Nonquasiparticle states and nature of the electron spectrum in iron and nickel

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A new model is proposed for the strong ferromagnetism of $3d$ metals. This model occupies an intermediate position between the Hubbard model and the s–d exchange model. The role of nonquasiparticle (spin-polaron) states lying near E_F is discussed. In particular, the role of these states in an interpretation of experimental data on the spin polarization of electrons and the temperature dependence of the resistance is discussed.

Despite the major theoretical effort devoted to the study of the magnetism of the transition metals, several points concerning the description of local magnetic moments remain unresolved. The spin-fluctuation theories[1] put the problem of local magnetic moments in the high-temperature region, with the ground state being described in the standard Stoner theory. At the same time, the very fact that local magnetic moments exist is difficult to reconcile with a quasiparticle description even at $T = 0$ (Refs. 2–4). The "model-free" version of the spin-fluctuation theory, which is based on the density-functional method,[5] fails to explain the presence of local magnetic moments near T_c in Ni, and it underestimates their values in Fe. On the other hand, the applicability of the standard Hubbard model to $3d$ metals is also questionable: A systematic calculation of the Hubbard parameter leads to an unreasonably high value of 6 eV for U for Fe (Ref. 6). In the present letter we wish to propose a new picture of the ferromagnetism of iron-group metal.

The results of band-theory calculations[7] for Fe suggest distinguishing a group of "magnetic" states which form a peak in the density of electron states $N(E)$ with a width Γ of 0.1 or 0.2 eV and with a capacity on the order of one electron per spin. This peak constitutes a two-dimensional Van Hove singularity from the P–N line (these states have symmetry e_g and are well localized in direct space). Upon the transition to a ferromagnetic state, the peak splits, retaining its shape. The spin splitting Δ is 2 eV (compare with the value of Γ). The situation in Ni is similar. In a zeroth approximation, the "magnetic" electrons can thus be described by a narrow-band Hubbard model with a band width on the order of Γ (compare with Δ) and an electron density $n > 1$. Their interaction with the other "s electrons" can then be dealt with in an s–d exchange model.[8]

We write the Hamiltonian of the model in the form

$$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} X^{2\sigma}_{-\vec{k}} X^{\sigma 2}_{\vec{k}} + H_s + H_{sd},$$

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where $\epsilon_{\vec{k}}$ is the spectrum of "magnetic" electrons, H_s is the Hamiltonian of the s electrons, H_{sd} is the exchange interaction between the two groups of electrons, and X_k^{q2} are the Fourier transforms of the generalized Hubbard projection operators which correspond to a transition from doubly occupied states ("doubles") to singly occupied states with a spin projection σ. For $n>1$ the vacant states are eliminated by any sufficiently strong electron–electron interaction (which need not be a contact interaction).

Since the peak with spin up is completely occupied in both Fe and Ni, we are dealing with a saturated or "semimetallic" ferromagnet (so far, we are ignoring the s electrons). The narrow-band Hubbard model (the first term in Hamiltonian H) has been studied thoroughly for this case. The Green's functions $G_{\vec{k}}^{-\sigma}(E) = \langle\langle X_k^{q2}|X_{-\vec{k}}^{2\sigma}\rangle\rangle_E$, which determine the electron spectrum are given by the following expression at $T=0$:

$$G_{\vec{k}}^{\downarrow}(E) = (E - \epsilon_{\vec{k}})^{-1}; \quad G_{\vec{k}}^{\uparrow}(E) = \left\{ E - \epsilon_{\vec{k}} - \left[\sum_{\vec{q}} \frac{f_{\vec{k}+\vec{q}}}{E - \epsilon_{\vec{k}+\vec{q}} + \omega_{\vec{q}}} \right]^{-1} \right\}^{-1},$$

where $f_{\vec{k}} = f(\epsilon_{\vec{k}})$ is the Fermi distribution function, and $\omega_{\vec{q}}$ is the magnon spectrum. If the density of doubles, $n_2 = n-1$, is not too large, the quantity $G_k^{\downarrow}(E)$ has no poles below E_F, but there is a "nonquasiparticle" (spin-polaron) component of the density of states, $N_\uparrow(E) = (-1/\pi)\mathrm{Im}\Sigma G_k^{\downarrow}(E)$, which is caused by a cut and which vanishes rapidly (over an interval on the order of the characteristic magnon energy $\overline{\omega}$) as $E\to E_F - 0$; here $N_\uparrow(E\to E_F) \sim [(E_F - E)/\overline{\omega}]^{3/2}$ (Fig. 1). On the other hand, the nonquasiparticle states [which are not associated with the poles of $G_k^q(E)$] do not affect the characteristics of the Fermi surface at $T \ll \overline{\omega}$. These states also lead to the

