is expected to exhibit the qualitative features of the Cr-group metals; whilst the spin-up Fermi level is placed near the top of the band and, according to this model, the relevant portions of its Fermi surface are expected to consist of hole pockets around H for three bands, and other more or less spherical hole regions around Γ for two bands.

As mentioned above, the Fermi surface is very sensitive to the details of the $E(\mathbf{k})$ curve, and thus to the approximations assumed. The s-d mixing, for instance, certainly induces some modification; but this effect is hard to evaluate, principally because of the uncertainty in the relative positions of the s and d bands, which, as pointed out above, depend critically on the assumed potential. Nevertheless, a comparison between the results obtained by tight-binding and APW calculations[16,17] in ΓNH plane for the Cr-group transition metals, for instance, shows the same qualitative features of the Fermi surface and suggests that, at least in some regions of the Brillouin zone, even such a simplified model can give some useful suggestions.

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Electron-Magnon Interaction in Ferromagnetic Transition Metals*

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The self-energy of an electron in a ferromagnetic transition metal due to the virtual emission and absorption of magnons has been calculated. It was found that the mass correction due to the electron-magnon interaction may be as large as that due to the electron-phonon interaction. Furthermore, it was noted that singularities in the density of states should occur at $\epsilon_F \pm \hbar\omega_0$, where ω_0 is the frequency of the magnon emitted or absorbed when electrons or holes forward-scatter from the Fermi surface of one spin band to the other spin band.

EXPERIMENTAL studies of the ferromagnetic transition metals may soon indicate the extent to which the electron mass at the Fermi surface is renormalized by the electron-magnon interaction.[1,2] The purpose of this paper is to report some results of a theoretical calculation of this mass correction and other effects associated with the self-energy of an electron due to the virtual emission and absorption of magnons.

We take the interaction Hamiltonian in second quantized form to be

$$H_{\rm int} = J\Omega_0 \int d^3r\, \mathbf{s}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r}), \qquad (1)$$

where $\mathbf{s}(\mathbf{r}) = \frac{1}{2}\psi^\dagger(\mathbf{r})\boldsymbol{\sigma}\psi(\mathbf{r})$ [$\psi(\mathbf{r})$ is the electron field operator and σ_i is a Pauli spin matrix, $\hbar = 1$] and $\mathbf{S}(\mathbf{r})$ is the net spin polarization per unit volume. The exchange constant is J, and Ω_0 is the volume of a unit cell. We introduce magnon creation and annihilation operators in a fashion similar to Kittel's[3]:

$$S^+(\mathbf{r}) = \left[\frac{2}{\Omega}\left(\frac{S}{\Omega_0}\right)\right]^{1/2} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}} b_{\mathbf{q}},$$

$$S^-(\mathbf{r}) = \left[\frac{2}{\Omega}\left(\frac{S}{\Omega_0}\right)\right]^{1/2} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} b_{\mathbf{q}}^\dagger, \qquad (2)$$

and

$$S_z(\mathbf{r}) = \frac{S}{\Omega_0} - \Omega^{-1} \sum_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{r}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}'}.$$

(Ω is the volume of the crystal.) In the ground state, $S_z(\mathbf{r}) = S/\Omega_0$, where S is the net spin polarization per atom.

The electron energies are $\epsilon_\sigma(\mathbf{k}) = \epsilon(\mathbf{k}) + (\sigma/2)JS$, so that the exchange splitting is JS. We assume that the magnon or spin-wave frequencies $\omega(\mathbf{q})$ are known.

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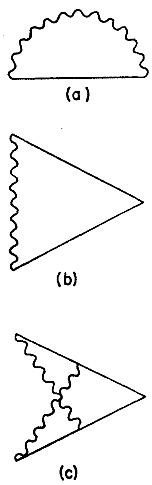

FIG. 1. (a) Approximation for self-energy (the solid line represents an electron and the wavy line, a magnon); (b) first-order vertex correction which is forbidden by spin conservation; and (c) lowest-order allowed vertex correction.

