Spin-wave spectra in rare-earth metals

A. V. Vedyaev and M. Yu. Nikolaev

Moscow State University (Submitted 15 October 1981) Zh. Eksp. Teor. Fiz. 82, 1287-1290 (April 1982)

We investigate the connection between the presence of a "ribbon bridge" on the Fermi surface of a rare-earth element and the onset, at a certain temperature, of a singularity in the ferromagnon spectrum at excitations $\mathbf{q} = 2\mathbf{k}_{F}$, which leads to instability of the ferromagnetic phase. It is shown that if the anisotropy in the antiferromagnon spectrum is neglected, no singularities due to the presence of the ribbon bridge arise if the equilibrium magnetic order is a helix with wave vector $\mathbf{q}_0 = 2\mathbf{k}_F$, i.e., the antiferromagnetic phase is stable.

PACS numbers: 75.30.Ds, 75.50.Cc

1. INTRODUCTION

Rare earth metals are known to have very curious and diverse properties (Ref. 1, p. 194 of Russ. translation). For example, dysprosium is ferromagnetic up to 85 K. At $T_c = 85$ K it goes over into an antiferromagnetic phase, and a "simple helix" magnetic structure is established. Holmium and terbium have similar properties. At the same time, gadolinium goes over directly from the ferromagnetic into the paramagnetic state. It is known that the Fermi surfaces of Dy, Ho, and Tb have flat sections-the so-called "ribbon" bridges"-and the wave vector of the simple helix coincides with the thickness of this ribbon bridge (Ref. 1, p. 148 of transl.). In addition, the Fermi surface of gadolinium has no such ribbon bridge and has no antiferromagnetic phase. It is natural to assume (Ref. 1, p. 214 of transl.) that the appearance of the antiferromagnetic phase is due to the presence of the ribbon bridge.

A phase transition from the paramagnetic into the antiferromagnetic phase of a rare earth metal, due to the topological features of the Fermi surface, was considered earlier by Dzyaloshinskiť.²

The purpose of the present paper is to investigate the connection between the presence of a ribbon bridge on the Fermi surface of a rare-earth metal, on the one hand, and the transition from its ferromagnetic into the antiferromagnetic phase, on the other. In Sec. 2 we investigate the spin-wave spectrum in the ferromagnetic phase, with account taken of the anisotropy, and show that at a certain temperature T^* there appears in the spectrum a singularity at $\mathbf{q} = 2\mathbf{k}_F$, meaning instability of the ferromagnetic phase. In Sec. 3 we obtain and investigate the spin-wave spectrum in the antiferromagnetic phase, neglecting anisotropy, and show that this phase is stable if the wave vector \mathbf{q}_0 of the simple helix is equal to the thickness of the ribbon bridge $2\mathbf{k}_F$.

2. SPIN-WAVE SPECTRUM OF FERROMAGNETIC PHASE

The magnetic order in rare-earth metals is due to s-f exchange.³ The Hamiltonian of this interaction is given by

$$H_{*} = \sum_{n} J S_{n} s(\mathbf{R}_{n}), \qquad (1)$$

where J is the indirect-exchange integral, S_n is the spin localized at the *n*-th site, and $s(\mathbf{R}_n)$ is the spin of the conduction electrons located near the *n*-th site.

The spin-wave dispersion law for the ferromagnetic phase was obtained by Vonsovskii and Izyumov with the aid of the Green's function method, by summing a "ladfer" sequence of diagrams of the form

where the dashed lines correspond to the magnon Green's functions, and the solid lines correspond to the electron functions⁴:

$$E_{\mathbf{q}} = E_{\mathbf{0}} + \Pi(\mathbf{q}), \quad E_{\mathbf{0}} = \frac{J}{N} \sum_{\mathbf{k}} (n_{\mathbf{k}}^{\dagger} - n_{\mathbf{k}}^{\dagger}), \quad (3)$$

$$\Pi(\mathbf{q}) = \frac{2J^2S}{N} \sum_{\mathbf{k}} \frac{n_{\mathbf{k}}^{\dagger} - n_{\mathbf{k}-\mathbf{q}}^{\downarrow}}{\mathbf{e}_{\mathbf{k}}^{\dagger} - \mathbf{e}_{\mathbf{k}-\mathbf{q}}^{\downarrow} + E_{\mathbf{q}}}, \qquad (4)$$

$$n_{\mathbf{k}}^{\sigma} = \left[\exp\left(\frac{e_{\mathbf{k}}^{\sigma} - \mu}{T}\right) + 1 \right]^{-1}, \tag{5}$$

$$\varepsilon_{\mathbf{k}}^{\sigma} = \begin{cases} \varepsilon_{\mathbf{k}} - JS, & \sigma = \uparrow \\ \varepsilon_{\mathbf{k}} + JS, & \sigma = \downarrow \end{cases}, \tag{6}$$

