

THE THEORY OF HELICOIDAL STRUCTURES IN ANTIFERROMAGNETS. II. METALS

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A theory of magnetic structures in antiferromagnetic metals is developed. In this case the periods of the structure are determined by the interaction between conduction electrons and the spins of the magnetic ions and are approximately equal to the inverse extremal diameters of the Fermi surface. The corresponding small parameter is $(\Theta/\epsilon_F)^{1/2}$, where Θ is the antiferromagnetic transition temperature and ϵ_F is the Fermi energy.

1. INTRODUCTION

IN a previous paper^[1] ¹⁾ the author developed the theory of the helicoidal structures in nonmetallic antiferromagnets. The method used in I was based on an examination of the symmetry properties of the thermodynamic potential Φ as a function of the "wave vector" of the magnetic structure \mathbf{f} ($f = 2\pi/L$, where L is the period of the magnetic structure) relative to the symmetry transformations of the paramagnetic phase. In particular, at temperatures close to the transition point Θ , it was sufficient to investigate the symmetry properties of the coefficients of the expansion of Φ in a power series in the mean spin density. (See I, Secs. 2 and 5.)

It was made clear that symmetry considerations permit two types of magnetic structure. To the first belong structures with vectors \mathbf{f} that take on special, highly symmetrical positions in the reciprocal cell of the paramagnetic phase. As shown by the analysis of E. Lifshitz^[2] (see also^[3]), these \mathbf{f} correspond to periods rigorously equal to 1, 2, 3, 4 (but not more) periods of the paramagnetic lattice. To the second type belong helicoidal superstructures with long periods. To a first approximation (at distances of the order of the interatomic spacings) the orientations of the spins in the superstructure are the same as in the structures just mentioned of the first type with a period equal to 1, 2, 3, 4 periods of the original lattice. In higher approximations, however, (at distances much greater than interatomic) beats with a greater period $2\pi/k$ ($k \ll 1/a$) are superposed on the "coarse" structure, with the result that the "coarse" structure "gradually" rotates from point to point about some selected axis. The

"wave vector" \mathbf{k} of the superstructures is small because they arise either from relativistic interactions or from strong anisotropy of the exchange forces.

It is obvious that symmetry considerations cannot eliminate "accidental" magnetic structures, which arise if the function $\Phi(\mathbf{f})$ has a minimum at those values of \mathbf{f} where symmetry does not require it. There is an essential difference between "accidental" structures and the aforementioned ones, however. In the latter case the "wave vectors" \mathbf{f} (but not the superstructure vector \mathbf{k} !) depend very weakly on temperature²⁾: in structures of the first type they vary only with the interatomic spacings, and in the structure of the second type also by virtue of changes in the vector \mathbf{k} , which itself represents a small addition. On the other hand, for an "accidental" structure the vector \mathbf{f} will change by an order of its magnitude with a change in the temperature T by an amount of order Θ . This circumstance readily permits recognition of the "accidental" structures from the experimental data.

The analysis presented in I started from the assumption that the thermodynamic potential $\Phi(\mathbf{f})$ and the coefficients of the quadratic terms of $a(\mathbf{f})$ in Landau's theory are analytic functions of the vector \mathbf{f} and can be expanded in a series in the vicinity of any point of the reciprocal lattice

²⁾It can be shown (this will be done in a following paper) that the period of the magnetic structure is always a multiple of the period of the paramagnetic phase, i.e., the vectors \mathbf{f} always have rational coordinates. Therefore, the variation of \mathbf{f} with temperature occurs by means of jumps from one rational point to another. In fact, however, the energies associated with these jumps are extremely small, and to the first approximation it can be assumed that \mathbf{f} varies continuously with temperature.

¹⁾Henceforth this paper will be referred to as I.

of the paramagnetic phase. This assumption did not evoke any doubts in the case of the nonconducting antiferromagnets considered in I. The situation changes, however, for magnetic metals and alloys. As we shall see, the interaction of the spins of the magnetic ions with the conduction electrons leads to singularities in the dependence of Φ and a on \mathbf{f} , resulting in minima in the functions $\Phi(\mathbf{f})$ and $a(\mathbf{f})$ that lie close to the singular points. The position of the singular points themselves is determined not by the symmetry properties of the lattice, but by the properties of the electronic Fermi surfaces—by the extremal diameters of the Fermi surfaces or by multiples of the latter. Hence the possible types of magnetic structures in metals are more diverse than in insulators; in particular, structures are possible in which the vector \mathbf{f} takes on an arbitrary asymmetrical position. The latter circumstance is confirmed by the large number of neutron diffraction investigations on rare-earth metals (see, for example, [4,5]).

The interaction between the spins of the magnetic ions and the conduction electrons is described by a Hamiltonian of the form

$$H_{int} = J \int \hat{\mathbf{s}}(\mathbf{r}) \psi^\dagger(\mathbf{r}) \boldsymbol{\sigma} \psi(\mathbf{r}) d\mathbf{r}, \quad (1)$$

where $\hat{\mathbf{s}}(\mathbf{r})$ is the spin density associated with the magnetic ions:

$$\hat{\mathbf{s}}(\mathbf{r}) = \sum_a \hat{\mathbf{S}}_a \delta(\mathbf{r} - \mathbf{r}_a),$$