Although the conduction electrons and $\mathbf{S}(\mathbf{r})$ are intimately related in an itinerant ferromagnet, the magnons are well-defined excitations and we do not inquire further into the calculation of $\omega(\mathbf{q})$ or of the dynamics of $\mathbf{S}(\mathbf{r})$. The portion of the interaction which concerns us, H_1, is that in which a magnon is emitted or absorbed. The remainder of the interaction gives rise to the exchange splitting, to contributions to the magnon frequencies, or to higher-order processes. We have, then,

$$H_1=J\left(\frac{S}{2N}\right)^{1/2}\sum_{\mathbf{k},\mathbf{q}}(c_{\mathbf{k}-\mathbf{q}\downarrow}{}^{\dagger}c_{\mathbf{k}\uparrow}b_{\mathbf{q}}+c_{\mathbf{k}+\mathbf{q}\uparrow}{}^{\dagger}c_{\mathbf{k}\downarrow}b_{\mathbf{q}}{}^{\dagger}), \quad (3)$$

where $c_{\mathbf{k}\sigma}{}^{\dagger}$ and $c_{\mathbf{k}\sigma}$ are the electron creation and annihilation operators and $N=\Omega/\Omega_0$.

From second-order perturbation theory, it can be shown that the second-order correction $\Sigma_\sigma(\mathbf{k})$ (there is no first-order correction) to $\epsilon_\sigma(\mathbf{k})$ is given by

$$\Sigma_\sigma(\mathbf{k})=\frac{J^2S}{2N}\sum_{\mathbf{q}}\left[\frac{(1-f_\uparrow(\mathbf{k}+\mathbf{q}))\delta_{\sigma\downarrow}}{\epsilon_\downarrow(\mathbf{k})-\epsilon_\uparrow(\mathbf{k}+\mathbf{q})-\omega(\mathbf{q})}+\frac{f_\downarrow(\mathbf{k}+\mathbf{q})\delta_{\sigma\uparrow}}{\epsilon_\uparrow(\mathbf{k})-\epsilon_\downarrow(\mathbf{k}+\mathbf{q})+\omega(\mathbf{q})}\right], \quad (4)$$

where $f_\sigma(\mathbf{k})=f(\epsilon_\sigma(\mathbf{k}))$ is the Fermi distribution function. In Eq. (4), we take $q<q_m$, where q_m is some maximum wave vector or Debye cutoff. If we were to include umklapp processes, we should take account of the $\mathbf{q}$ dependence of J.

$\Sigma_\sigma(\mathbf{k})$ is the self-energy of Green's-function theory[4] $\Sigma_\sigma(\epsilon,\mathbf{k})$ evaluated at $\epsilon_\sigma(\mathbf{k})$. In Fig. 1(a), we show diagrammatically the approximation in which we calculate the self-energy. In Fig. 1(b), we show the first-order vertex correction of the corresponding problem in the electron-phonon interaction. Because of the conservation of spin, Fig. 1(b) is, however, identically equal to zero in the magnon problem. The lowest-order allowed vertex correction is shown in Fig. 1(c). We do not include any vertex correction in this paper since 1(c) is presumably quite small.

Let us rewrite Eq. (4) as follows:

$$\Sigma_0(\mathbf{k})=\frac{J^2S}{2N}\int_{\epsilon_F-D}^{\epsilon_F+D}d\epsilon\int d\omega\times\left[\frac{(1-f(\epsilon))\delta_{\sigma\downarrow}}{\epsilon_\downarrow(\mathbf{k})-\epsilon-\omega}+\frac{f(\epsilon)\delta_{\sigma\uparrow}}{\epsilon_\uparrow(\mathbf{k})-\epsilon+\omega}\right]F_0(\epsilon,\omega,\mathbf{k}), \quad (5)$$

where

$$F_\sigma(\epsilon,\omega,\mathbf{k})=\int\frac{d^3q}{(2\pi)^3}\delta(\epsilon-\epsilon_{-\sigma}(\mathbf{k}+\mathbf{q}))\delta(\omega-\omega(\mathbf{q})). \quad (6)$$