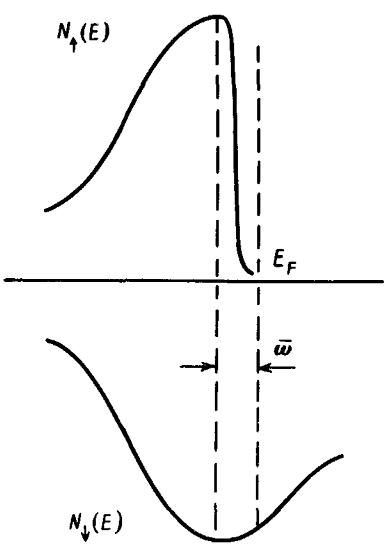

FIG. 1. Schematic diagram of the density of states of "doubles" near the Fermi level. The occupied peak with spin up corresponds to the lower Hubbard subband, which is off to the left (not shown in this figure).

value $M_0 = (n_\uparrow - n_\downarrow)/2 = (1 - n_2)/2$ and to a decay of the magnetization with the temperature in accordance with the Bloch law.[4]

The assertion that a picture of this sort—a familiar one in the Hubbard narrow-band model—is valid for Fe and Ni is not a trivial one and can be tested experimentally. The model which we are discussing here does not contradict the fact that the band theory is capable of giving a correct description of the Fermi surface and the values of M_0 for Fe and Ni. On the other hand, the spin polarizations of the emitted electrons, $P(E)$, are radically different in the two pictures. While P in our model is small when an average is taken over an energy interval $|\Delta E| \gg \overline{\omega}$ [by virtue of $N_\uparrow(E<E_F) \approx N_\downarrow(E)$], according to the band theory of Ref. 7, we would have $N_\downarrow(E_F) \gg N_\uparrow(E_F)$, and P should be large and negative. The experimental data on Ni (Ref. 11) definitely yield small values $P \approx -5\%$ to $+10\%$. The scatter in the data for Fe is considerably larger because of the difficulties in preparing the surface.[11] It follows from this model that P should be small if the samples are prepared carefully.

An old and still unresolved problem is explaining the temperature dependence of the electrical resistance of ferromagnetic metals at $T \ll T_c$. According to Ref. 8, we have $\rho(T) = aT + bT^2$ or $\rho(T) \propto T^{3/2}$. A term on the order of T^2 is observed at values of T much lower than predicted by the standard theory, which explains it in terms of one-magnon processes. The coefficient a is three orders of magnitude greater than the value stemming from relativistic processes. In our model, a $T^{3/2}$ dependence can be explained in terms of scattering by impurity centers with a nonquasiparticle component

$$\delta\rho(T) \sim \int dE \left(-\frac{\partial f(E)}{\partial E}\right) \delta N_\uparrow(E) \sim T^{3/2}.$$

In highly pure samples, this component should vanish. The component on the order of T^2 may arise by virtue of a scattering of "s electrons" by "magnetic" ones, as in the ordinary s–d model. The one-magnon processes come into play at low temperatures (since the s–d exchange parameter is small).[8]

The assertion that Hubbard's narrow-band model applies to Fe and Ni leads to a natural explanation for such manifestations of local magnetic moments as the spontaneous "spin" splitting above the Curie point T_c (interpreted as a Hubbard splitting) and the Curie-Weiss law.[9] The temperature T_c is estimated as $\Gamma\varphi(n)$, where $\varphi(n) \sim 1$ is the electron distribution function. The fact that $T_c \sim 10^3$ K is small in comparison with the "Stoner" splitting Δ—a fact which has been regarded as a serious problem for strong magnetic materials[1,8]—might thus be a consequence of the narrowness of the region of "magnetic" states: $\Gamma \ll \Delta$.

According to this model, only some of the d electrons (the e_g states near the Fermi level) are highly correlated ("Hubbard") electrons in Fe. This circumstance should be kept in mind in calculations of U of the type in Ref. 6; in particular, one should keep in mind that it is screened by t_{2g} electrons (not only by sp electrons).

We note in conclusion that the important role played by the "nonquasiparticle" contributions ("nonquasiparticle" in the sense that it stems from a cut in the Green's functions) in this model does not, in general, mean that the phenomenological theory of a Fermi liquid is inapplicable, since one can always introduce some "static" quasiparticles which are not directly related to poles of the Green's functions.[10] In particular, states with $\sigma = \uparrow$ make a linear contribution to the specific heat in the narrow-band Hubbard model, according to Ref. 4. That contribution is formally analogous to the difference between the contributions of "static" and "dynamic" quasiparticles.

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