$\hat{\mathbf{S}}_a$ are the spin operators of the ions, ψ and ψ^\dagger are second-quantization operators of the electrons, and $\boldsymbol{\sigma}$ are the Pauli matrices. The constant J determines the intensity of the interaction. For rare-earth metals J is readily related in order of magnitude with the temperature of transition Θ . Actually, the only source of the self-interaction of the spins of the f -shells of rare-earth ions is electron exchange (Kittel-Ruderman interaction). This interaction arises in the second-order perturbation theory approximation of the Hamiltonian (1) and its order of magnitude is J^2/ϵ_F , where ϵ_F is the Fermi energy. Comparing J^2/ϵ_F with the transition temperature Θ , we find

$$J \sim (\Theta \epsilon_F)^{1/2}. \quad (2)$$

In transition metals and alloys the situation is somewhat more complicated. If the principal contribution to the interaction between the magnetic ions comes from the Kittel-Ruderman interaction via s electrons, then the estimate (2) remains the same for J_{sd} . But if the principal role is played by effects associated with the overlap of wave

functions of the d band, then the quantity $(\Theta \epsilon_F)^{1/2}$ gives the upper limit for J_{sd} ($J_{sd} \lesssim (\Theta \epsilon_F)^{1/2}$). The interaction of the conduction electrons of the d band (if it is not filled) with the ionic core is in both cases equal in order of magnitude to $J_{dd} \sim \Theta$.

The first calculation of the periods of the magnetic structures in rare-earth metals at low temperatures on the basis of the interaction (1) was carried out by Yosida and Watabe.^[6] They calculated the Kittel-Ruderman exchange integral $J(a, b)$ as a function of the spacing between the ions and assumed that the minimum of the thermodynamic potential Φ as a function of \mathbf{f} coincided with the minimum of the Fourier component of this exchange integral $J(\mathbf{f})$. This situation, however, occurs only in the theories of magnetic structures of Yoshimori and Kaplan (see I, Sec. 5), against which serious objections were raised in I. We remark additionally that quasiclassical theories like those of Yoshimori and Kaplan are known to be inapplicable to the case of the so-called sinusoidal structures (see the beginning of Sec. 2), where the mean values of the spins of the ions are far from the nominal ones.³⁾

We present below a theory based on an exact calculation of the singularities in the thermodynamic potential Φ as a function of the vector \mathbf{f} .

2. MAGNETIC STRUCTURES AT LOW TEMPERATURES

We consider the two simplest variants of a magnetic structure: the so-called helicoidal structure (see I, Fig. 1) and the sinusoidal structure (Fig. 1). In addition, we restrict our-

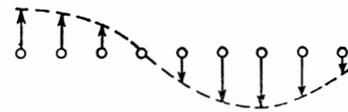


FIG. 1

selves to the case of a uniaxial crystal and assume that the “wave vector” of the structure is directed along the crystal axis. The corresponding mean density of the ion spin has the form

$$\mathbf{s}(\mathbf{r}) = \frac{1}{2}(\mathbf{s}_0 e^{i\mathbf{f}z} + \mathbf{s}_0^* e^{-i\mathbf{f}z}), \quad (3)$$

where for the sinusoidal structure \mathbf{s}_0 is a purely real or purely imaginary vector lying in some symmetrical direction, for example, to be specific, along the same z axis; for the helicoidal structure \mathbf{s}_0 is a complex vector lying in the xy plane.

³⁾A further discussion of the work of Yosida and Watabe is given in Sec. 2.

We shall now make clear what happens to the electronic spectrum and, in particular, to the Fermi surface when the metal becomes antiferromagnetic with spin density (3). Principally, the change in shape of the Fermi surface is due in this case to the change in the dimensions of the crystal cell in the direction z . As pointed out in the second footnote, the vector \mathbf{f} always has rational indices in the reciprocal lattice of the paramagnetic phase ($f = 2\pi p/qc$, where p and q are integers and c is the crystallographic cell dimension), and so, strictly speaking, the length of the new cell of the reciprocal lattice in the z direction will equal $2\pi/qc$. For our purposes, however, as can be shown (we shall not stop to do this), it can be assumed that the length of the new cell simply equals f in the first non-vanishing approximation for J/ϵ_F .

The most pronounced change in the character of the Fermi surface will occur if any part of it has an extremal diameter $2p_0$ directed along the z axis and f is close to $2p_0$ (see Fig. 2a, where the case of maximal diameter is shown, or Fig. 2b, where the chosen unit cell is shifted by $f/2$ relative to the cell in Fig. 2a). For $f > 2p_0$ the

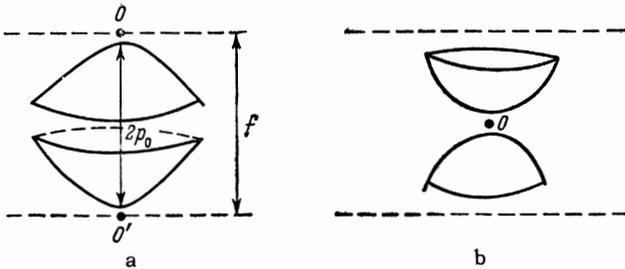


FIG. 2

Fermi surface near the point O , as can be seen from Fig. 2b, has the form of a two-cavity hyperboloid. For $f < 2p_0$ the Fermi surface begins to intersect itself (Fig. 3a); however, if account is taken of the interaction (1), then the degeneracy associated with the self-intersection is removed and the surface close to point O breaks up into two parts—a single-cavity hyperboloid and an enclosed elliptical surface (Fig. 3b).