 ε_k is the dispersion law of the electrons in the paramagnetic phase. Allowance for the anisotropy, which is comparable in rare earth metals with J (Ref. 4) and decreases rapidly (as the tenth power of the magnetization) with increasing temperature,^{1,5} adds to Eq. (3) a positive constant B(T) proportional to the anisotropy constant and decreasing rapidly with increasing temperature:

$$E_{\mathbf{q}} = E_{\mathbf{0}} + B(T) + \Pi(\mathbf{q}). \tag{7}$$

In the derivation of (7) it was assumed that the anisotropy separates the "easy plane" and separates also in this plane the direction of the magnetization vector. Our basic assumption is that the antiferromagnetic order in a rare-earth metal sets in because of the presence of a flat section on the Fermi surface. We shall therefore assume in this paper that the conductionelectron dispersion law is one-dimensional, since the flat section makes an additive contribution to the magnon energy, and it is precisely this contribution that we wish to examine.

In that case

$$\sum_{\mathbf{k}} \frac{n_{\mathbf{k}}^{\dagger} - n_{\mathbf{k}-q}^{\dagger}}{\varepsilon_{\mathbf{k}}^{\dagger} - \varepsilon_{\mathbf{k}-q}^{\dagger}}$$

$$\tag{8}$$

goes to $-\infty$ at $q_0 = 2k_F$ (Refs. 6 and 7). If we obtain graphically the solutions of (7), we find that at $q_0 \approx 2k_F$ a solution $E_{q_0} < 0$ exists at any temperature. If, however, we take into account the renormalization of the vertices in the diagrams (2), which make up a ladder, by solving the Dyson equation for the vertex part:

the polarization operator in (7) takes the form

$$\tilde{\Pi}(q) = \frac{g_0^2}{1 + g_0^2 \Gamma(q)} \sum_{k} \frac{n_k^{\dagger} - n_{k-q}^{\downarrow}}{\varepsilon_k^{\dagger} - \varepsilon_{k-q}^{\downarrow} + E_q},$$
(10)

where $g_0^2 = J^2 S$ and

$$\Gamma(q) = \sum_{\mathbf{k}} \frac{n_{\mathbf{k}}^{\dagger} - n_{\mathbf{k}-q}^{\mathbf{g}}}{\varepsilon_{\mathbf{k}}^{\dagger} - \varepsilon_{\mathbf{k}-q}^{\dagger} + E_{q}^{\dagger}} j(k) + \Delta \Gamma_{\mathrm{reg}}(q).$$
(11)

Here f(k) is a smooth function of k, i.e., $\overline{\Pi}(q)$ does not go to $-\infty$ at $q=q_0$ and $E_{q_0}=0$, but it can be shown that

$$\Pi(q_0) + E_0 < 0, \tag{12}$$

so that at $T > T^*$, when

$$\Pi(q_0) + E_0 + B(T) < 0, \tag{13}$$

there exists a solution $E_{q_0}^* < 0$, and at $T < T^*$, when

$$\Pi(q_0) + E_0 + B(T) > 0, \tag{14}$$

this solution vanishes. Consequently at $T < T^*$ all the solutions of (7) are positive and the ferromagnetic phase is stable, while at $T > T^*$ a solution $E_{q_0} < 0$ exists, i.e., the ferromagnetic phase is unstable.

3. SPIN-WAVE SPECTRUM IN THE ANTIFERROMAGNETIC PHASE

To find the spin-wave spectrum in an antiferromagnetic phase with a magnetic order of the simple helix type (Ref. 8, p. 26), two circumstances must be taken into account.

1. The Holstein-Primakoff transformation must be carried out in a "rotating" coordinate frame.⁹ As a result, the initial Hamiltonian breaks up into two terms, $H = H_0 + H_{sw}$, where all the terms containing magnon operators are included in H_{sw} , while H_0 , which contains no magnon operators, describes the system in the "ground state," when it has no spin waves.

