Contribution to the band theory of antiferromagnetism

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New properties due to the influence of the collectivization of magnetic electrons on the spatial distribution and the temperature dependence of the magnetic moment are predicted for collinear antiferromagnets. In contrast to the molecular-field theory, in which the local magnetic moment is proportional to the temperature-dependent energy of the electron spin splitting (to the molecular field), the new temperature dependence of the magnetic moment of antiferromagnets, adduced in this paper, is due to the variation of the electron wave functions with temperature. It is shown that the critical exponent β, which characterizes the behavior of the local moment ($\sim(T_N-T)^\beta$) near the Neel temperature T_N, takes on the value 1/2 that follows from the molecular field theory only for antiferromagnets whose chemical and magnetic unit cells coincide. When the cells do not coincide, the critical exponent turns out to be 3/2 in the model considered by us. New regularities have been observed, characterizing the properties of magnetic excitations of antiferromagnets, and due to the motion of the collectivized magnetic electrons. The effect of the interaction with the Stoner excitations on the dispersion law of the antiferromagnons is determined. It is shown that the magnon spectrum can differ significantly from the linear spectrum typical of dielectrics, and has a square-root singularity near the boundary of the region of the Stoner excitations. Interband spin waves and collisionless damping of antiferromagnons by single-particle interband excitations is considered; this damping can be predominant in pure crystals at low temperatures.

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1. Weiss's molecular-field hypothesis has led to substantial progress in the theory of magnetically ordered substances. A definite interpretation of this hypothesis is given by the model of direct (Heisenberg) exchange between electrons of neighboring atoms. In this model, each of the atoms has its own magnetic moment with a value determined by Hund's rule. The deviations between the atomic magnetic moments of real magnets from those predicted by Hund's rule has led to the development of the band theory of magnetism, the success of which is due to Stoner's relatively simple molecular-field model.[1] In Stoner's theory, the collectivized electrons are situated in an effective magnetic field due to the self-consistent action of the electrons and proportional to the magnetization. This theory is not directly applicable to the description of complex magnetic structures, say antiferromagnets, in which there is no macroscopic magnetization. In the theory of antiferromagnetism the approach mainly developed is one with an assumed localization of the magnetic moments on atoms that interact either directly (direct exchange) or indirectly (via the conduction electrons or via the localized electrons of nonmagnetic atoms).[2-4]

The band theory of antiferromagnetism deals also with conducting antiferromagnets, in which the ground state of the collectivized electrons is the spin-density wave.[5] The study of such substances was initiated by Overhauser[6] and has led to a definite success because of the observation of the unusual magnetic properties of pure chromium, in which, in particular, the period of the magnetic structure turned out to be commensurate with the period of the crystal lattice.

It can be stated that the band theory of collinear antiferromagnets (AF) is still not sufficiently advanced. A simple model of a collinear band AF was proposed by Englert and Antonoff.[7] They have considered a nonconducting AF with two bands in which the electrons were fully polarized in opposite directions. Neglecting the intraband interaction of the electrons, they obtained the spectrum of the transverse spin waves, antiferromagnons, which have, just as the Heisenberg AF, a linear dispersion law.

The excitations in an antiferromagnetic Fermi liquid, using a model of two degenerate band, were considered by Akhiezer and Chudnovskiĭ,[8] who obtained for the antiferromagnons, just as in[7], a linear dispersion law.

In the present paper we discuss, on the basis of the electron-fluid theory,[9,10] the spatial distribution and the temperature dependence of the magnetic moment in a collinear AF. We show here that the magnetic moment per lattice site is, generally speaking, not a linear function of the energy of the spin splitting of the bands, $\hbar\Omega_{0\mathbf{f}}$, as it is assumed, following Weiss,[2] in the molecular-field theory, and has a complicated temperature dependence governed not only by the functional $\Omega_{0\mathbf{f}}$ dependence, but also by the variation of the wave functions of the electron-fluid quasiparticles with changing temperature. Analysis of magnetic excitations in conducting AF has revealed that the motion of the collectivized magnetic d-electrons leads to a substantial change of the spectrum of the transverse spin waves in comparison with the case of dielectrics. For waves that are not too long, the magnon spectrum differs significantly from linear because of the interaction with the single-particle (Stoner) excitations of the magnetic electrons, which leads under certain conditions also to a collisionless damping of the spin waves. In addition to magnons, conducting AF can have also interband spin-wave modes having a zero-sound character. We discuss also the possibility of collisionless damping of antiferromagnons, due to the decay of the spin wave into single-particle interband excitations.

