to those of the dc scattering rate found in other theories of the electrical conductivity.

II. THE MODEL

We shall be considering the high-frequency electrical conductivity in pure, paramagnetic transition-metal compounds. In these materials there exist degenerate, partially occupied d bands, which strongly hybridize with conduction bands of s and p character. Since the d-band wave functions retain a significant amount of the character of the localized atomic d orbitals, two electrons within the Wannier orbitals of the same lattice site experience large Coulombic interactions. It is these Coulomb interactions between the d electrons which are responsible for the magnetic properties of the transition metals.

We shall model this system by a single hybrid band, the states in which both have itinerant and local character, and the electrons interact via a local Coulomb repulsion U_{dd}. This picture should be contrasted with the two band models used by Lederer and Mills[5] and by Kaiser and Doniach.[8] In those two band pictures the conductivity occurs in a conduction band of s character, while the spin fluctuations occur in the d band. The conduction electrons are scattered from the d-band spin fluctuation via a weak interaction that could be envisaged as a Schrieffer-Wolf type of exchange interaction that involves the hybridization of the bands. Our picture is that of strongly hybridized bands and is complementary to that of Lederer and Mills,[5] namely for two weakly hybridized bands.

The Hamiltonian is written as the sum of two parts:

$$\hat{H}=\hat{H}_0+\hat{H}_1 \ . \tag{2.1a}$$

The term $\hat{H}_0$ describes the motion of the noninteracting electrons in a nondegenerate hybridized band. It is expressed as

$$\hat{H}_0=\sum_{\vec{k}_\sigma}\epsilon(\vec{k})d_{\vec{k}_\sigma}d_{\vec{k}_\sigma} \ , \tag{2.1b}$$

where $d^\dagger_{\vec{k}_\sigma}$ and $d_{\vec{k}_\sigma}$, respectively, create and destroy an electron of spin σ in the state labeled by the Bloch wave vector $\vec{k}$. The interaction between two electrons within the same Wannier orbitals is described by H_1, and is written as

$$\hat{H}_1=\frac{U_{dd}}{2}\sum_{i\sigma}d^\dagger_{i\sigma}d^\dagger_{i-\sigma}d_{i-\sigma}d_{i\sigma} \ . \tag{2.1c}$$

In this expression $d^\dagger_{i\sigma}$ and $d_{i\sigma}$ are the creation and destruction operators for an electron of spin σ in the Wannier orbital at site i. Since the band is nondegenerate the Coulomb interaction is restricted to occur between up- and down-spin electrons via the Pauli exclusion principle. The transformation from the Wannier representation to Bloch representation is given by

$$d^\dagger_{\vec{k}\sigma}=\frac{1}{N}\sum_i \epsilon^{i\vec{k}\cdot\vec{R}_i}d^\dagger_{i\sigma} \ . \tag{2.2}$$

As mentioned previously, for values of U slightly less than some critical value U_c, the dominant low-temperature excitations of the system are the spin fluctuations. In the random-phase approximation, the transverse spin fluctuations are described as an electron and a hole of opposite spin, which interact repeatedly (Fig. 1). The multiple Coulomb interactions tend to bind the electron-hole pair causing them to form a bosonlike excitation with a spin one.

The spin-fluctuation propagator $D(q,\omega)$ is found from the solution of the Bethe-Salpeter equation,

$$\begin{aligned}D(q,\omega)=&\frac{1}{\beta}\sum_{\vec{k}\omega_n}G(\vec{k}+\vec{q}\,|\,\omega_n+\omega)G(\vec{k}\,|\,\omega_n)\\&+\frac{1}{\beta}\sum_{\vec{k}\omega_n}G(\vec{k}+\vec{q}\,|\,\omega_n+\omega)G(\vec{k}\,|\,\omega_n)\\&\times UD(\vec{q},\omega) \ ,\end{aligned} \tag{2.3}$$

in which ω_n is the Matsubara frequency $\omega_n=(\pi/\beta)(n+1)$, and n is an integer. If we introduce $\chi(q,\omega)$ as the susceptibility of a noninteracting gas of electrons, we have

$$\chi(q,\omega)=\frac{1}{\beta}\sum_{\vec{k}\omega_n}G(\vec{k}+\vec{q}\,|\,\omega+\omega_n)G(\vec{k}\,|\,\omega_n) \ . \tag{2.4a}$$

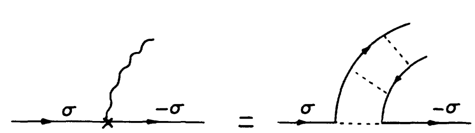

FIG. 1. Emission or absorption of spin fluctuation by an electron of spin σ. The electron is represented by the solid line —➤—, and the spin fluctuation by the wiggly line ∿∿. The spin fluctuation is also represented in terms of multiple scattering between an electron of spin σ and a hole of spin σ.

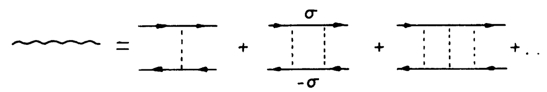

FIG. 2. Correspondence between a spin fluctuation and multiple-scattering events.