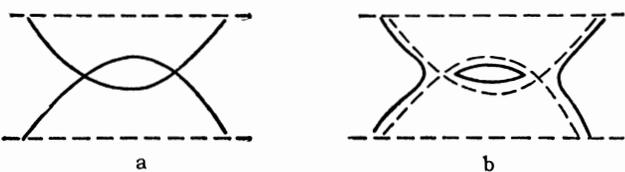


FIG. 3

Thus, at the point $f = 2p_0$ a change occurs in the topology of the Fermi surface: the closed surface

of Fig. 2a, b transforms to an open one (Fig. 3b), and besides this an additional, new closed surface arises. The first singularities in thermodynamic quantities associated with similar changes in topology were treated by I. Lifshitz.^[7] From his results it follows immediately that near $f = 2p_0$ the thermodynamic potential $\Phi(f)$ has a singularity of the form $J^{1/2}(f - 2p_0)^{5/2}$. For our purposes, however, it is necessary to take $\Phi(f)$ for $f - 2p_0 \sim Jp_0$, and so we shall carry out the calculation to the accuracy of terms of the order $J^2(f - 2p_0)$.

Then $\Phi(f)$ breaks up near to $f_0 = 2p_0$ into a sum of three terms:

$$\Phi(f) = \Phi(f_0) + \Phi_{\text{sing}}(f - f_0) + A \cdot (f - f_0), \quad (4)$$

$A \sim J^2$. The singular part of the potential Φ_{sing} arises because at $f - f_0 \lesssim f_0 J/\epsilon_F$, when the self-intersection of the Fermi surface takes place, the perturbation theory with respect to J/ϵ_F is inapplicable and it is necessary to take into account the change in the electronic spectrum near the point O (Fig. 2).

In Φ_{sing} we also include terms $\sim J^2$, but which have a non-analytic character with respect to $f - f_0$. Such terms arise only for $f - f_0 \gg f_0 J/\epsilon_F$; they include for example the well known Kohn singularity^[8]

$$\Phi_{\text{sing}} \sim J^2(f - f_0) \ln \frac{f_0}{|f - f_0|}.$$

It is important that only the electrons lying close to the Fermi surface, more precisely that part of it in the vicinity of the point O , give a contribution to Φ_{sing} . We note further that since only those electrons which are separated from the Fermi surface by a distance ζ such that $J \lesssim \zeta \ll \epsilon_F$ are important to us, we can neglect the scattering of electrons by spin waves and phonons, since, according to (2), $J \gg \Theta$, and the corresponding inverse relaxation times do not exceed in order of magnitude Θ and Θ_D (the Debye temperature), and for all magnetic metals $\Theta \sim \Theta_D$. (It is understood that the latter pertains only to temperatures T that are not too close to the transition temperature, when J becomes very small.) For this same reason, when $T - \Theta \sim \Theta$ we can neglect the effect of temperature ($T \lesssim \Theta \ll J$) and carry out the calculation for $T = 0$.

Thus, in calculating Φ_{sing} we can regard the electrons as noninteracting particles with some arbitrary dispersion law⁴⁾ $\epsilon_0(p)$. The situation

⁴⁾We observe, incidentally, as shown by Migdal^[9], that the form of the function $\epsilon_0(p)$ for $\epsilon_0 \gg \Theta$, Θ_D can differ substantially from its form for $\epsilon_0 \ll \Theta$, Θ_D .

is different with the term $A(f - f_0)$ in Eq. (4). It appears as the mean value of the effective spin Hamiltonian

$$\hat{H}_{\text{ion}} = \sum_{a,b} I(a, b) \hat{S}_a \hat{S}_b, \quad I \sim J^2 \sim \Theta. \quad (5)$$

The "exchange integral" $I(a, b)$ in Eq. (5) arises from the second-order perturbation theory with respect to the interaction (1) and contains the contribution of electrons situated far from the Fermi surface as well as from other Fermi surfaces, if such exist. (It is implied in this that in $I(a, b)$ there are no parts associated with Kohn singularities, the contribution of which has already been included in Φ_{sing} .) To say nothing of the impossibility of averaging over the ion spins in Eq. (5), since in general there is no small parameter in the problem, it is not even possible to calculate the "exchange integral" $I(a, b)$ itself, since for this it is necessary to know the energy level density of the electrons far from the Fermi surface, where the electrons can by no means be considered free. On the other hand, it is clear that the contribution \hat{H}_{ion} is a smooth function of f and can therefore be expanded in a power series in $f - f_0$. Moreover, since the vector \mathbf{f}_0 takes an arbitrary asymmetrical position in the reciprocal cell of the paramagnetic phase, this expansion begins, according to I, with terms linear in $f - f_0$, so that the contribution from the Hamiltonian (5) can be described by one phenomenological parameter $A \sim J^2$. The parameter A , of course, depends on temperature, and $dA/dT \sim A/\Theta$ for $T \sim \Theta$.

We proceed to calculate Φ_{sing} . For this it is necessary to determine how the spectrum of the electrons changes near the point O in Fig. 2 by virtue of their interaction (1) with the ion spin. Here the effect of the spins can obviously be taken into account by introducing an effective field acting on the electrons. It is important only to realize that this field by no means coincides with the mean spin density of the ions (3). The effective field will contain not only harmonics of the form e^{ifz} but also all the multiple harmonics e^{inifz} , where n is an arbitrary odd integer, with coefficients that in general agree in order of magnitude with the coefficient of the first harmonic. In addition, besides the harmonics of form e^{ifz} , it can include also harmonics of the form $e^{i(f+2\pi K)z}$, where K is an arbitrary period of the reciprocal lattice of the paramagnetic phase. Therefore in what follows we shall understand by f the quantity $nf + 2\pi K$, where f is the true magnetic-structure "wave vector" entering in (3), for when $f \sim 2p_0$ the contribution of each harmonic of the effective field to Φ_{sing} can be considered independently.