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We consider first the ground state of an AF, which we shall assume to be determined essentially by the d-electrons of the transition-element atoms. The influence of the "nonmagnetic" s and p electrons will henceforth be assumed small. Neglecting the weak spin-orbit interaction, the wave function $\varphi_{t\mathbf{p}\sigma}(\mathbf{r})$ of the quasiparticles of the electron fluid of a magnet is the product of the spin wave function $\varphi_{t\mathbf{p}}(\mathbf{r})$ and of a coordinate-independent spinor. The band subscript t, the quasimomentum $\mathbf{p}$, and the spin variable $\sigma=\pm1$ are here the quantum numbers of the Bloch representation. The density of the magnetic moment in the ground state of a collinear magnet is determined here mainly by the relation

$$M(\mathbf{r})=\mu_0\sum_{t\mathbf{p}}|\varphi_{t\mathbf{p}}(\mathbf{r})|^2[n_F(\varepsilon_{t\mathbf{p}}^+)-n_F(\varepsilon_{t\mathbf{p}}^-)], \tag{1}$$

where $n_F(\varepsilon_{t\mathbf{p}}^\sigma)$ is the Fermi distribution function of quasiparticles with energy $\varepsilon_{t\mathbf{p}}^\sigma=\varepsilon_{t\mathbf{p}}-\sigma\hbar\Omega_{0t}(\mathbf{p})/2$. The spin-splitting energy $\hbar\Omega_{0t}$ is determined from the equation[11]

$$\hbar\Omega_{0t}(p)=-2\sum_{t_1p_1}\Psi(t\mathbf{p},t_1\mathbf{p}_1;t_1\mathbf{p}_1,t\mathbf{p})[n_F(\varepsilon_{t_1\mathbf{p}_1}^+)-n_F(\varepsilon_{t_1\mathbf{p}_1}^-)]. \tag{2}$$

The function $\hat{\Psi}$, as is customary in Fermi-liquid theory, takes into account here, in addition to the exchange effects, also the correlation interaction of the electrons. In the Hartree-Fock approximation the expression for the function $\hat{\Psi}$ is given in the Appendix.

Integrating (1) over the crystal volume we obtain the magnetization M (per unit volume). In the antiferromagnetic state there is no magnetization:

$$M=\sum_t m_t=0, \tag{3}$$

but since the electrons are polarized in each d band, it follows that

$$m_t=\mu_0\sum_{\mathbf{p}}[n_F(\varepsilon_{t\mathbf{p}}^+)-n_F(\varepsilon_{t\mathbf{p}}^-)]\neq0. \tag{4}$$

It is convenient to expand the functions $\varphi_{t\mathbf{p}}(\mathbf{r})$, which correspond to magnetic d electrons, in the atom-like wave functions $\Phi_\mu(\mathbf{r}-\mathbf{n}_\alpha)$:

$$\varphi_{t\mathbf{p}}(\mathbf{r})=N^{-1/2}\sum_{\mathbf{n}_\alpha\alpha\mu}\exp(i\mathbf{p}\mathbf{n}_\alpha/\hbar)a_{t\mu}(\mathbf{p},\alpha)\Phi_\mu(\mathbf{r}-\mathbf{n}_\alpha), \tag{5}$$

in analogy with the procedure used in the strong-coupling approximation (see[12]). The subscript μ ($\mu=1,2,\ldots,5$) numbers here the states of the d electron in the atom; $\mathbf{n}_\alpha$ are the lattice vectors corresponding to the magnetic sites of sort α; N is the number of magnetic atoms in the crystal. We neglect here the effect exerted here on the d-band structure by the nonmagnetic atoms contained in the AF, and assume that the magnetic atom are chemically indistinguishable. The non-equivalence of the (magnetic) sites in the AF leads to a dependence of the expansion coefficients $a_{t\mu}(\mathbf{p},\alpha)$ on the sort of site α.

Confining ourselves to AF with two sorts of site ($\alpha=1,2$), we consider for simplicity only two d bands (t, $\mu=1,2$), and neglect the dependence of the coefficients $a_{t\mu}(\mathbf{p},\alpha)$ on the momentum $\mathbf{p}$. In this case we obtain for the magnetic-moment density (1), using relations (2)–(5) and regarding as usual the overlap of the atomic functions $\Phi_\mu(\mathbf{r}-\mathbf{n}_\alpha)$ corresponding to different sites as small, the simple expression

$$M(\mathbf{r})=\frac{m_1}{N}\sum_{\mathbf{n}\alpha\alpha\mu}[|a_{1\mu}(\alpha)|^2-|a_{2\mu}(\alpha)|^2]|\Phi_\mu(\mathbf{r}-\mathbf{n}_\alpha)|^2, \tag{6}$$

where the coefficients $a_{t\mu}(\alpha)$ are connected by the relation

$$\sum_{\alpha,\mu}|a_{t\mu}(\alpha)|^2=2, \tag{7}$$

which follows from the normalization of (5) to unity.