In Eq. (5), the principal value of the integral is to be taken, and $2D$ is the bandwidth. (ϵ_F is chosen at the center of the band only for convenience.) The important contributions to Eq. (5) [or to (4)] come from small q and $\epsilon_\sigma(\mathbf{k})$ near ϵ_F so we take

$$\epsilon_k=k^2/2m,\qquad m=\text{some band mass},$$

$$\omega(q)=q^2/2M\quad\text{and}\quad\epsilon_\sigma(\mathbf{k}+\mathbf{q})=\epsilon_\sigma(\mathbf{k})+v_Fq\cos\theta.$$

The angle between $\mathbf{v}(\mathbf{k})$ and $\mathbf{q}$ is θ, and we ignore anisotropies in $\epsilon_\sigma(\mathbf{k})$ and $\omega(\mathbf{q})$. With these approximations, we can evaluate $F_\sigma(\epsilon,\omega,\mathbf{k})$.

$$F_\sigma(\epsilon,\omega,\mathbf{k})=\frac{M}{4\pi^2v_F}\times1,\qquad\omega_m>\omega>\omega(q'),$$
$$\times0,\qquad\text{otherwise}, \quad (7)$$

where $\omega_m=\omega(q_m)$ and $v_Fq'=|\epsilon-\epsilon_{-\sigma}(\mathbf{k})|$.

Substituting Eq. (7) into Eq. (5), we have

$$\Sigma_\sigma(\mathbf{k})=\frac{J^2S\Omega_0M}{8\pi^2v_F}\left[-\int_{\epsilon_F}^{\epsilon_F+D}d\epsilon\ln\left|\frac{\epsilon_\downarrow(\mathbf{k})-\epsilon-\omega_m}{\epsilon_\downarrow(\mathbf{k})-\epsilon-\omega(q')}\right|\delta_{\sigma\downarrow}+\int_{\epsilon_F-D}^{\epsilon_F}d\epsilon\ln\left|\frac{\epsilon_\uparrow(\mathbf{k})-\epsilon+\omega_m}{\epsilon_\uparrow(\mathbf{k})-\epsilon+\omega(q')}\right|\delta_{\sigma\uparrow}\right]. \quad (8)$$

We are primarily interested in $\partial\Sigma_\sigma/\partial\epsilon_\sigma(\mathbf{k})$, which can be easily evaluated for $\epsilon_\sigma(\mathbf{k})$ near ϵ_F:

$$\frac{\partial\Sigma_\sigma}{\partial\epsilon_\sigma(\mathbf{k})}=\frac{JS}{\epsilon_F}J\rho_0\frac{M}{8m}\left[\ln\left|\frac{\epsilon_\downarrow(\mathbf{k})-\epsilon_F-\omega_0}{\omega_m}\right|\delta_{\sigma\downarrow}+\ln\left|\frac{\epsilon_\uparrow(\mathbf{k})-\epsilon_F+\omega_0}{\omega_m}\right|\delta_{\sigma\uparrow}\right], \quad (9)$$

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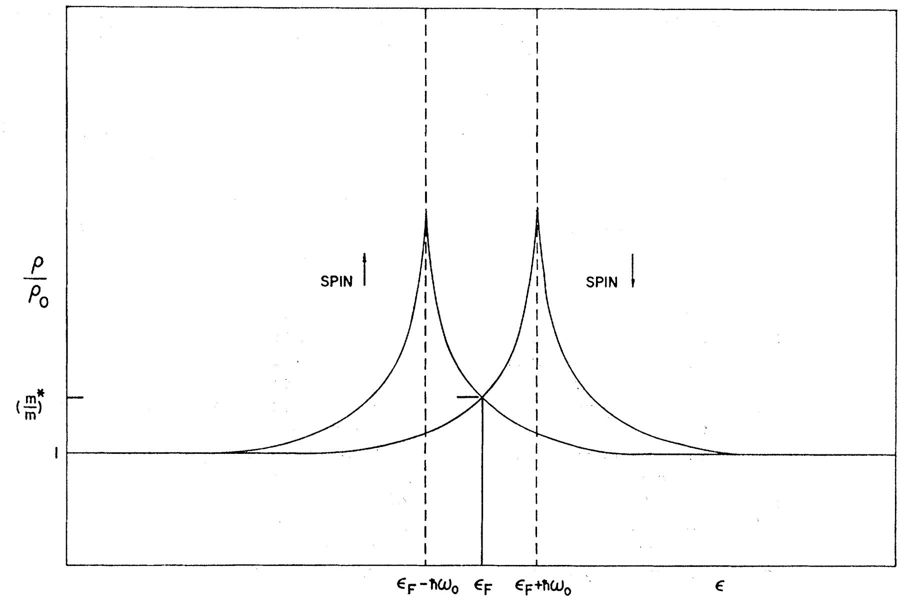