Thus the problem has been reduced to a determination of the spectrum of the electrons in a periodic external field of the type (3). Since we are interested in the spectrum near the points O and O' in Fig. 2, with coordinates $(0, 0, f/2)$ and $(0, 0, -f/2)$, i.e., near the zone intersection, it is necessary to solve the corresponding secular equation (see, for example, [10]). For the case of the sinusoidal structure it has the form

$$\begin{vmatrix} \epsilon_0(\mathbf{p}) - \epsilon & j\sigma_z \\ j\sigma_z & \epsilon_0(\mathbf{p} - \mathbf{f}) - \epsilon \end{vmatrix} = 0,$$

where j is some constant ($j \sim J \sim (\Theta/\epsilon_F)^{1/2}$). Solving this, we find

$$\begin{aligned} \epsilon_{1,2} &= 1/2(\epsilon_0(\mathbf{p}) + \epsilon_0(\mathbf{p} - \mathbf{f})) \\ &\mp [1/4(\epsilon_0(\mathbf{p}) - \epsilon_0(\mathbf{p} - \mathbf{f}))^2 + j^2]^{1/2}, \\ \epsilon_{3,4} &= \epsilon_{1,2}. \end{aligned} \quad (6)$$

For the helicoidal case the equation is somewhat different:

$$\begin{vmatrix} \epsilon_0(\mathbf{p}) - \epsilon & j\sigma_x \\ j\sigma_x & \epsilon_0(\mathbf{p} - \mathbf{f}) - \epsilon \end{vmatrix} = 0,$$

$\sigma_{\pm} = \sigma_x \pm i\sigma_y$. Two of its solutions coincide with $\epsilon_{1,2}$ of (6), and $\epsilon_3 = \epsilon_0(\mathbf{p})$, $\epsilon_4 = \epsilon_0(\mathbf{p} - \mathbf{f})$. Thus in the helicoidal structure in the lowest order of j/ϵ_F the degeneracy associated with the intersection is not completely lifted. The lifting occurs for $\epsilon_{3,4}$ only if terms of the order j^4/ϵ_F^3 , which we shall neglect, are taken into account. We shall therefore consider only the solution $\epsilon_{1,2}$. All the following formulas will be written for the case of the helicoidal structure; to change to sinusoidal structure one must double the coefficients α and β in all formulas.

For the case of maximum diameter shown in Fig. 2a, the functions $\epsilon_0(\mathbf{p})$ and $\epsilon_0(\mathbf{p} - \mathbf{f})$ have near the point $(0, 0, f/2)$ the form ($p_3 \equiv p_z$)

$$\begin{aligned} \epsilon_0(\mathbf{p}) &= \epsilon_f + (p_1^2 + p_2^2) / 2m + u(p_3 - f/2), \\ \epsilon_0(\mathbf{p} - \mathbf{f}) &= \epsilon_f + (p_1^2 + p_2^2) / 2m - u(p_3 - f/2), \end{aligned} \quad (7)$$

$\epsilon_f = \epsilon_0(\mathbf{f}/2)$, where m is a quantity of the order of the mass of the free electron m_0 , and u is equal in order of magnitude to the Fermi velocity

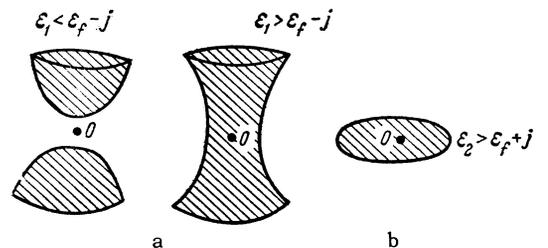


FIG. 4

v_F. Substituting (7) in (6), we find

$$\epsilon_{1,2} = \epsilon_f + (p_1^2 + p_2^2) / 2m \mp (u^2 p_3^2 + j^2)^{1/2}; \quad (8)$$

here we have transferred the origin to the point (0, 0, f/2) (point O in Fig. 2b).

The constant-energy surfaces are shown in Fig. 4a, b. From this it can be seen how the Fermi surface (i.e., the surface $\epsilon_1 = \epsilon_2 = \mu$, where μ is the chemical potential) changes with a change in f. For $\epsilon_f > \mu + j$ the Fermi surface near the point O is a two-cavity hyperboloid; for $\epsilon_f < \mu + j$ this hyperboloid turns into a single-cavity one; finally, for $\epsilon_f < \mu - j$ a new closed Fermi surface appears.

In calculating Φ_{sing} we proceed in the following manner. We first determine the change in the electron spin density $\delta\nu(\epsilon)$ near the point O in Fig. 4 due to the appearance of a magnetic structure. To this end we first calculate $\nu(\epsilon)$ for the spectrum (8) from the formula

$$\nu(\epsilon) = \frac{1}{(2\pi)^3} \oint \frac{dS}{v},$$

where dS is an element of area of the surface $\epsilon(\mathbf{p}) = \epsilon = \text{const}$, and v is the velocity of the electron on this surface ($v = |\nabla_{\mathbf{p}}\epsilon(\mathbf{p})|$), and subtract from it the corresponding expression for $j \rightarrow 0$. The quantity obtained in this way will be, with accuracy to terms $\sim j^2$ for $\epsilon \gg j$, the part of $\nu(\epsilon)$ singular in ϵ . After this we determine the change in the number of particles $\delta N(\mu)$ as a function of the chemical potential:

$$\delta N(\mu) = \int_0^{\mu} \delta\nu(\epsilon) d\epsilon$$

and finally the singular part of the thermodynamic potential in the variables T, V, and $\mu - \Omega_{\text{sing}}$ from the formula

$$\Omega_{\text{sing}} = - \int_0^{\mu} d\mu' [\delta N(\mu', \epsilon_f) - \delta N(\mu', \mu)].$$

In the last formula we performed a subtraction corresponding to our expanding the potential Ω in powers of f near the point f_0 such that $\epsilon_{f_0} = \mu$. All the integrals over ϵ encountered in this calculation converge at the upper limit, in accord with the fact that only electrons near the Fermi surface give a contribution to Ω_{sing} . There is one exception—a weak logarithmic divergence in the last formula for Ω_{sing} , which is easily eliminated by cutting off at $\epsilon \sim \epsilon_f$.