The density of the magnetic moment, as seen from formula (6), is concentrated to a considerable degree near the (magnetic) lattice sites, because of the spatial localization of the atomic functions $\Phi_\mu(\mathbf{r}-\mathbf{n}_\alpha)$. According to (6) and (7) we have for the magnetic moment M_α per site of sort α

$$M_1=-M_2\equiv M_0=\frac{m_1}{N}\sum_\mu[|a_{1\mu}(1)|^2-|a_{2\mu}(1)|^2]. \tag{8}$$

In the band model of antiferromagnetism, where it is assumed that the overlap of the atomic functions corresponding to neighboring sites is small, just as in the Neel model (see, e.g.,[2]), we can therefore speak of two magnetic sublattices with magnetizations $\pm NM_0/2$.

It follows from (8) that in the band theory of antiferromagnetism the atomic magnetic moment has in the general case a fractional value (in units of the electron magnetic moment μ_0). For a nonconducting AF, whose magnetic electrons are fully polarized, we have

$$n_F(\varepsilon_{1\mathbf{p}}^+)=n_F(\varepsilon_{2\mathbf{p}}^-)=1,\quad n_F(\varepsilon_{1\mathbf{p}}^-)=n_F(\varepsilon_{2\mathbf{p}}^+)=0.$$

In our model of two d bands, we have one d electron per atom, and accordingly Eq. (8) takes the form

$$M_0=\mu_0\left\{1-\frac{1}{2}\sum_\mu[|a_{1\mu}(2)|^2+|a_{2\mu}(1)|^2]\right\}. \tag{9}$$

The whole-number result $M_0=\mu_0$, which corresponds to the Heisenberg theory of magnetism, follows from (9) only when the electrons of the t-th band are localized near the sites of sort $\alpha=t$ of the dielectric:

$$a_{1\mu}(2)=a_{2\mu}(1)=0.$$

Let us discuss briefly the temperature dependence of the magnetic moment $M_0(T)$ per site. This dependence, just as in ferromagnets, can be the result of the redistribution of the Bloch electrons over the energy states following a change of temperature. As follows from (2), the spin splitting energy $\hbar\Omega_{0t}(T)\sim m_1(T)$ depends then on the temperature. Furthermore, the magnetic moment (8) has an additional temperature dependence because of the variation of the coefficients $a_{t\mu}(\alpha)$ with temperature; this variation appears in the electron-fluid theory because the wave function of the quasiparticles is deter-

mined not only by the crystal potential of the lattice ions but also by the temperature-dependent self-consistent potential of the electrons.[1)] [11,13] To make this clear, we consider first the case when the chemical and magnetic unit cells of the AF coincide (as, e.g., in MnF_2). Then the (magnetic) sites of the two types have not only different magnetic moments concentrated near them, but also non-equivalent positions in the crystal lattice. In the absence of magnetic order ($\Omega_{0t}=0$) the sites therefore remain non-equivalent: $a_{t\mu}(1)\neq a_{t\mu}(2)$ and, as follows from (7), the quantity

$$Q=\sum_{\mu}[|a_{1\mu}(1)|^2-|a_{2\mu}(1)|^2]$$

is generally speaking different from zero. In the magnetically ordered state under conditions when the spin splitting energy $\hbar\Omega_0(T)\approx\hbar|\Omega_{0t}(T)|$ is small, the quantity $Q(T)$ can be approximately regarded as independent of the temperature. This situation arises near the Neel point, when $T\approx T_N\sim\hbar\Omega_0(0)$, or in weakly antiferromagnetic metals, in which $\hbar\Omega_0/2$ is small compared with the Fermi energy. Formula (8) then leads, just as in the molecular-field theory, to the linear relation

$$M_0(T)\sim\Omega_0(T) \tag{10}$$

between the magnetic moment and the energy of the spin splitting (the molecular field).

The situation is entirely different if the chemical cell contains one magnetic atom and does not coincide with the magnetic cell (e.g., MnO). Then in the disordered state ($\Omega_0=0$) there is no difference between the sites. This means that $a_{t\mu}(1)=a_{t\mu}(2)$ and, as follows from (7), Q vanishes. At small $\Omega_0(T)$, since the state of the crystal is not changed when the quantization axis is reversed ($\Omega_{0t}\to-\Omega_{0t}$), we assume that $Q(T)\sim\Omega_0^2(T)$. Under this assumption it turns out that the atomic magnetic moment (8) depends on the temperature like the cube of the spin splitting energy

$$M_0(T)\sim\Omega_0^3(T). \tag{11}$$

Near the antiferromagnetic-transition point $T=T_N$ the spin splitting energy depends on temperature, just as in ferromagnets,[1] but like $\Omega_0(T)\sim(T_N-T)^{1/2}$. We emphasize that in our microscopic model of antiferromagnetism the magnetic order is characterized by a bans spin splitting energy $\hbar\Omega_0(T)$ that corresponds to the order parameter in the theory of phase transitions. Near the Neel temperature we obtain for the diamagnetic moment from (10) and (11)

$$M_0(T)\sim(T_N-T)^{\beta}, \tag{12}$$

where the exponent β can take on the value 1/2 that follows from the usual molecular-field theory only if the chemical and magnetic cells of the AF coincide. If they do not, then $\beta=3/2$.