Then the spin-fluctuation propagator can be expressed as

$$D(q,\omega)=\frac{\chi(q,\omega)}{1-u\chi(q,\omega)} . \tag{2.4b}$$

The spin fluctuations interact with the electrons, the coupling constant being U (Fig. 2).

A spin fluctuation may be emitted or absorbed by an electron. A coupling constant U is associated with the electron-spin fluctuation vertex. The repeated interaction between an up-spin electron $+\sigma$ and a down-spin hole $-\sigma$ can be represented as a spin fluctuation (see Figs. 1 and 2).

III. THE HIGH-FREQUENCY ELECTRICAL CONDUCTIVITY

The frequency- and wave-vector-dependent electrical conductivity is calculated from the Kubo formula

$$\sigma_{\alpha\beta}(\vec{q},\omega)=\frac{1}{i\omega}[F_{\alpha\beta}(\vec{q},\omega)-F_{\alpha\beta}(0,0)] , \tag{3.1}$$

where $F_{\alpha\beta}(\vec{q},\omega)$ is the space and time Fourier transform of the current-current correlation function. $F(q,\omega)$ can be expressed as

$$F_{\alpha\beta}(\vec{q},\omega)=-i\int d\vec{r}\epsilon^{i\vec{q}\cdot\vec{r}}\int_{-\infty}^{\infty}dt\,\epsilon^{i\omega t}\Theta(\tau)\langle j_\alpha(\vec{r},t);j_\beta(0,0)\rangle , \tag{3.1a}$$

in which $j_\alpha(\vec{r},t)$ is the α component of the paramagnetic current operator

$$j_\alpha(\vec{r},0)=\sum_{\vec{k}\vec{q}\sigma}\epsilon^{i\vec{q}\cdot\vec{r}}a^\dagger_{\vec{k}-\vec{q}\sigma}a_{\vec{k}\sigma}\vec{V}_{\vec{k};\vec{q}} , \tag{3.1b}$$

where $\vec{V}_{\vec{k};-\vec{q}}$ is the velocity.

In the high-frequency limit we can evaluate $\sigma_{\alpha\beta}(0,\omega)$ by diagrammatic expansion. We shall follow Holstein's[10] work on the electron-phonon gas quite closely. We find that the leading terms of the conductivity are of the form

$$\sigma_{\alpha\beta}(0,\omega)=\frac{-ine^2}{m^*\omega}\delta_{\alpha\beta}+\frac{ne^2}{m^*\omega^2\tau} , \tag{3.2}$$

in which the effective mass m^* is defined by

$$\frac{n}{m^*}=-\sum_{\vec{k}_\sigma}\frac{\partial f(k)}{\partial\epsilon(\vec{k})}\frac{\vec{V}_{\vec{k}}\cdot\vec{V}_{\vec{k}}}{3} . \tag{3.3}$$

The scattering rate τ^{-1} is calculated from the processes depicted diagrammatically in Figs. 3(a) and 3(b). Thus the high-frequency conductivity exhibits a Drude-type tail, and it is expected that the Drude formula

$$\sigma(\omega)=\frac{ne^2}{m^*}\frac{\tau(1+i\omega\tau)}{1+\omega^2\tau^2} \tag{3.4}$$

will be a good intrapolation formula between the high-frequency limit and the dc conductivity

$$\sigma(0)=\frac{ne^2\tau}{m^*} . \tag{3.5}$$

The diagrams in Fig. 3(a) constitute the Fermi golden-rule expression for scattering due to the emission or absorption of spin fluctuations. These processes, by themselves, do not constitute a conserving approximation since they do not satisfy the Ward identities. It is necessary to incorporate the diagrams shown in Fig. 3(b) in order that the momentum-conserving Coulomb interactions do not constitute to the transport scattering rate. We shall show that within this approximation only the umklapp scattering processes contribute to the scattering rate. In the umklapp scattering processes the whole crystal acts as a momentum sink for the electronic system.

We shall evaluate the contributions to the scattering rate from Figs. 3(a) and 3(b) separately. The spin-fluctuation self-energy correction to the electron propagator contributes, to τ^{-1}, the term

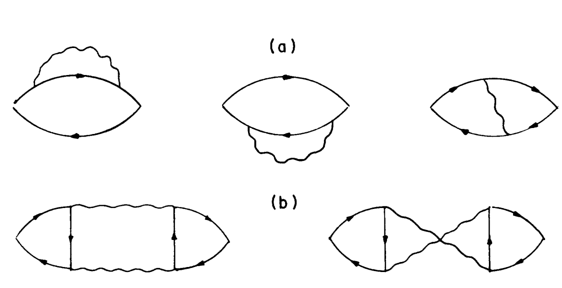

FIG. 3. We depict diagrammatically the scattering processes that result in a conserving approximation for the transport scattering rate. In Fig. (a) we depict the scattering of an electron by a spin fluctuation. These terms constitute the usual Fermi golden-rule scattering rate. In Fig. (b) we depict processes that are responsible for dragging the spin fluctuations out of thermal equilibrium.