The calculation leads to the following expression for $\delta\nu(\epsilon)$:

$$\delta\nu(\epsilon) = \begin{cases} -\alpha\eta, & |\eta| < j, \\ -\alpha\eta + \alpha(\eta^2 - j^2)^{1/2} \text{sign } \eta, & |\eta| > j, \end{cases} \quad (9)$$

where $\eta = \epsilon - \epsilon_f$ and $\alpha = m/2\pi^2 u$. For Ω_{sing} we obtain from this formula

$$\Omega_{\text{sing}}(\mu) = -\frac{1}{6} \alpha \zeta^3 + \frac{1}{2} \alpha j^2 \zeta \ln \frac{\Lambda}{2j} + \frac{1}{6} \alpha j^3 \Psi\left(\frac{\zeta}{j}\right), \quad (10)$$

where $\zeta = \epsilon_f - \mu$, Λ is a constant of the order of the Fermi energy ϵ_f , and

$$\Psi(x) = \begin{cases} 0, & |x| < 1, \\ [(x^2 + 2)(x^2 - 1)^{1/2} - 3|x| \text{Arch } |x| \text{sign } x], & |x| > 1. \end{cases} \quad (11)^*$$

The corresponding addition to Φ_{sing} is obtained from (10) (to terms $\sim j^4$), if one replaces the μ therein by $\mu_0(p, T)$, the chemical potential of the metal in the paramagnetic state as a function of pressure and temperature. Then $\zeta = \epsilon_f - \mu$ transforms to the quantity $\zeta = 1/2 u (f - 2p_0)$, where $2p_0$ is the maximum diameter of the Fermi surfaces.

For $\zeta \gg j$, the expression for Φ_{sing} takes the form

$$\Phi_{\text{sing}} = \frac{1}{2} \alpha j^2 \zeta \ln \frac{\Lambda}{|\zeta|}, \quad (12)$$

which corresponds to the Kohn singularity.^[8] Near the points $\zeta_0 = \pm j$, the function Φ_{sing} has a Lifshitz type of singularity^[7]:

$$\Delta\Phi = \pm^{4/15} \alpha \sqrt{2j} (|\zeta| - j)^{3/2}, \quad |\zeta| > j. \quad (13)$$

As was mentioned at the beginning of this section, to the expression Φ_{sing} there must be added a term $A\zeta$ with the constant A equal in order of magnitude to $\alpha j^2 \sim \Theta p_0^3 / \epsilon_f$:

$$\delta\Phi(\zeta) = \Phi_{\text{sing}}(\zeta) + A(\zeta). \quad (14)$$

The “wave vector” of the magnetic structure is determined from the minimum condition for the function $\delta\Phi$ with respect to ζ . We begin with the case where j is so small that not only is the condition $j \ll \epsilon_f$ fulfilled but also the much stronger inequality $\ln(\epsilon_f/j) \gg 1$. Then over the entire range of variation of ζ where a minimum in Eq. (14) is possible, we can use Eq. (12) for Φ_{sing} , so that

$$\delta\Phi(\zeta) = \frac{1}{2} \alpha j^2 \zeta \ln \frac{\Lambda}{|\zeta|} + A\zeta. \quad (15)$$

For $A > 0$ Eq. (15) is a monotonically increasing function with no minimum. For $A < 0$ it has a minimum and a maximum situated respectively at the points $-\zeta_{\text{min}}$ and ζ_{min} , where

$$\zeta_{\text{min}} = \Lambda e^{-\gamma}, \quad \gamma = 1 - 2A / \alpha j^2 \quad (16)$$

*Arch = cosh⁻¹.

(see Fig. 5). The condition of applicability of Eqs. (15) and (16) is $\zeta_{\min} \ll \Lambda \sim \epsilon_F$; but since $|A| \sim j^2$, this inequality, even if fulfilled, is not fulfilled with a very large numerical margin of the type $e \gg 1$, so that it is perfectly possible that in general no minimum at all will exist within the limits of applicability of (15) and (16).

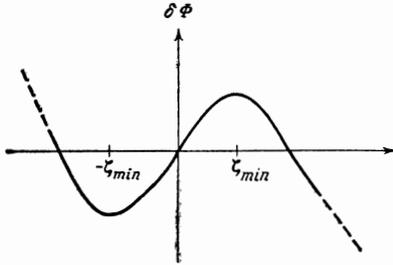


FIG. 5

For real antiferromagnetic metals the condition $\ln(\epsilon_F/j) \gg 1$ is apparently not fulfilled in general; their transition temperatures are of the order of 10^2 °K, and $j/\epsilon_F \sim 10^{-1}$. In this case it is necessary to use the exact formula (10) for Φ_{sing} . An investigation of this shows that Eq. (14) has a minimum and a maximum only under the condition $0 > A > -1/2\alpha j^2 \ln(\Lambda/2j)$. For $A > 0$, Eq. (14) is again a monotonic increasing function, and for $A < -1/2\alpha j^2 \ln(\Lambda/2j)$ the function $\delta\Phi$ decreases monotonically.

The minimum and maximum of $\delta\Phi$ are located at the symmetrical points $\pm\zeta_{\min}$, as in Fig. 5, and are determined from the transcendental equation

$$x_0^2 - 1/3\psi'(x_0) = \lambda,$$

where ψ' is the derivative of the function ψ in Eq. (11), $x_0 = \zeta_{\min}/j$, and $\lambda = \ln(\Lambda/2j) + 2A/\alpha j^2$ is a dimensionless positive parameter of order unity. Clearly, ζ_{\min} is of the order of j ($\zeta_{\min} \sim j$).