2. We proceed to consider the magnetic excitations in collinear AF at low temperatures, confining ourselves to transverse excitations that are described by a nonequilibrium spin density matrix $\delta\hat{\sigma}\sim e^{i\omega t}$, which is polarized in a plane perpendicular to the quantization axis. For circularly polarized components $\delta\hat{\sigma}^{\pm}$ of the density matrix we have in the absence of a constant magnetic field the equation[11]

$$(\hbar\omega+\varepsilon_{t'\mathbf{p}-\hbar\mathbf{k}}^{\pm}-\varepsilon_{t\mathbf{p}}^{\mp}+i0)\,\delta\sigma^{\pm}(t\mathbf{p},t'\mathbf{p}-\hbar\mathbf{k})-2[n_F(\varepsilon_{t'\mathbf{p}-\hbar\mathbf{k}}^{\pm})-n_F(\varepsilon_{t\mathbf{p}}^{\mp})]$$
$$\times\sum_{t_1t_1'\mathbf{p}_1}\Psi(t\mathbf{p},t_1'\mathbf{p}_1-\hbar\mathbf{k};t_1\mathbf{p}_1,t'\mathbf{p}-\hbar\mathbf{k})\,\delta\sigma^{\pm}(t_1\mathbf{p}_1,t_1'\mathbf{p}_1-\hbar\mathbf{k})=0. \tag{13}$$

This equation does not take into account the magnetic anisotropy and the alternating magnetic field of the excitations, that lead in our case to small changes in the spin-wave spectrum.

Being interested in the qualitative differences between the properties of conducting AF and dielectrics, we shall approximate, for simplicity, the energy structure of the crystal d bands by two degenerate bands with a quadratic dispersion law $\varepsilon_{t\mathbf{p}}=p^2/2m$. From Eqs. (2)–(4), letting $\Omega_{0t}(\mathbf{p})$ on the Fermi surface tend to zero, we obtain the condition for the onset of the antiferromagnetic state:

$$B_2-B_1-1>0,$$
$$B_1=-2\sum_{\mathbf{p}_1}\Psi(t\mathbf{p},t\mathbf{p}_1;t\mathbf{p}_1,t\mathbf{p})\frac{\partial n_F(\varepsilon_{t\mathbf{p}_1})}{\partial\varepsilon},$$
$$B_2=-2\sum_{\mathbf{p}_1}\Psi(t\mathbf{p},t_1\mathbf{p}_1;t_1\mathbf{p}_1,t\mathbf{p})\frac{\partial n_F(\varepsilon_{t_1\mathbf{p}_1})}{\partial\varepsilon},\quad t\neq t_1. \tag{14}$$

where the function $\Psi(t\mathbf{p},t_1\mathbf{p}_1;t_1\mathbf{p}_1,t\mathbf{p})$ for vectors $\mathbf{p}$ and $\mathbf{p}_1$ lying on the Fermi surface depends only on the angle between them.

On the basis of the results of[11] we can state that the dependence of the correlation function $\hat{\Psi}$ on the momenta leads, just as in ferromagnets, to the existence of polar spin waves (cf.[14]) with frequencies $\omega\sim\Omega_0$. We shall, however, not investigate here such high-frequency waves and confine ourselves to low-frequency excitations. The dependence of $\hat{\Psi}$ on the momenta can be neglected for these excitations and it can be assumed, following Englert and Antonoff,[7] that

$$\Psi(t\mathbf{p},t_1'\mathbf{p}_1-\hbar\mathbf{k};\,t_1\mathbf{p}_1,t'\mathbf{p}-\hbar\mathbf{k})\approx\Psi(t,t_1';\,t_1,t';\,\mathbf{k}). \tag{15}$$

We note that the need for taking into account the dependence of the functions $\hat{\Psi}(k)$ on the wave vector $\mathbf{k}$ was demonstrated by Lowde and Windsor[15] in a study of inelastic scattering of neutrons in ferromagnetic nickel.[2)]

The correlation function Ψ has symmetry properties that decrease the number of the independent components. Besides the relations

$$\Psi(\beta,\beta_1';\beta_1,\beta')=\Psi(\beta_1,\beta';\beta,\beta_1')=\Psi(\beta_1',\beta;\beta',\beta_1),\quad \beta\equiv(t,\mathbf{p}),$$

which follow from hermiticity as well as from the fact that the function $\hat{\Psi}$ is the second variational derivative of the energy of the electron fluid with respect to the spin density matrix, we have also the equation[17]

$$\sum_{\beta_1}\Psi(\beta,\beta_1;\beta_1,\beta')[n_F(\varepsilon_{\beta_1}^{+})-n_F(\varepsilon_{\beta_1}^{-})]=0,\quad \beta\neq\beta', \tag{16}$$

which follow from the diagonality of the quasiparticle energy operator.[11]

In the case of two degenerate bands, $\hat{\Psi}$ has five independent components

$$\Psi(t,t;\ t,t)=\Psi_1,\quad \Psi(t,t_1;\ t_1,t)=\Psi_2,\quad \Psi(t_1,t;\ t_1,t)=\Psi_3,$$
$$\Psi(t,t;\ t_1,t_1)=\Psi_4,\qquad (17)$$
$$\Psi(t_1,t;\ t,t)=\Psi(t,t_1;\ t,t)=\Psi(t,t;\ t_1,t)=\Psi(t,t;\ t,t_1)=\Psi_5,\quad t\neq t_1,$$

which are even functions of **k**.