$$\frac{m^*}{n}\omega \sum_{\vec{k}\,\vec{q}_1\,\vec{q}_2\sigma} \frac{1}{\beta^2} \sum_{\omega_n \Omega_n} V^{\alpha}_{\vec{k}} V^{\beta}_{\vec{k}} U^2 \Delta(\vec{q}_1 - \vec{q}_2)$$
$$\times \mathrm{Im}[G_\sigma(\vec{k}\,|\,\omega+\omega_n) G_{-\sigma}(\vec{k}+\vec{q}_1\,|\,\omega+\omega_n+\Omega_n) D(\vec{q}_2,\Omega_n) G_\sigma(\vec{k}\,|\,\omega+\omega_n) G_\sigma(\vec{k}\,|\,\omega_n)], \tag{3.6}$$

while the self-energy correction to the hole propagator yields

$$\frac{m^*}{n}\omega \sum_{\vec{k}\,\vec{q}_1\,\vec{q}_2\sigma} \frac{1}{\beta^2} \sum_{\omega_n \Omega_n} V^{\alpha}_{\vec{k}} V^{\beta}_{\vec{k}} U^2 \Delta(\vec{q}_1 - \vec{q}_2) \mathrm{Im}[G_\sigma(\vec{k}\,|\,\omega+\omega_n) G_{-\sigma}(\vec{k}+\vec{q}_1\,|\,\omega+\Omega_n) D(\vec{q}_2,\Omega_n) G_\sigma(\vec{k}\,|\,\omega_n)] \,. \tag{3.7}$$

The first vertex correction contributes a term

$$\frac{m^*}{n}\omega \sum_{\vec{k}\,\vec{q}_1\,\vec{q}_2\sigma} \frac{1}{\beta^2} \sum_{\omega_n \Omega_n} V^{\alpha}_{\vec{k}} V^{\beta}_{\vec{k}} U^2 \Delta(\vec{q}_1 - \vec{q}_2) \mathrm{Im}[G_\sigma(\vec{k}\,|\,\omega+\omega_n) G_{-\sigma}(\vec{k}+\vec{q}_1\,|\,\omega_n+\omega+\Omega_n) D(\vec{q}_2,\Omega_n)$$
$$\times G_\sigma(\vec{k}\,|\,\omega_n) G_{-\sigma}(\vec{k}+\vec{q}_1\,|\,\omega_n+\Omega_n)] \,. \tag{3.8}$$

In these expressions $\delta(q_1 - q_2)$ represents the conservation of wave-vector modulo a reciprocal-lattice vector. After some manipulations these three terms may be combined as

$$\mathrm{Im}\frac{m^*}{n\omega} \sum_{\vec{k}\,\vec{q}_1\,\vec{q}_2\sigma} \frac{1}{\beta^2} \sum_{\omega_n \Omega_n} V^{\alpha}_{\vec{k}} (V^{\beta}_{\vec{k}\,\vec{q}_1} - V^{\beta}_{\vec{k}}) u^2 \Delta(\vec{q}_1 - \vec{q}_2) \frac{1}{1 - u\chi(\vec{q}_2\Omega_n)} \frac{1}{1 - u\chi(\vec{q}_2\Omega_n + \omega)}$$
$$\times [\chi(\vec{q}_2,\omega+\Omega_n) - \chi(\vec{q}_2,\Omega_n)] \left\{ \frac{f(\vec{k}) - f(\vec{k}+\vec{q}_1)}{i(\omega+\Omega_n) + \epsilon(\vec{k}) - \epsilon(\vec{k}+\vec{q})} - \frac{f(\vec{k}) - f(\vec{k}+\vec{q}_1)}{i\Omega_n + \epsilon(\vec{k}) - \epsilon(\vec{k}+\vec{q})} \right\} . \tag{3.9}$$

We shall use this form of the scattering rate from the processes in Fig. 3(a) to combine with those of Fig. 3(b). However, we shall first reexpress the rate for the normal scattering processes in a more recognizable form:

$$\frac{1}{\tau} = \frac{u^2}{nm\beta\omega} \int_0^\infty d\Omega \left[N\left[\Omega - \frac{\omega}{2}\right] - N\left[\Omega + \frac{\omega}{2}\right] \right] \sum_{\vec{k}\,\vec{q}} |q|^2 [f(\vec{k}) - f(\vec{k}+\vec{q})]$$
$$\times \left[\delta\left[\Omega - \frac{\omega}{2} + \epsilon(\vec{k}) - \epsilon(\vec{k}+\vec{q})\right] \mathrm{Im}D\left[\vec{q},\Omega + \frac{\omega}{2}\right] + \delta\left[\Omega + \frac{\omega}{2} + \epsilon(\vec{k}) - \epsilon(\vec{k}+\vec{q})\right] \mathrm{Im}D\left[\vec{q},\Omega - \frac{\omega}{2}\right] \right] , \tag{3.10}$$