The states just found are metastable, since the depth of the minimum in the potential $\delta\Phi$ in both cases considered is in order of magnitude respectively equal to $\Theta e^{-\gamma}$, $j^3/\epsilon_F^2 \sim \Theta(\Theta/\epsilon_F)^{1/2} \ll \Theta$, whereas the total change of $\delta\Phi$ is of the order of Θ (dashed lines in Fig. 5).

Turning to the case of very small j ($\ln(\epsilon_F/j) \gg 1$), we note that Eq. (15) for $\delta\Phi$ could be obtained in this case directly from the effective spin Hamiltonian (5) if in \hat{H}_{ion} we were to substitute the Kittel-Ruderman exchange integral $J(a, b)$ in place of $I(a, b)$. Consequently the inequality $\ln|\epsilon_F/J| \gg 1$ with J from Eq. (1) represents the condition under which the magnetic properties of the metal are truly described by a Heisenberg

Hamiltonian. This justifies to some extent the approach adopted by Yosida and Watabe^[6] (see end of Sec. 1). Nonetheless, their calculation can scarcely be regarded as correct. In the first place, in the calculation of the non-singular part of the Kittel-Ruderman exchange integral, where, as mentioned above, it is necessary to take into account the contribution of electrons that lie deeply under the Fermi surface, they used the free-electron model. Further, they completely neglected the term $A(f - f_0)$ by remaining in the framework of the theory of Yoshimori and Kaplan; as a result they succeeded in obtaining for $\delta\Phi$ a curve with a minimum only by the simultaneous calculation of several singular points of the type $2p_0 + 2\pi K$. These were found to be close, however, because of their choice of perfect spheres as Fermi surfaces, i.e., surfaces all of whose diameters are maximal. But the real Fermi surfaces in a metal surely do not possess such properties.

We shall consider another type of Fermi surface with an extremal diameter—a surface in the form of a ‘‘neck’’ (Fig. 6). In this case the spec-

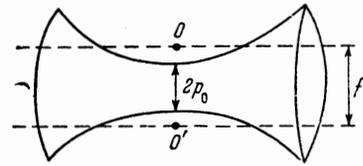


FIG. 6

trum of the electrons in the paramagnetic phase $\epsilon_0(\mathbf{p})$ close to the points O and O' in Fig. 6 has the form

$$\begin{aligned} \epsilon_0(\mathbf{p}) &= \epsilon_f + p_1^2/2m_1 - p_2^2/2m_2 + u(p_3 - f/2), \\ \epsilon_0(\mathbf{p} - \mathbf{f}) &= \epsilon_f + p_1^2/2m_1 - p_2^2/2m_2 - u(p_3 - f/2), \end{aligned}$$

$m_1, m_2 \sim m_0$, and the spectra $\epsilon_{1,2}$ in the presence of magnetic structure are expressed by the formulas

$$\epsilon_{1,2} = \epsilon_f + p_1^2/2m_1 - p_2^2/2m_2 \mp (u^2 p_3^2 + j^2)^{1/2}. \quad (17)$$

The shape of the corresponding surfaces of constant energy close to the point O (Fig. 6) is shown in Fig. 7a, b. Repeating the calculations presented above for the case of maximum diameter, we obtain the following expression for the increment $\delta\nu$ to the level density:

$$\delta\nu(\epsilon) = \begin{cases} -\beta(j^2 - \eta^2)^{1/2}, & |\eta| < j, \\ 0, & |\eta| > j, \end{cases} \quad (18)$$

$\beta = (m_1 m_2)^{1/2}/2\pi^2 u$, and for the singular part of the potential Φ_{sing} :

$$\Phi_{\text{sing}} = \begin{cases} 1/4 \pi \beta j^2 |\zeta|, & |\zeta| > j, \\ 1/2 \beta j^3 \varphi(\zeta/j), & |\zeta| < j, \end{cases} \quad (19)$$

where

$$\varphi(x) = x \arcsin x + (1-x^2)^{1/2} - 1/3(1-x^2)^{3/2}.$$

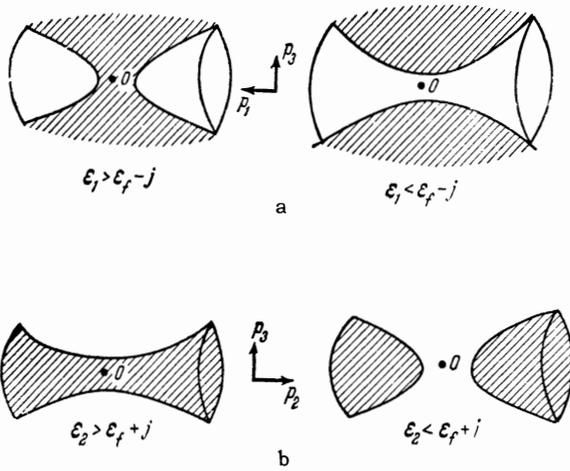


FIG. 7

A minimum of Eq. (14) for $\delta\Phi$ with the Φ_{sing} of Eq. (19) exists only under the condition $|A| < 1/4\pi\beta j^2$ and is determined by the equation

$$\arcsin \frac{\zeta}{j} + \frac{\zeta}{j} \left(1 - \frac{\zeta^2}{j^2}\right)^{1/2} = -\frac{2A}{\beta j^2}. \quad (20)$$

The quantity ζ_{min} is always less than j and agrees with the latter in order of magnitude. For $|A| > 1/4\pi\beta j^2$ the function monotonically increases ($A > 0$) or decreases ($A < 0$). The form of the dependence of $\delta\Phi$ on ζ for $|A| < 1/4\pi\beta j^2$ is shown in Fig. 8.