The assumed "isotopic invariance" used by Akhiezer and Chudnovskiĭ [8] (see also [18]) reduces the number of independent components of the correlation function to two: $\Psi_1, \Psi_2 \neq 0$. In this case

$$2\Psi_3=\Psi_1-\Psi_2,\qquad \Psi_4=\Psi_5=0. \qquad (18)$$

However, as shown in the Appendix, this model can hardly be justified in the analysis of phenomena connected with antiferromagnetic order.

Using relations (3), (4) and (15), we have for the energy of the spin splitting from Eq. (2) at zero temperature

$$\Omega_{01}=-\Omega_{02}=\Omega_0,\qquad (\hbar\Omega_0/\varepsilon_F)^2=96[B_2(0)-B_1(0)-1]. \qquad (19)$$

We have introduced here the notation $B_i(\mathbf{k})=\Psi_i(\mathbf{k})\nu_F$, where ν_F is the electron state density in one zone on the Fermi surface. The Fermi energy ε_F is assumed here large in comparison with $\hbar\Omega_0/2$, which in our case is of the order of the Neel temperature.

We note that if not too strong a magnetic field **B** ($\mu_0 B \ll \hbar\Omega_0$) is present in the AF, then the magnetic structure differs insignificantly from the simple collinear one. The magnetization vectors m_i lie then in the plane of the vector **B** and the angles they make with it are $\sim \pm \arccos(\mu_0 B/\hbar\Omega_0)$. This result for the magnetization m_i agrees with the theory of a Heisenberg AF in a magnetic field.[2]

From (13) and (15) we obtain a dispersion relation that determines the spectrum of the transverse magnetic excitations

$$\|\delta_{tt'}\delta_{t_1t_1'}-\Psi(t,t_1';\ t_1,t';\ \mathbf{k})S_{tt'}^{\pm}(\omega,\mathbf{k})\|=0, \qquad (20)$$

where

$$S_{tt'}(\omega,\mathbf{k})=2\sum_{\mathbf{p}}\frac{n_F(\varepsilon_{t'\mathbf{p}-\hbar\mathbf{k}}^{\pm})-n_F(\varepsilon_{t\mathbf{p}}^{\mp})}{\hbar\omega+\varepsilon_{t'\mathbf{p}-\hbar\mathbf{k}}^{\pm}-\varepsilon_{t\mathbf{p}}^{\mp}+i0}. \qquad (21)$$

We assume first for simplicity that $\Psi_5=0$. It will be shown below that many qualitative results obtained in this approximation remain in force also in the general case. The dispersion equation (20) then splits into two:

$$(1-\Psi_1 S_{11}^{\pm})(1-\Psi_1 S_{22}^{\pm})-\Psi_2^2 S_{11}^{\pm}S_{22}^{\pm}=0, \qquad (22)$$

$$(1-\Psi_3 S_{12}^{\pm})(1-\Psi_3 S_{21}^{\pm})-\Psi_4^2 S_{12}^{\pm}S_{21}^{\pm}=0. \qquad (23)$$

The first of these equations determines the intraband excitations—the antiferromagnons and the single-particle excitations, which are analogous to the Stoner excitations of ferromagnets and are described by the diagonal (in the band index) components $\delta\hat{\sigma}^{\pm}(t,t)$ of the density matrix. Equation (23) corresponds to interband excitations described by the matrix $\delta\hat{\sigma}^{\pm}(t,t')$ $(t\neq t')$.

3. We consider first the intraband-excitation spectrum defined by Eq. (22). Single-particle excitations with spin flip, which we shall call Stoner excitations as in the case of ferromagnets, correspond to the frequency and wave-vector region defined by the inequality

$$|\omega-\Omega_0-\hbar k^2/2m|\leqslant kv^+. \qquad (24)$$

In the region (24), the intraband spin wave attenuate strongly because of the possibility of decay into Stoner excitation (Landau damping).