namely, the Fermi golden rule for frequency-modulated processes. We note the presence of the factor $|q|^2$, which weighs large-angle scattering, as is typical of transport scattering rates. The terms depicted in Fig. 3(b) represent processes by which the system of spin fluctuations is dragged out of equilibrium by the scattering with the conduction electrons. The contributions from these processes are the following:

$$\frac{m^*}{n\omega}\sum_{\substack{\vec{k}\vec{k}',\sigma\\ \vec{q}_1\vec{q}_2}}\frac{1}{\beta^3}\sum_{\substack{\omega_n\omega_m\\ \Omega_n}} V^{\alpha}_{\vec{k}}V^{\beta}_{\vec{k}}U^2\Delta(\vec{q}_1-\vec{q}_2)$$

$$\times\operatorname{Im}\left[G_\sigma(\vec{k}\,|\,\omega+\omega_n)\frac{1}{1-uX(\vec{q}_1,\omega-\Omega_n)}G_\sigma(\vec{k}'\,|\,\omega+\omega_m)G_{-\sigma}(\vec{k}+\vec{q}_2\,|\,\omega_n+\Omega_n)\right.$$

$$\left.\times\, G_\sigma(\vec{k}\,|\,\omega_n)\frac{1}{1-uX(\vec{q}_1,\Omega_n)}G_\sigma(\vec{k}'\,|\,\omega_m)G_{-\sigma}(\vec{k}'+\vec{q}_2\,|\,\omega_m+\Omega_n)\right]$$

$$+\frac{m^*}{n\omega}\sum_{\substack{\vec{k}\vec{k}',\sigma\\ \vec{q}_1\vec{q}_2}}\frac{1}{\beta^3}\sum_{\substack{\omega_n\omega_m\\ \Omega_n}} V^{\alpha}_{\vec{k}}V^{\beta}_{\vec{k}}U^2\Delta(\vec{q}_1-\vec{q}_2)\operatorname{Im}\left[G(\vec{k}\,|\,\omega+\Omega)G(\vec{k}\,|\,\omega)G(\vec{k}'+\vec{q}\,|\,\omega+\omega)G(\vec{k}'+\vec{q}\,|\,\omega)\right.$$

$$\times\frac{1}{1-VX(\vec{q}_2,\Omega_n+\omega)}G_0(\vec{k}'\,|\,\omega_m-\Omega_n)$$

$$\left.\times\, G_{-\sigma}(\vec{k}'+\vec{q}_1\,|\,\omega+\omega_n)G_{-\sigma}(\vec{k}'+\vec{q}_1\,|\,\omega_n)\right]. \tag{3.11}$$

Upon combining the spin-fluctuation drag terms we obtain

$$\operatorname{Im}\frac{m^*}{n\omega}\sum_{\substack{\vec{k}\vec{k}',\sigma\\ \vec{q}_1\vec{q}_2}}\frac{1}{\beta}\sum_{\Omega_n}V^{\alpha}_{\vec{k}}(V^{\beta}_{\vec{k}'}-V^{\beta}_{\vec{k}'+\vec{q}_2})U^2\Delta(\vec{q}_1-\vec{q}_2)\frac{1}{1-uX(\vec{q}_1,\Omega_n)}\,\frac{1}{1-uX(\vec{q}_1,\Omega_n+\omega)}$$

$$\times\left[\frac{f(\vec{k})-f(\vec{k}+\vec{q}_2)}{i(\Omega_n+\omega)+\epsilon(\vec{k})-\epsilon(\vec{k}+\vec{q}_2)}-\frac{f(\vec{k})-f(\vec{k}+\vec{q}_2)}{i\Omega_n+\epsilon(\vec{k}')-\epsilon(\vec{k}'+q_2)}\right]$$

$$\times\left[\frac{f(\vec{k}')-f(\vec{k}'+\vec{q}_2)}{i(\Omega_n+\omega)+\epsilon(\vec{k}')-\epsilon(\vec{k}'+\vec{q}_2)}-\frac{f(\vec{k}')-f(\vec{k}'+\vec{q}_2)}{i\Omega_n+\epsilon(\vec{k}')-\epsilon(\vec{k}'+\vec{q}_2)}\right]. \tag{3.12}$$

Upon combining the terms of Figs. 3(a) and 3(b), we find

$$\operatorname{Im}\frac{m^*}{n\omega}\sum_{\substack{\vec{k}\vec{k}',\sigma\\ \vec{q}_1\vec{q}_2}}\frac{1}{\beta}\sum_{\Omega_n}V^{\alpha}_{\vec{k}}(V^{\beta}_{\vec{k}}-V^{\beta}_{\vec{k}+\vec{q}_1}-V^{\beta}_{\vec{k}'}+V^{\beta}_{\vec{k}'+\vec{q}_2})\mu^2\Delta(\vec{q}_1-\vec{q}_2)\frac{u}{1-uX(\vec{q}_1,\Omega_n)}\,\frac{u}{1-uX(\vec{q}_1,\Omega_n+\omega)}$$