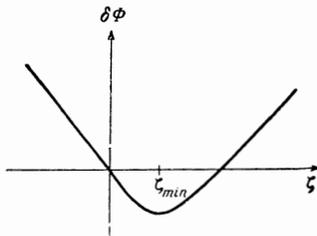


FIG. 8

We note that since it is always true that $|\zeta_{\text{min}}| < j$, then the results for the "neck" type of Fermi surface cannot be obtained with the aid of the Heisenberg-type Hamiltonian (5) nor from any relation between j and ϵ_F .

3. MAGNETIC STRUCTURES NEAR THE PHASE TRANSITION POINT

At temperatures close to the transition point

⊙ the parameter j tends to zero⁵⁾ together with the average spin of the ions s ($j = bs$). Hence the perturbation theory becomes valid for all values ζ ($\sim f - f_0$) and to find the singular part of the potential Φ (or the coefficient a of the quadratic terms in the Landau theory: $\Phi = as^2$) one can use the effective Hamiltonian (5) of the Heisenberg type, understanding by $I(a, b)$ the total Kittel-Ruderman exchange integral $J(a, b)$. However, it is necessary to keep in mind that even when $T \rightarrow \ominus$ electrons that are at a distance $\zeta \lesssim \ominus$ from the Fermi surface cannot be considered free. This is because the scattering of the electrons by the ion spin fluctuations, which is maintained even in the paramagnetic region, i.e., when $j = 0$, leads to a smearing of the electronic spectrum precisely by an amount of order \ominus , which must be taken into account in the calculation of $J(a, b)$. At the same time we must also consider the influence of temperature, which effectively smears the spectrum to the same extent.

The calculation of the dependence $\Phi(f)$ close to the transition point has been carried out by de Gennes and Saint-James.^[11] They started from an equation for $\Phi(f)$ in the form

$$\delta\Phi(f) = J(f)s^2, \quad (21)$$

where $J(f)$ is the Fourier component of the Kittel-Ruderman exchange integral $J(a, b)$ calculated with account of scattering by the fluctuations of the ion spins and by the impurities. Equation (21), however, is obtained if it is assumed in the calculation of the mean value of the spin Hamiltonian (5) that not only is the average spin s small, but also its fluctuations $\langle \hat{S}_a \hat{S}_b \rangle$. This latter assumption is by no means justifiable, since the fluctuations (accounted for, incidentally, in^[11] in a calculation of the electron motion) are not only not small, but on the contrary become anomalously large when $T \rightarrow \ominus$. In addition, the effect of temperature was not considered in^[11], and a free-particle model was used for the electrons lying deep below the Fermi surface.

We shall now show that basic qualitative judgments can be made without unwieldy calculations in the region $\zeta \lesssim \ominus$. For this we consider the dependence $\delta\Phi(f)$ [or $\delta a(f)$] for f such that $\zeta \gg \ominus$. In this region one can neglect the depend-

⁵⁾We note that the amplitudes of the highest harmonics (mentioned on p. 226) of the effective field of the type e^{inf} , $n > 1$ and odd, go to zero like s^n and can be neglected. It is understood at the same time that "harmonics" with "wave vectors" of the form $f + 2\pi K$, where K is an arbitrary period of the reciprocal lattice of the crystal, are retained.

ence on the temperature and on the mean free path, and use directly the results of the preceding section for $\zeta \gg j$. We have

$$\delta a(f) = \frac{1}{2} \alpha b^2 \zeta \ln \frac{\Lambda}{|\zeta|} + d\zeta \quad (22)$$

for the maximum diameter, and

$$\delta a(f) = \frac{1}{4} \pi \beta b^2 |\zeta| + d\zeta \quad (23)$$

for a "neck" type Fermi surface. The term $d\zeta$ ($d \approx \alpha b^2$), like the quantity $A\zeta$ ($A \sim j^2 \alpha$) in the equations of the preceding section, accounts for the contribution of the deep electrons and the fluctuations of the ion spins.

Since Eq. (22) completely agrees in form with Eq. (15), all the conclusions made in connection with the latter carry over also to the case $T \rightarrow \Theta$. Equation (22) will have a minimum and maximum at the points $\mp \zeta_{\min}$, $\zeta_{\min} \gg \Theta$, if $d < 0$, and $\Theta \ll \epsilon_F \exp(-1 + 2d/\alpha b^2)$. In all the remaining cases $\delta a(f)$ for $\zeta \gg \Theta$ is a monotonic function. In principle it is impossible to eliminate the appearance of an additional minimum in the region $\zeta \sim \Theta$. Its depth, estimated according to dimensional considerations, equals⁶⁾ $\Theta \zeta_{\min} / \epsilon_F \sim \Theta^2 / \epsilon_F$, which is very much less than the value of $\delta a(f)$ for $\zeta \gg \Theta$ ($\delta a(f) \sim \Theta \zeta / \epsilon_F$). Consequently, the state for $\zeta_{\min} \sim \Theta$ will in the best case be metastable (Fig. 9), and thus the calcula-

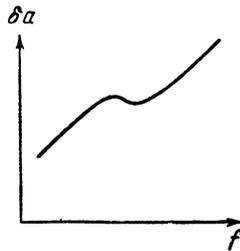


FIG. 9

tion of electron scattering in the case of maximal diameter does not bring in anything new.