In the absence of a magnetic field and of anisotropy effects, Eq. (22) yields a doubly degenerate spin-wave branch corresponding to antiferromagnons with two different polarizations. Not too close to the boundary of region (24) we have for the antiferromagnon spectrum

$$\omega^2=2B_2(0)D(\mathbf{k})\left[\frac{2B_2}{(k_0^2-k^2)v_F^2}-\frac{B_2+B_1}{(2kv_F)^2}\ln^2\left|\frac{k_0+k}{k_0-k}\right|\right]^{-1}. \qquad (25)$$

Here $k_0=m(v^+-v^-)/\hbar\approx\Omega_0/v_F$ corresponds to the intersection of the boundary of the region (24) with the line $\omega=0$, $v^{\sigma}=[2(\varepsilon_F+\sigma\hbar\Omega_0/2)/m]^{1/2}$ is the velocity of the particles with spin σ on the Fermi surface, $p_F=mv_F=(2m\varepsilon_F)^{1/2}$,

$$D(\mathbf{k})=(\hbar k/p_F)^2/12+B_1(\mathbf{k})-B_1(0)+B_2(0)-B_2(\mathbf{k}). \qquad (26)$$

Formulas (25) and (26) are valid if

$$|k_0-k|/k_0\gg(\hbar\Omega_0/\varepsilon_F)^2.$$

It follows from (26) that in the long-wave limit $k^2\ll k_0^2$, just as in dielectric, the antiferromagnons have a linear dispersion law

$$\omega^2=2B_2(0)D(\mathbf{k})\Omega_0^2. \qquad (27)$$

The first term in expression (26) to $D(\mathbf{k})$, which enters in the right-hand part of (27), is determined here by the motion of the collectivized magnetic electrons. The remaining terms in the right-hand side of formula (26) for $D(\mathbf{k})$ are due to the dependence of the correlation function $\hat{\Psi}$ on the wave vector **k** and are of the same nature as in dielectrics where, for example at $\Psi_1=0$, the magnon frequency is determined according to [7] by the relation

$$\omega^2=\Omega_0^2[1-\Psi_2^2(\mathbf{k})/\Psi_2^2(0)].$$

According to (26) and (27), the magnon frequency is real, and therefore the antiferromagnetic state is stable to intraband spin oscillations if

$$B_1(0)<0,\qquad B_2(0)>0. \qquad (28)$$

We note that the magnetically ordered state arises at zero temperature if

$$1+B_1(0)>|B_2(0)|.$$

The ferromagnetic state in a magnet with two degenerate bands is stable under the conditions

$$1+B_1(0)<|B_2(0)|;\qquad B_1(0),B_2(0)<0.$$

With increasing wave vector $\mathbf{k}$, the antiferromagnon dispersion law differs substantially from the linear law typical of dielectrics, because of the interaction of the spin waves with the Stoner excitations. As follows from (25), near the boundary of the region of the Stoner excitations, when $\mathbf{k}$ approaches the value $k=k_0$, the magnon frequency decreases like

$$\omega=\Omega_0[2D(\mathbf{k}_0)(k_0-k)/k_0]^{1/2}. \tag{29}$$

The singularity of (29) in the antiferromagnon spectrum is of the square-root type, in contrast to the comparatively weak logarithmic spectrum in the ferromagnon spectrum[19] (see also[20]). It is to be expected that a similar strong singularity will appear in the AF spectrum in the case of an arbitrary Fermi surface. The dispersion curve of the antiferromagnons crosses the boundary of the region (24) of the Stoner excitations at an end-point wave vector value $\mathbf{k}_{ep}=\mathbf{k}_0[1-\omega(\mathbf{k}_{ep})/\Omega_0]$. The frequency of the spin wave at the end point of the spectrum, $\omega(\mathbf{k}_{ep})$, is given by

$$\omega(\mathbf{k}_{ep})=\frac{4D(\mathbf{k}_0)\Omega_0}{\ln(4\varepsilon_F/\hbar\Omega_0)+1}. \tag{30}$$

At wave-vector values $k>k_{ep}$, the conditions (24) for collisionless spin-wave damping due to decay into Stoner excitations are satisfied. This leads to a strong damping of the antiferromagnons $\mathrm{Re}\,\omega\sim-\mathrm{Im}\,\omega>0$. For example, at $|k_0-k|/k_0\ll 1$ we have

$$-\mathrm{Im}\,\omega\approx\pi(k-k_0)v_F/2\approx 3^{-1/2}\,\mathrm{Re}\,\omega.$$

We note that the results (24)–(30) remain valid also in the presence of a magnetic field if the wavelengths of the antiferromagnons are not too large: $kv_F\gg\mu_0 B/\hbar$.

In a number of cases, for example under conditions of the quantization of the motion of electrons in a magnetic field or in thin films, collisionless damping may turn out to be suppressed. Formula (25) will then give in the wave-vector region $k>k_0$ imaginary values of ω, corresponding to perturbations that increase with time. This indicates that the collinear AF considered by us is unstable. A more complicated magnetic structure may be realized in this case.