$$\times\left[\frac{f(\vec{k})-f(\vec{k}+\vec{q}_1)}{i(\Omega_n+\omega)+\epsilon(\vec{k})-\epsilon(\vec{k}+\vec{q}_1)}-\frac{f(\vec{k})-f(\vec{k}+\vec{q}_1)}{i\Omega_n+\epsilon(\vec{k}')-\epsilon(\vec{k}'+\vec{q}_1)}\right]$$

$$\times\left[\frac{f(\vec{k}')-f(\vec{k}'+\vec{q}_2)}{i(\Omega_n+\omega)+\epsilon(\vec{k}')-\epsilon(\vec{k}'+\vec{q}_2)}-\frac{f(\vec{k}')-f(\vec{k}'+\vec{q}_2)}{i\Omega_n+\epsilon(\vec{k}')-\epsilon(\vec{k}'+\vec{q}_2)}\right]. \tag{3.13}$$

Apart from the magnetic enhancement factors, this is the scattering rate appropriate for electron-electron collisions. As is discussed by Ziman, the normal scattering processes conserve the total momentum of the electronic system and thereby do not contribute the the transport scattering rate. This is most simply seen by separating out the normal and umklapp contributions to the velocity

$$V_{\vec{k}}=\alpha_{\vec{k}}\vec{k}+\sum_{G}\beta_{\vec{k}}\vec{G}\ ,$$

in which $\vec{G}$ runs over the set of reciprocal-lattice vectors. Then, the factor

$$(V_{\vec{k}+\vec{q}}-V_{\vec{k}}+V_{\vec{k}'}-V_{\vec{k}'+\vec{q}})=0$$

for the normal components of the velocity. As shown in the work of Lawrence and Wilkens[11] a proper treatment of the umklapp processes is very complicated and depends critically on the close proximity of the Brillouin-zone boundary and the Fermi surface. Since we are only interested in the frequency and temperature dependence of the scattering rate, we shall not be interested in the exact value of the scattering rate. It will be sufficient for our purposes to utilize the result of the Lawrence and Wilkens[11] calculations, which is that the scattering occurs mainly at wave vectors close to the Brillouin-zone boundary. The scattering rate may then be approximated by

$$\frac{1}{\tau}\propto\frac{|\vec{G}|^2}{nm^*\omega^2}u^2\mathrm{Im}\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi i}N(\Omega)$$
$$\times\left[\frac{[\chi(\Omega+i\omega)-\chi(\Omega+i\eta)]^2}{[1-u\chi(\Omega+i\omega)][1-u\chi(\Omega+i\eta)]}-\frac{[\chi(\Omega+i\omega)-\chi(\Omega-i\omega)]^2}{[1-u\chi(\Omega+i\omega)][1-u\chi(\Omega-i\eta)]}\right.$$
$$\left.+\frac{[\chi(\Omega+i\eta)-\chi(\Omega-i\omega)]^2}{[1-u\chi(\Omega+i\eta)][1-u\chi(\Omega-\omega)]}-\frac{[\chi(\Omega-i\eta)-\chi(\Omega-\omega)]^2}{[1-u\chi(\Omega-i\eta)][1-u\chi(\Omega-i\omega)]}\right], \tag{3.14}$$

where $\chi(\Omega\sim\chi(q,\Omega)$ for large q. After some manipulation we have

$$\frac{1}{\tau}\propto\frac{|G|^2}{nm^*\omega}u^2\int_{-}^{\infty}d\Omega\left[N\left[\Omega-\frac{\omega}{2}\right]-N\left[\Omega+\frac{\omega}{2}\right]\right]\mathrm{Im}\chi\left[\Omega+\frac{\omega}{2}\right]\mathrm{Im}\chi\left[\Omega-\frac{\omega}{2}\right]$$
$$\times\left[\frac{1}{|1-u\chi(\Omega-\omega/2)|^2}+\frac{1}{|1-u\chi(\omega+\omega/2)|^2}\right], \tag{3.15}$$

which is analogous to the scattering rate calculated from the nonconserving approximation in which the spin-fluctuation drag terms have been neglected [Eq. (3.10)]. We shall follow Lederer and Mills[5,6] and Kaiser and Doniach[8] by assuming $\chi(\omega)$ to have the following ω dependence:

$$\mathrm{Re}\chi(\omega)=\chi_0\ ,$$
$$\mathrm{Im}\chi(\omega=\omega\tilde{\chi}_0\ . \tag{3.16}$$

The effects of a q dependence in $\chi(q,\omega)$ are discussed in the Appendix. This is consistent with the large-q limit of the imaginary part of the dynamic susceptibility, as calculated in RPA, being given by a Lorentzian

$$\mathrm{Im}D(q,\omega)=\frac{\omega\tilde{\chi}_0}{(1-u\chi_0)^2+\omega^2u^2\tilde{\chi}_0^2}\ , \tag{3.17}$$

while the real part of the susceptibility is

$$\mathrm{Re}D(q,\omega)=\frac{\chi_0(1-u\chi_0)+\omega^2u\tilde{\chi}_0^2}{(1-u\chi_0)^2+\omega^2u^2\tilde{\chi}^2}\ . \tag{3.18}$$