In the case of a "neck" type Fermi surface, Eq. (23) shows that when $|d| < \frac{1}{4} \pi \beta b^2$, $\delta a(f)$ increases on both sides of the point $\zeta = 0$ at large distances from the latter. The calculation of the position of the minimum requires extremely unwieldy computations that take into account the effect of finite temperature and electron scattering; it is clear, however, that in order of magnitude $\zeta_{\min} \lesssim \Theta$.

We shall now discuss the dependence of the periods of the magnetic structure on temperature (see also the second footnote). In all the selected

⁶⁾It should be taken into account that $\delta a(f)$ vanishes at the point $\zeta = 0$.

cases the "wave vector" of the structure is rather rigidly "tied-in" with the value of the corresponding extremal diameter or with a quantity that is a whole number of times less (or, finally, with a quantity that differs from the first two by an arbitrary period of the reciprocal lattice): $\zeta_{\min} \lesssim \Theta$ for $T \rightarrow \Theta$, $\zeta_{\min} \lesssim (\Theta \epsilon_F)^{1/2}$ at arbitrary temperatures. On the other hand, the variation with temperature of the coefficients A and d in Eqs. (14), (22), and (23) is the only source of the temperature dependence of ζ_{\min} . Hence, although A and d themselves change strongly with temperature ($\Delta A/A \sim \Delta d/d \sim \Delta T/\Theta$), because of the aforementioned "rigidity" of the quantities ζ_{\min} the relative changes of the "wave vector" are equal in order of magnitude to

$$\frac{\Delta f}{f} \sim \frac{\Delta \zeta_{\min}}{\epsilon_F} \sim \left(\frac{\Theta}{\epsilon_F}\right)^{1/2} \frac{\Delta T}{\Theta} \sim 10^{-1} \frac{\Delta T}{\Theta}$$

at low temperatures and

$$\frac{\Delta f}{f} \sim \frac{\Theta}{\epsilon_F} \frac{\Delta T}{\Theta} \sim 10^{-2} \frac{\Delta T}{\Theta}$$

for $T \rightarrow \Theta$. This situation is evidently observed over a wide temperature interval in Er and Ho.^[4,5]

The situation changes sharply if with changing temperature the coefficients A and d begin to approach values at which the inequalities that are the conditions for the existence of minima are violated. Then the structure either abruptly transforms to some other (like the transition from the antiferromagnetic state to a purely ferromagnetic state in Dy^[4,5]), or the period begins rapidly to change with temperature, as in Er^[4,5] (we ignore here the possible change in the orientation of the spins of the ions).

As a result of the interaction of the spins with the electrons there arises a tendency toward the formation of the "accidental" structures mentioned in the introduction, the period of which changes by one order of its magnitude when $\Delta T \sim \Theta$. In fact, let us consider any Fermi surface with a maximum diameter $2p_0$. Near $f = 2p_0$ the singular part of the potential Φ is an increasing function of f or $\zeta \sim f - 2p_0$ (curve 1 in Fig. 10).

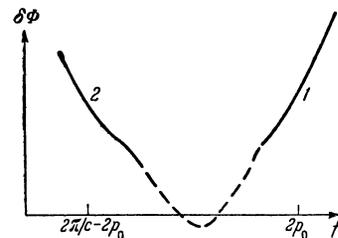


FIG. 10

On the other hand, there always exists a vector f' "auxiliary" to f such that $2\pi/c - f'$ is also close to $2p_0$ (c is the period of the lattice of the paramagnetic phase), so that for the structure with vector f' the effective-field harmonic $\exp[i(f' - 2\pi K)z]$ with $K = 1/c$ will also be "resonant." The singular part of Φ close to $f = 2\pi/c - 2p_0$ (an increasing function of $\zeta = 2\pi/c - f - 2p_0$) now becomes a decreasing function of f (curve 2, Fig. 10). For $p_0 > \pi/2c$ the arrangement of curves 1 and 2 will be such, as in Fig. 10, as to produce an "accidental" minimum. The helicoidal structure in Dy ^[4,5] is apparently an "accidental" structure of this type.

In conclusion, we remark that in actual cases of a different kind the extremal diameters and quantities that are multiples of them can in principle be arranged close to each other, and it will no longer be possible to take the contribution of each of them into account independently, as was done above. It would scarcely be worthwhile, however, to carry through the corresponding calculations until reliable experimental information about the shape of the Fermi surfaces in rare-earth metals appears.

¹I. E. Dzyaloshinskiĭ, JETP 46, 1420 (1964), Soviet Phys. JETP 19, 960 (1964).

²E. M. Lifshitz, JETP 11, 253 (1941).

³L. D. Landau and E. M. Lifshitz, *Statisticheskaya fizika* (Statistical Physics), Gostekhizdat, 1951 (Engl. Transl., Addison-Wesley, Reading, Mass., 1958).

⁴Wilkinson, Koehler, Wollan, and Cable, J. Appl. Phys. 32, 48S, 49S (1961).

⁵Koehler, Cable, Wollan, and Wilkinson, J. Phys. Soc. Japan 17, Supplement BIII, 32 (1962).

⁶K. Yosida and A. Watabe, Progr. Theoret. Phys. (Kyoto) 28, 361 (1962).

⁷I. M. Lifshitz, JETP 38, 1569 (1960), Soviet Phys. JETP 11, 1130 (1960).

⁸W. Kohn, Phys. Rev. Letters 2, 393 (1959).

⁹A. B. Migdal, JETP 34, 1438 (1958), Soviet Phys. JETP 7, 996 (1958).

¹⁰R. E. Peierls, Quantum Theory of Solids, Clarendon Press, Oxford, 1955 (Russ. Transl., IIL, 1956).

¹¹P. G. de Gennes, J. phys. radium 23, 630 (1962); P. G. de Gennes and D. Saint-James, Solid State Communications 1, 62 (1963).