4. Proceeding to a discussion of the properties of the interband magnetic excitations described by (23), we note that such excitations have heretofore not been considered for AF. To solve (23) in a region with not too short waves, we represent the quantities $S^{\pm}_{tt'}$, with $t\neq t'$ in the form

$$S_{21}^{\pm}=S_{12}^{\mp}=-\nu_F\frac{v^{\pm}}{v_F}f\left(\frac{\omega+i0}{kv^{\pm}}\right), \tag{31}$$

where

$$f(x)=1-(x/2)\ln[(x+1)/(x-1)].$$

Equations (23) and (31) yield, besides the single-particle interband excitations that occur in the region $\omega\leq kv^+$, two spin-wave branches with a linear dispersion typical of zero-sound oscillations.[9] Each of the branches is doubly degenerate with respect to the two possible polarizations of the transverse spin waves. The phase velocity of such waves is close to the velocity of the v^+d electrons on the Fermi surface. We note that under certain conditions, one interband branch (when $|B_3|<|B_4|$) or both branches (when $B_3<-|B_4|$) will attenuate strongly because of decay into single-particle interband excitations (Landau damping). These waves will not increase with time if the inequality

$$1+B_3(0)>|B_1(0)|, \tag{32}$$

which corresponds to stability of the electron fluid of antiferromagnets relative to interband spin oscillations, is satisfied. The interband spin waves are due to motion of collectivized electrons in partially filled d bands of conducting AF and do not take place in dielectrics.

We have neglected so far the influence of the nonmagnetic s and p conduction electrons. According to Kondratenko,[21] in antiferromagnetic metals such electrons are not polarized and can lead to the onset of one more zero-sound branch of spin waves with a phase velocity close to the velocity of the s (p) electrons on the Fermi surface. Besides the differences in velocity, the interband branches of the spin waves and the branch corresponding to nonmagnetic electrons can differ also in their behavior in a magnetic field, which lifts the degeneracy in the polarizations of the transverse spin waves in the AF and leads to the onset of nonzero end-point frequencies $\omega(\mathbf{k}=0)\sim\mu_0 B/\hbar$. Each of the doubly degenerate interband branches splits in this case into two branches, for which the dispersion law remains linear in the region of not too large wavelengths $kv^+\gg\mu_0 B/\hbar$. The magnetic field leads also to the possible existence of such interband waves that attenuate strongly in the absence of a field. There are thus altogether in a magnetic field four different undamped interband spin-wave branches. The branch corresponding to the nonmagnetic electrons can have a left-hand polarization (described by a density matrix $\delta\sigma^+\sim e^{-i\omega t}$) in the presence of a magnetic field and behaves in the same way as in a normal metal.[10]

5. In the general case $\Psi_5(\mathbf{k})\neq 0$, as follows from (9), it is necessary to take into account the interaction of the intraband and interband excitations that are defined by (22) and (23), respectively. Since the phase velocity of the interband spin waves is close to the Fermi velocity v^+ and exceeds significantly the velocity $\sim\hbar\Omega_0/p_F$ of the antiferromagnons the interaction with the intraband excitations leads to small corrections to the frequency of the interband spin waves, of the order of $B_5^2(\hbar\Omega_0/\varepsilon_F)^2$.

The antiferromagnon spectrum is not changed qualitatively in this case and is given by formulas (25)–(27), in which it is necessary to make the substitution

$$B_i(\mathbf{k})\to\tilde{B}_i(\mathbf{k})=B_i(\mathbf{k})-2B_5^2(0)/[1+B_3(0)+B_1(0)]. \tag{33}$$

Near the boundary of the region of the Stoner excitations, the magnon frequency is determined as before by relations (29) and (30), and the antiferromagnon spectrum has likewise in the general case $\Psi_5\neq 0$ a square-root singularity.

It follows from (27) and (33) that for the antiferromagnetic state to be stable in the general case it is necessary to stipulate, besides satisfaction of conditions (14), (28), and (32), also

$$B_2(0)>0$$

or

$$2B_5^2(0)<B_2(0)\,[1+B_3(0)+B_4(0)]. \tag{34}$$

The substantial difference from the case $\Psi_5=0$ lies in the appearance in the antiferromagnon spectrum of collisionless damping due to the decay of the spin wave into single-particle interband excitations. This damping of the magnons, in contrast to collisionless damping due to decay into Stoner excitations, which occurs at relatively short wavelengths $k>k_0$, is possible also in the region of large wavelengths if the condition $\omega \leqslant kv^*$ is satisfied. For the magnon damping decrement $\gamma=-\operatorname{Im}\omega$ we obtain from (20)

$$\gamma(\mathbf{k})=\pi B_5^2\frac{1+B_3-B_4}{(1+B_3+B_4)^2}\frac{D(\mathbf{k})\Omega_0^2}{kv_F}\left(\frac{k_0}{2k}\ln\left|\frac{k_0+k}{k_0-k}\right|\right)^2$$
$$\times\left[2\bar{B}_2\frac{k_0^2}{k_0^2-k^2}-(\bar{B}_2+\bar{B}_4)\left(\frac{k_0}{2k}\ln\left|\frac{k_0+k}{k_0-k}\right|\right)^2\right]^{-2}. \tag{35}$$