2. Since the crystal has a magnetic structure of the simple helix type, the conduction-electron spectrum is renormalized. A split and an unsplit spectrum modes appear, and subbands are produced. To find the spin-wave spectrum it suffices to take into account the exis-

tence of only the two lowest ones. We denote the unsplit branches by $\varepsilon_k^1 = \varepsilon_k$, $\varepsilon_k^2 = \varepsilon_{k^-q_0}$ and the split ones by

$${}^{\mathbf{s},\mathbf{s}}_{k} = \{(\varepsilon_{k} + \varepsilon_{k-q_{0}}) \mp [(\varepsilon_{k} - \varepsilon_{k-q_{0}})^{2} + (2JS)^{2}]^{\frac{1}{2}}\}/2.$$
(15)

The renormalized electron spectrum is the result of diagonalization of H_0 with the aid of the Bogolyubov transformation (Ref. 8, p. 111). To find the spin-wave spectrum we use the Green's function method. H_{int} is replaced in our case by H_{sw} . Summing a ladder sequence of diagrams of the type (2) and finding the pole of the magnon Green's function, we obtain the spectrum

$$E_q = E_s + \Pi(q), \quad E_s = \sum_{\mathbf{k},\mathbf{\ell}} \beta B_i^{\mathbf{k}} n(\varepsilon_{\mathbf{k}}^{\mathbf{i}}), \tag{16}$$

$$\Pi(q) = \sum_{k,i,j} \alpha^2 (A_{ij}{}^{kq} A_{ji}{}^{kq}) \frac{n(\varepsilon_k{}^i) - n(\varepsilon_k{}^j-q)}{\varepsilon_k{}^i - \varepsilon_{k-q}{}^j + E_q}, \qquad (17)$$

where

 $\alpha^2 = J^2 S/4N$, $\beta = J/2N$, $n(\varepsilon_k^i) = [\exp((\varepsilon_k^i - \mu)/T) + 1]^{-1}$, i, j = I, 2, 3, 4, B_i^k and A_{ij}^{kq} are smooth functions of ε_k^i and ε_{k-q}^i . It is important that

$$A_{11}{}^{kq} = A_{22}{}^{kq} = A_{12}{}^{kq} = A_{21}{}^{kq} = A_{33}{}^{kq} = A_{34}{}^{kq} = A_{44}{}^{kq} = A_{44}{}^{kq} = 0.$$
(18)

As a result, the denominator of (17) can contain only differences of the split and unsplit energies. No divergences of $\Pi(q)$, as in the spectrum of the ferromagnetic phase, arise therefore at $E_q = 0$, if q_0 (the wave vector of the simple helix) is such that the Fermi energy lies between the split branches ε_k^3 and ε_k^4 , i.e., $q_0 = 2k_F$.

It can be shown that $E_q > 0$ for any $q \neq 0$, and for $q \ll k_F$ there exists an acoustic solution $E_q \sim q$, if no account is taken of the presence of anisotropy, which is small at high temperature. Allowance for the anisotropic terms, as is clear from consideration of the ferromagnetic phase, should lead to the onset of an instability of an antiferromagnetic phase with decreasing temperature.

- ¹M. I. Darby and K. N. R. Taylor, Physics of Rare Earth
- Solids, Chapman & Hall, 1972 [Russ. transl., Mir, 1974].
 ²N. E. Dzyaloshinskii, Zh. Eksp. Teor. Fiz. 47, 336 (1964)
 [Sov. Phys. JETP 20, 223 (1965)].
- ³M. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954). T. Kasuya, Progr. Theor. Phys. (Kyoto), **16**, 45 (1956). K. Yosida, Phys. Rev. **106**, 893 (1957).
- ⁴S. V. Vonsovskii, Magnetism, Halsted, 1975.
- ⁵H. Calen and E. Calen, J. Phys. Chem. Sol. 27, 1271 (1966).
- ⁶A. M. Afanas'ev and Yu. P. Kagan, Zh. Eksp. Teor. Fiz. 43,
- 1456 (1962) [Sov. Phys. JETP 16, 1030 (1963)].
- ⁷A. V. Vedyaev and M. Kh. Usmanov, Fiz. Tverd. Tela (Leningrad) 23, 1456 (1981) [Sov. Phys. Solid State 23, 848 (1981)].
- ⁸S. V. Tyablikov, Metody kvantovoľ teorii magnetizma (Methods of Quantum Theory of Magnetism), Nauka, 1965 [Plenum, 1967].
- ⁹R. Elliott and F. Wedgwood, Proc. Phys. Soc. **81**, 846 (1963).

Translated by J. G. Adashko