FIG. 2. The enhanced density of states (in units of the one-electron density of states) near the Fermi energy ϵ_F. Singularities at $\epsilon_F \pm \hbar\omega_0$ are due to the forward scattering of electrons or holes from one spin band to the other with emission or absorption of a magnon.

where $\omega_0 = \omega(JS/v_F)$. We neglect $\epsilon_\sigma(k) - \epsilon_F$ compared to JS. The density of states in a unit cell at the Fermi energy is $\rho_0 = \Omega_0 m p_F / 2\pi^2$. The effective mass at the Fermi surface for both spin bands is given by[4]

$$m^*/m = 1 - [\partial\Sigma_\sigma/\partial\epsilon_\sigma(\mathbf{k})]_{\epsilon_\sigma(\mathbf{k})=\epsilon_F}$$
$$= 1 + (JS/\epsilon_F) J\rho_0 (M/8m) \ln|\omega_m/\omega_0|. \quad (10)$$

From estimates of the parameters involved[5,6]

$$(JS \sim 1 \text{ eV}, \epsilon_F \sim 5 \text{ eV}, J\rho \sim 1, M \sim 10m),$$

it is not unreasonable to expect corrections as much as 50% or more, i.e., $m^*/m \approx 1.5$, depending upon what we take ω_m/ω_0 to be. We cannot take ω_m too large since if we were to include a q dependence in J, J would surely drop off significantly by $q = p_F$. In view of the fact that the electron-phonon contribution to m^*/m is ~ 0.2 in Cu,[7] it would appear that the electron-magnon enhancement may be as significant as the electron-phonon enhancement in ferromagnetic transition metals. The size of the correction is consistent with that suggested by Phillips and Mattheiss[8] for Ni.

It should also be noted that a singularity occurs in $\partial\Sigma_\downarrow/\partial\epsilon_\downarrow(\mathbf{k})$ when $\epsilon_\downarrow(\mathbf{k}) = \epsilon_F + \omega_0$ and in $\partial\Sigma_\uparrow/\partial\epsilon_\uparrow(\mathbf{k})$ when $\epsilon_\uparrow(\mathbf{k}) = \epsilon_F - \omega_0$. These conditions correspond to the forward scattering of an electron or hole near ϵ_F from one spin band to the other with the emission or absorption of a magnon. For example, when a ↓ electron with energy ϵ_F flips its spin, it must give up momentum JS/v_F in the forward direction, say, to remain near ϵ_F in the ↑ band. This is accomplished by emitting a magnon of momentum JS/v_F. However, the magnon also carries away energy $\omega_0 = \omega(JS/v_F)$ so that the spin-flipped electron scatters into the ↑ band at an energy $\approx \omega_0$ below ϵ_F. This is the physical origin of the divergence at $\epsilon_\uparrow(\mathbf{k}) = \epsilon_F - \omega_0$ in the ↑ band, and a similar process occurs in the ↓ band at $\epsilon_\downarrow(\mathbf{k}) = \epsilon_F + \omega_0$. There results a kink (in a sense, a Kohn anomaly) in the electron energy spectrum. ω_0 corresponds to an energy of ~ 5 mV or a temperature of ~ 60°K.

Since the correction to the density of states goes as $-\partial\Sigma_\sigma/\partial\epsilon_\sigma(\mathbf{k})$, one should see a singular enhancement of the density of ↓ states at $\epsilon_F + \omega_0$ and a singular enhancement in the density of ↑ states at $\epsilon_F - \omega_0$. (See Fig. 2.) In real systems, the singularities will, of course, be replaced by finite peaks due to thermal scattering and the finite lifetime of the magnons. Anisotropies in $\epsilon_\sigma(\mathbf{k})$ and $\omega(\mathbf{q})$ will reduce and broaden the peaks, and possibly give rise to other peaks.

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