As follows from (35), in the region of not too short wavelengths ($k_0-k\sim k_0$) the relative damping is $\gamma/\mathrm{Re}\omega \sim B_5^2\hbar\Omega_0/\varepsilon_F$. As the wave vector approaches $k=k_0$, the ratio $\gamma/\mathrm{Re}\omega$ decreases like

$$\frac{\gamma}{\mathrm{Re}\,\omega}\sim B_5^2\frac{\hbar\Omega_0}{\varepsilon_F}\left(\frac{k_0-k}{k_0}\right)^{1/2}\ln^2\frac{2k_0}{k_0-k}.$$

At not too small values of the ratio $\hbar\Omega_0/\varepsilon_F$ and of B_5^2, the relative damping at $k<k_0$ may turn out to be large: $\gamma/\mathrm{Re}\omega\sim 1$. The antiferromagnons have no long-wave spectrum in this case. On the otherhand if $B_5^2\hbar\Omega_0/\varepsilon_F \ll 1$, the magnons constitute a well defined collective mode everywhere in the region $k<k_{ep}$. We emphasize that the collisionless mechanism of the magnon damping may be the principal one in sufficiently pure AF at low temperatures.

APPENDIX

In the Hartree-Fock approximation, the function Ψ, which describes the exchange interaction between the electrons, is of the form[11]

$$\Psi(t\mathbf{p},t_1'\mathbf{p}_1';t_1\mathbf{p}_1,t'\mathbf{p}')$$
$$=-\frac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\,\varphi_{t\mathbf{p}}^*(r)\varphi_{t_1'\mathbf{p}_1'}^*(r')U(\mathbf{r},\mathbf{r}')\varphi_{t_1\mathbf{p}_1}(\mathbf{r})\varphi_{t'\mathbf{p}'}(\mathbf{r}'), \tag{A.1}$$

where $U(\mathbf{r},\mathbf{r}')$ is the energy operator of the electron-electron interaction. Substituting in (A.1) the expansion (5) of the Bloch functions $\varphi_{t\mathfrak{p}}(\mathbf{r})$ in the atomlike functions $\Phi_\mu(\mathbf{r}-\mathbf{n}_\alpha)$, we get

$$\Psi(t\mathbf{p},t_1'\mathbf{p}'-\mathbf{q};t_1\mathbf{p}-\mathbf{q},t'\mathbf{p}')$$
$$=-\frac{1}{2N^2}\sum_{\substack{n_{\alpha_1}'n_{\alpha_1}n_{\alpha'}n_\alpha\\ \alpha_1'\alpha_1\alpha'\alpha\mu_1'\mu_1\mu'\mu}}\exp\left\{\frac{i}{\hbar}\left[\mathbf{p}(\mathbf{n}_{\alpha_1}-\mathbf{n}_\alpha)+\mathbf{p}'(\mathbf{n}_{\alpha'}-\mathbf{n}_{\alpha_1'})+\mathbf{q}(\mathbf{n}_{\alpha_1'}-\mathbf{n}_{\alpha_1})\right]\right\}$$
$$\times a_{t\mu}^*(\alpha)a_{t_1'\mu_1'}^*(\alpha_1')a_{t_1\mu_1}(\alpha_1)a_{t'\mu'}(\alpha')\int d\mathbf{r}\,d\mathbf{r}'\,\Phi_\mu^*(\mathbf{r}-\mathbf{n}_\alpha)\Phi_{\mu_1'}^*(\mathbf{r}'-\mathbf{n}_{\alpha_1'})$$
$$\times U(\mathbf{r},\mathbf{r}')\Phi_{\mu_1}(\mathbf{r}-\mathbf{n}_{\alpha_1})\Phi_{\mu'}(\mathbf{r}'-\mathbf{n}_{\alpha'}). \tag{A.2}$$

Since we consider antiferromagnetic ordering under conditions of small overlap of the atomic functions corresponding to different sites, we confine ourselves in (A.2) to "two-center" integrals.

If we assume that the electrons of the different bands have identical spatial wave functions $\varphi_{t\mathfrak{p}}(\mathbf{r})=\varphi_{\mathfrak{p}}(\mathbf{r})\chi_t$, where the spinor χ_t describes the band state of the electron ($\chi_t^*\chi_{t'}=\delta_{tt'}$ because of the orthogonality of the wave functions), then the general expression (A.2) leads to relations (18) of the "isotopic invariance" model of Akhiezer and Chudnovskiĭ.[8] In this case, however, the magnetic-moment density (6) and the atomic magnetic moment (8) are zero everywhere. This means that in the Hartree-Fock approximation the "isotopic invariance" model cannot be used to describe phenomena connected with magnetic order.

[1)] The effect of spin wave on the magnetization has been investigated theoretically in relatively great detail (see, e.g., [2,3]) and will not be discussed here.

[2)] Such a dependence of the correlation function on the wave vector was used in the theory of a ferromagnetic electron fluid by Akhiezer and Chudnovskiĭ.[16]

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