This ansatz is in agreement with the observation that the width Γ of the inelastic neutron scattering cross section $\mathrm{Im}D(q,\omega)$ correlates with the static susceptibility $D(0,0)$:

$$\Gamma=\frac{1-U\chi_0)}{u\tilde{\chi}_0}\ , \tag{3.19a}$$

while

$$D(0,0)^{-1}=\frac{1-U\chi_0}{\chi_0}\ . \tag{3.19b}$$

Upon substituting the assumed form for $\chi(\omega)$, we may perform the Ω integration by expressing the Bose-Einstein distribution function in terms of the digamma function Ψ:

$$N(\Omega)=-\frac{1}{2}+\frac{1}{\Omega\beta}+\frac{1}{2\pi i}\left[\psi\left[1+\frac{i\beta\Omega}{2\pi}\right]-\psi\left[1-\frac{i\beta\Omega}{2\pi}\right]\right]\ . \tag{3.20}$$

The final result for the frequency-dependent scattering rate is

$$\frac{1}{\tau(\omega)}=\frac{1}{4\tau_0\omega}\left\{\frac{2\pi\omega}{\beta\Gamma}-2\omega+-i\Gamma\left[\psi\left[1+\frac{\beta\Gamma}{2\pi}+i\frac{\beta\omega}{2\pi}\right]-\psi\left[1+\frac{\beta\Gamma}{2\pi}-\frac{-\beta\omega}{2\pi}\right]\right]\right.$$
$$\left.+\omega\left[\psi\left[1+\frac{\beta\Gamma}{2\pi}+\frac{i\beta\omega}{2\pi}\right]+\psi\left[1+\frac{\beta\Gamma}{2\pi}-\frac{i\beta\omega}{2\pi}\right]-2\psi\left[1+\frac{\beta\Gamma}{2\pi}\right]\right]\right\}, \qquad (3.21)$$

where τ_0 is a constant. This is the central result of this paper. In the next section we shall exhibit the temperature and frequency variation explicitly. We shall also examine some asymptotic limits by analytic methods. The experimental implications will also be discussed.

IV. RESULTS AND DISCUSSION

The high-frequency limit of the conductivity exhibits a Drude-type tail, and the scattering rate is frequency dependent. We shall now examine some special limits of the ac scattering rate.

A. $T=0$

At zero temperature the scattering rate varies as

$$\frac{1}{\tau(\omega)}=\frac{1}{4\tau_0}\left[\frac{2\Gamma}{\omega}\tan^{-1}\frac{\omega}{\Gamma}+\ln\left[1+\frac{\omega^2}{\Gamma^2}\right]-2\right]. \qquad (4.1)$$

At large frequencies $\omega/\Gamma \gg 1$, the scattering rate varies logarithmically with ω,

$$\frac{1}{\tau(\omega)}\sim\frac{1}{2\tau_0}\left[\ln\frac{\omega}{\Gamma}-1\right], \qquad (4.2)$$

while at low frequencies $\omega/\Gamma \ll 1$, the scattering rate is proportional to ω^2,

$$\frac{1}{\tau(\omega)}\sim\frac{1}{12\tau_0}\frac{\omega^2}{\Gamma^2}. \qquad (4.3)$$

The vanishing of $1/\tau(\omega)$ as ω^2 at $T=0$ is a direct consequence of the phase space available for electron-electron collisions.

B. High temperature $\beta\Gamma \ll 1$

For temperatures much greater than Γ, the spin-fluctuation temperature, the scattering rate is of the form

$$\frac{1}{\tau(\omega)}=\frac{1}{4\tau_0}\left\{\frac{2\pi}{\beta\Gamma}\left[1-\frac{\Gamma^2}{\omega^2}\right]+\frac{\pi\Gamma}{\omega}\coth\frac{\beta\omega}{2}\right.$$
$$\left.+2\left[\mathrm{Re}\psi\left[1-\frac{i\beta\omega}{2\pi}\right]+\gamma-1\right]\right\}. \qquad (4.4)$$

For high frequencies compared to temperature, the above formula simplifies to

$$\frac{1}{\tau(\omega)}\sim\frac{1}{4\tau_0}\left[\frac{2\pi}{\beta\Gamma}+\frac{\pi\Gamma}{\omega}+2\left[\ln\frac{\beta\omega}{2\pi}+\gamma-1\right]\right], \qquad \beta\omega \gg 1 \quad (4.5)$$

while in the opposite limit $\beta\omega \ll 1$ we obtain

$$\frac{1}{\tau(\omega)}=\frac{1}{4\tau_0}\frac{2\Pi}{\beta\Gamma}-\frac{8\pi^2}{4\Pi^2+\beta^2\omega^2}$$
$$+[1-\xi(3)]\frac{\beta^2\omega^2}{4\pi^2}. \qquad (4.6)$$

We note that in the dc limit the expression reduces to the T law, found at high temperatures, in Kaiser and Doniach's theory[8] of the dc conductivity due to spin-fluctuation scattering.

