Ferromagnetism of 3*d* metals

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It is shown that the narrowness of the d band in comparison with the s band in metals of the iron group can lead to an effective attraction between the spins of the d electrons, and by the same token to ferromagnetism regardless of the signs of the initiating exchange interactions.

The development of a theory of the ferromagnetism of iron-group metals encounters difficulties when it comes to explaining the sign and order of magnitude of the effective exchange interaction between the d-electron spins (see[1]).

We shall show that a simple model of a two-component Fermi liquid of s and d electrons, under the only requirement

$$g_d >> g_s \tag{1}$$

(g_d and g_s are the densities of the electronic states at the Fermi level) leads to an effective attraction between the spins of the d electrons regardless of the signs of the initiating exchange interactions.

We call attention to the fact that in transition 3d metals the ratio g_d/g_s increases with increasing atomic number, owing to the decrease of the radius of the 3d shell. Therefore the inequality (1) is particularly well satisfied for Fe, Co, and Ni, which, as is well known, are indeed ferromagnetic.

Generalizing the analysis of[2] to include the case of a two-component Fermi liquid, we write down the energies of the single-particle electronic states in the form

$$\epsilon_\alpha(\mathbf{p}, s) = \epsilon_\alpha^{(0)}(\mathbf{p}) + 2\beta_\alpha \mathbf{m} s; \quad \alpha = s, d. \tag{2}$$

Here $\epsilon_\alpha^{(0)}$ are the energies of the s and d electrons in the paramagnetic phase, $\mathbf{m}$ is the magnetization,

$$\mathbf{m} = 2\mu_e \operatorname{Sp} \sum_\alpha s \int \frac{d^3p}{(2\pi)^3} n_\alpha(\mathbf{p}, s), \tag{3}$$

n_α are single-particle Fermi density matrices, and μ_e is the Bohr magneton.

According to the Landau theory of the Fermi liquid,[3] the small perturbations of the single-particle energy and of the density matrices, due to the perturbation of the magnetization, are connected by the relations

$$\delta\epsilon_\alpha(\mathbf{p}, s) = \operatorname{Sp} \sum_\gamma \int \frac{d^3p}{(2\pi)^3} 4\psi_{\alpha\gamma}(\mathbf{p}, \mathbf{p}')(s, s')\delta n_\gamma(\mathbf{p}', s'), \tag{4}$$

where ψ_{ss}, ψ_{dd}, and $\psi_{sd} = \psi_{ds}$ are respectively the values of the ss, dd, and sd exchanges.

From (3) and (4) we obtain an expression for the quantities:

$$\beta_d = -(\mu_e g_d F)^{-1}\left[F_d + F_s F_d - F_{sd}^2 - F_{sd}\sqrt{\frac{g_d}{g_s}}\right], \tag{5}$$

$$\beta_s = (\mu_e g_s F)^{-1}\left[F_s + F_s F_d - F_{sd}^2 - F_{sd}\sqrt{\frac{g_s}{g_d}}\right], \tag{6}$$

$$F = F_d - F_s - F_{sd}\left(\sqrt{\frac{g_d}{g_s}} - \sqrt{\frac{g_s}{g_d}}\right), \tag{7}$$

where $F_d = \psi_{dd} g_d$, $F_s = \psi_{ss} g_s$, and $F_{sd}\sqrt{g_s g_d}$ are dimensionless parameters of the exchange interaction (we confine ourselves for simplicity to the zeroth harmonic in the expansion of the functions $\psi_{\alpha\gamma}$ in Legendre polynomials).

The case of a single-component Fermi liquid corresponds, obviously, to $F_s = F_d = F_{sd}$ and $g_s = g_d$. Formulas (5)–(7) then result in an uncertainty; the quantity $\beta = \beta_s = \beta_d$ can in this case, however, be readily determined directly from (4):

$$\beta = \frac{\psi}{\mu_e}. \tag{8}$$

In order for ferromagnetism to occur, it is necessary that β be negative; therefore ferromagnetism in the single-component model appears only at $\psi < 0$.

The situation is different in a two-band model with $g_d \gg g_s$. In this case we obtain from (5)–(7)

$$\beta_d = -(\mu_e g_d)^{-1}; \quad \beta_s = (\mu_e \sqrt{g_s g_d})^{-1} \frac{F_{sd}^2 - F_s F_d - F_s}{F_{sd}}. \tag{9}$$

We see that in this case the d electrons (the contribution of which to the magnetization is decisive) turn out to be ferromagnetic ($\beta_d < 0$) regardless of the signs of the initiating exchange interactions.

It is interesting that the spin splitting $\Delta = \beta_d m$ of the d band can be obtained without knowing the absolute values of the exchange parameters, since β_d is determined only by the density of the d states at the Fermi level. The values of Δ for the experimental values of the magnetization at $T = 0$ are listed in the table. The densities of states were taken from measurements of the specific heat[4] [with account taken of the inequality (1)].

TABLE I.

Metal	Δ, eV
Fe	1.06
Co	0.86
Ni	0.21

[1]S. V. Vonsovskiĭ, Magnetizm (Magnetism) Moscow, Nauka, 1972.
[2]A. A. Abrikosov and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. 35, 771 (1958) [Sov. Phys.-JETP 8, 535 (1959)].
[3]L. D. Landau, Zh. Eksp. Teor. Fiz. 30, 1058 (1956) [Sov. Phys.-JETP 3, 920 (1956)].
[4]S. A. Nemnonov, Fiz. Met. Metaloved. 19, 550 (1965).