C. Low temperature $\beta\Gamma \gg 1$

In the low-temperature regime the scattering rate is given by

$$\frac{1}{\tau(\omega)}\simeq\frac{1}{4\tau_0}\left[\frac{2\pi}{\beta\Gamma}+\frac{2\Gamma}{\omega}\tan^{-1}\left[\frac{\beta\omega/2\pi}{1+\beta\omega/2\pi}\right]+\frac{1+\beta\Gamma/2\pi}{(1+\beta\Gamma/2\pi)^2+(\beta\omega/2\pi)^2}+\ln\left[1+\frac{(\beta\omega/2\pi)^2}{(1+\beta\Gamma/2\pi)^2}\right]\right.$$
$$\left.-2-\frac{(\beta\omega/2\pi)^2}{[(1+\beta\Gamma/2\pi)^2+(\beta\omega/2\pi)^2][1+\beta\Gamma/2\pi]}\right]. \qquad (4.7)$$

We note that the dc limit gives

$$\frac{1}{\tau}=\frac{\pi^2}{3\tau_0}\frac{1}{\beta^2\Gamma^2}\left[1-\frac{4}{5}\frac{\pi^2}{\beta^2\Gamma^2}+\cdots\right], \qquad (4.8)$$

The T^2 law as calculated by Lederer and Mills[5] and by Kaiser and Doniach.[8] The T^2 variation comes from the phase space available for electron-electron collisions.

Thus as we have shown, $1/\tau(\omega)$ can have many different types of frequency dependences, which can be quite complicated. The scattering rate reduces to the well-known form in the dc limit. The dc scattering rate shows a T^2 law at low temperatures, followed by a T law at higher temperatures. At even higher temperatures one may suspect that Γ will be temperature dependent. One may see this from examining the form of $\chi(q,\omega)$ as calculated for the free-electron gas, or if one assumes that $\chi(q,\omega)$ is roughly independent of q, then one may correlate with the dc susceptibility. At low temperatures, when the dc susceptibility $D(0,0)$ is temperature independent, Γ should be temperature independent too. At higher temperatures the susceptibility shows a Cure-type tail; for these temperatures one expects that Γ should be proportional to T (Ref. 11). We model this dependence of Γ by

$$\Gamma=\begin{cases}\Gamma_0, & T<T_\sigma \\ \Gamma_0\dfrac{T}{T_\sigma}, & T>T_\sigma\ .\end{cases} \tag{4.9}$$

Thus at the temperature $T>\Gamma$, the dc scattering saturates to a constant value the de Gennes—Friedel limit of spin disorder scattering.

As Kaiser and Doniach[8] have noted, the dc scattering time shows a crude type of universality, scaling with $\beta\Gamma$. As Mills[12] has shown, this is marred by the q dependence of $\chi(q,\omega)$ and by the spread of q values which contribute to scattering. In our single-band model the q dependence comes almost entirely from the scattering at the Brillouin-zone boundary. Thus the scaling with $\beta\Gamma$ should be more precise. As seen in Eq. (3.21) this scaling property should also be found in the ac scattering time as measured in the infrared-absorption measurements. Experimental data on the infrared conductivity exists for Pd.[13,14] The data is complicated by the presence of interband transitions at $\omega=0.46$ eV, which makes the extraction of the Drude background quite difficult. For example, Duisbaeva *et al.*[13] have performed reflectance measurements on Pd at room temperature, in the frequency range 0.14—1.4 eV. From the data they have extracted an optical collision rate that varies from $1/\tau=3.3\times10^{14}$ Hz at $\omega=0.35$ eV to $1/\tau=2.23\times10^{14}$ Hz at $\omega=0.14$ eV. There is too much scatter and too few data points to allow for a power law and a logarithmic frequency variation to be distinguished. Weaver and Benbow[14] have performed absorbance measurements on Pd at 4.2 K, in the frequency range 0.15—4.4 eV. They find that the interband structure at 0.46 eV is about 3 times smaller than the structure found by Duisbaeva *et al.*[13] Since the slope near the Drude tail is strongly affected by the interband transitions, it is no surprise that Weaver and Benbow[14] find $1/\tau=20\times10^{14}$ Hz, which strongly differs from that given by Duisbaeva *et al.* In order that this discrepancy in the magnitude of $1/\tau$ and its frequency dependence be removed more measurements should be made. These should be performed at the longest wavelengths possible in order that the effects of the interband transitions be minimized. The quality of the sample surface should be strictly controlled.

A temperature-dependent study of $1/\tau$ would allow the phonon contribution to be subtracted. The temperature dependence of the spin-fluctuation contribution is shown in Fig. 4. The spin-fluctuation temperature Γ found from the optical collision rate $1/\tau$ could then be compared with the halfwidths obtained from the inelastic neutron scattering cross section,

$$\frac{d\sigma}{d\omega d\Omega}=\frac{h}{\Pi}\frac{k_f}{k_i}\left[\frac{\gamma e^2}{mc^2}\frac{q}{2}\right]^2[N(\omega)+1]ImD(q,\omega) \tag{4.10}$$

for large q, or from the width of the NMR line.[12,15] The NMR width is expressed as

$$\frac{1}{T_1}=\frac{2}{\beta}\left[\frac{\gamma_N}{\gamma_e h}\right]\sum_q|H(q)|^2\frac{\mathrm{Im}D(q,\omega_N)}{\omega_N}\ , \tag{4.11}$$

where $H(q)$ is the strength of the hyperfine field and $\omega_N\sim0$ is the NMR frequency. The values of Γ extracted from these measurements should have the

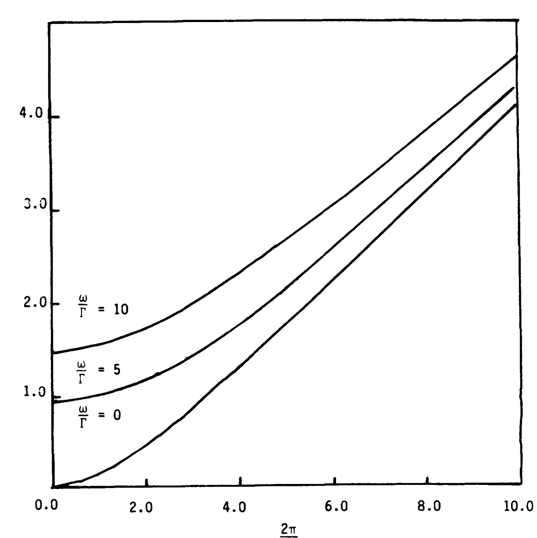

FIG. 4. Scattering rate $1/\tau$, in dimensionless units, as a function of the dimensionless temperature $2\pi/\beta\Gamma$ for various frequencies.

same temperature variations and allow the scaling behavior of $1/\tau(\omega)$ to be exhibited. Of course, it is not expected that the same type of scaling should occur from the value of Γ taken from the static susceptibility, since $D(q,0)$ is expected to show a rapid variation near ~ 0. The larger enhancement of $D(q,0)$ near $q \sim 0$ stems from the proximity of the ferromagnetic transition for larger values of U.

In summary, we have calculated the high-frequency ac electrical conductivity. The conductivity shows a Drude-type tail in which the scattering rate is frequency dependent. The dc limit of the scattering time is of the form calculated by Kaiser and Doniach. The scattering rate calculated is a universal function of $\beta\Gamma$ and $\beta\omega$. The temperature dependence of the factor Γ is experimentally measurable from either the widths of the inelastic neutron scattering spectrum or the NMR width. These may then be used to show the scaling of the $1/\tau(\omega)$ as should be found in infrared-absorption experiments.

APPENDIX

In this appendix we shall discuss the effects of including a q dependence in the noninteracting susceptibility $\chi^0(q,\omega)$. In general, the noninteracting susceptibility will be a complicated function that depends on all the details of the electronic band structure. In this appendix we shall assume that $\chi^0(q,\omega)$ has the form associated with the low-frequency behavior of the $T=0$ K Lindhart function,

$$\mathrm{Re}\chi^0(q,\omega)=\chi^0\left[1-\frac{q^2}{3q^2}\right]$$

and

$$\mathrm{Im}\chi^0(q,\omega)=\frac{3\pi}{4\mu}\frac{\omega}{vq} .$$

The dc scattering rate can be written at low temperatures as being proportional to

$$1/\tau \propto T^2 \int dq\, q \frac{1}{[1-U\chi^0(q,0)]^2} ,$$

and at high temperatures to

$$1/\tau \propto T \int dq \frac{1}{[1-U\chi^0(q,0)]} .$$

The approximation made by Kaiser and Doniach[8] is that of neglecting the q^2 dependence in the real part of $\chi^0(q,\omega)$. This leads to the scattering rate being proportional to

$$1/\tau = S^2T^2$$

at low temperatures, and to

$$1/\tau = ST$$

at higher temperatures where S is the Stoner enhancement factor $S=[1-U\chi^0(0,0)]^{-1}$. If one retains the q^2 dependence of the real part of $\chi^0(q,\omega)$, then one obtains the behavior

$$1/\tau = T^2\left[\frac{S^2}{1+(S/3)}+\frac{S^{3/2}}{\sqrt{3}}\tan^{-1}\frac{S^{1/2}}{3}\right]$$

and

$$1/\tau = T\ln\left[1+\frac{S}{3}\right]$$

at low and high temperatures, respectively. The analogous case in which spin-fluctuation drag effects had been neglected has been considered by Mills.[12] Experiments have not been able to distinguish between the various dependences on the Stoner enhancements S. Further complications set in since it seems that it is necessary to use a screened Coulomb interaction rather than the local Hubbard interaction U in order to obtain smaller mass enhancements as found in experiment. In view of the model dependences of the ac conductivity we have neglected the q dependence of $\mathrm{Re}\chi^0(q,\omega)$ in the main text. For reasonable values of S the differences will not be important.

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