Short-range order in quasi-two-dimensional band antiferromagnets with a spin-density wave

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A "local-band" theory for an antiferromagnetic metal with a "nesting" singularity of the electron spectrum is constructed, and the spin-fluctuation contribution to the energy is obtained in the form of the classical Heisenberg Hamiltonian. It is shown that thermodynamic transverse spin-density fluctuations have a fundamental influence on the formation of the long-range magnetic order, sharply lowering the Néel temperature T_N^{SF} relative to the "mean-field" temperature T_N^0 for the appearance of a spin-density-wave amplitude. In a wide range of temperatures $T_N^{SF} < T < T_N^0$ a regime of short-range magnetic order is realized, and a pseudogap, with smeared-out peaks of the density of states near its edges, is preserved in the electron spectrum. In a quasi-two-dimensional system there is a crossover regime in the paramagnetic phase, and the temperature T_N^{SF} vanishes in the purely two-dimensional case.

1. INTRODUCTION

In the modern theory of band magnetism it is customary to assume that the responsibility for the destruction of the long-range magnetic order with increase of temperature is carried by comparatively low-energy collective excitations of the spin density of the quasiparticles—spin fluctuations, while one-particle (Stoner) excitations do not play an essential role in this process. The problem of calculating the transition temperature T_k reduces, therefore, to taking into account more or less correctly the contribution of the spin fluctuations to the free energy F of the band magnet.[1] No universal consistent scheme for doing this exists at the present time, although attempts to construct one are being constantly undertaken (see, e.g., the relevant discussion in Ref. 1). The difficulties that arise on this path are rather diverse, but the chief of them is evidently the problem of specifying *a priori* the type of fluctuations (in particular, the degree of their spatial localization) that make the principal contribution to F.

In saturated ("strong") band magnets with a spin-density amplitude close to the maximum, two groups of theories, corresponding to different assumptions about the degree of localization of the fluctuations, can be distinguished. In "alloy" theories (of Hasegawa,[2] Hubbard,[3] *et al.*) it is assumed that the principal contribution to F is made by uncorrelated fluctuations of almost local spins on the lattice sites. The field of such fluctuations, with an almost fixed spin-density amplitude at a site, is described by introducing a self-consistent coherent potential in analogy with the theory of alloys in metals. In the theories of Refs. 2 and 3 the destruction of the long-range order occurs by way of a phase transformation without the formation of a significant temperature region with short-range order.

The other approach, based on the idea of a special role for long-wavelength transverse fluctuations in the destruction of the long-range order, was put forward by Korenman *et al.*[4,5] and has become known as "local-band theory." The picture of the spin fluctuations that arises in this approach is closest to the behavior of a system of Heisenberg classical spins. Above the transition temperature T_k at which the destruction of the long-range order occurs, a phase with partial spatial correlation of the spin-density distribution on macroscopic scales is preserved. With increase of temperature this correlation is destroyed in a certain interval $\Delta T_{SRO} \sim T_k$, after which the system can be assumed to be completely disordered (in theories of the type of Refs. 2 and 3 it is assumed, in effect, that $\Delta T_{SRO} \ll T_k$ and the phase of short-range order is absent).

In the theory of "weak" (unsaturated) magnets the Moriya–Kawabata method of renormalized spin fluctuations is used.[6] The high-temperature approximation of this method corresponds to the Murata–Doniach scheme[7] for extremely long-wavelength static fluctuation modes of small amplitude. For cases of long-wavelength modes of large amplitude, Hertz and Klenin[8] proposed a generalization of the scheme of Ref. 6. We note that in the theories of the type of Refs. 6–8 the longitudinal (amplitude) and transverse (orientational) spin fluctuations are taken into account in equal measure in the random-Gaussian-field approximation, and there was no special discussion of the question of the short-range order. Here, too, we shall not set ourselves the task of constructing a theory of the short-range order in all types of "weak" band magnets (in particular, we shall not be discussing ferromagnets of the Stoner type, in which the presence of a sufficiently large interaction constant $U > 1$ is necessary). We shall confine ourselves to the standard band-antiferromagnetism model of the "spin-density-wave" (SDW) type, which is formally valid in the limit $U \ll 1$ (see, e.g., Ref. 9).

Usually, in the SDW model, mean-field theory makes it possible to give a satisfactory description of the thermodynamics of the system, although a regular technique for taking fluctuation corrections into account has not been worked out. Hasegawa[10] has calculated in the framework of the scheme of Ref. 6 corrections to the Néel temperature T_N and SDW amplitude. The use here of a simple one-loop approximation for the renormalized susceptibility was not justified in any way. Allowance by Volkov and Tugushev[11] for a more complicated renormalization in the ladder approximation has displayed the presence of nonanalytic behavior of the functional F in the vicinity of T_N, and, as a consequence, has led to a change of the transition from second-order to first-

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order. We note that these papers discussed only SDW amplitude fluctuations, and, in essence, the presence of long-wavelength fluctuations of the direction of the spin-polarization vector was not taken into account, inasmuch as the analysis was performed in the so-called "Z-representation," with a fixed quantization axis, which is extremely inconvenient for this purpose.

As shown in this paper, fluctuations of the direction of the SDW vector have a fundamental influence on the formation of long-range antiferromagnetic order, sharply lowering the Néel temperature from the value T_N^0 (the "mean-field" temperature of the appearance of a nonzero SDW amplitude) to a value $T_N^{SF} \ll T_N^0$. In a wide range of temperatures $T_N^{SF} < T < T_N^0$ a regime of short-range magnetic order is realized, the spin-density correlation function has a sharply expressed peak at the wave vector of the AFM structure, and a pseudogap, with smeared-out peaks of the density of states near its edges, is preserved in the electron spectrum.

Another aspect of the problem of short-range magnetic order, discussed in this paper, involves the increase of the role of this effect in systems with lower dimensionality. In particular, in a quasi-two-dimensional system with SDW the temperature interval in which short-range AFM order exists expands in the low-temperature direction, a crossover regime obtains in the paramagnetic phase, and the temperature of the onset of long-range order decreases, vanishing in the purely two-dimensional case. The structure of the short-range AFM order and the possibility of a transition of the Kosterlitz–Thouless type in a quasi-two-dimensional system with SDW are not considered in detail in this paper, although it is apparent that we may expect the appearance of complicated SDW vortex structures and of associated unusual behavior of the thermodynamic characteristics.

2. TRANSVERSE SDW FLUCTUATIONS AND THE "LOCAL-BAND" METHOD IN ANTIFERROMAGNETS WITH SHORT-RANGE ORDER

Before proceeding to the original part of the paper, for the convenience of the reader we recall briefly a number of familiar techniques used in the spin-fluctuation theory of band magnetism (see the detailed account in Ref. 12).

The starting point of the analysis is the one-band Hubbard model with Hamiltonian

$$H=H_0+H_{int},$$
$$H_0=\sum_{ij\sigma} t_{ij} c_{i\sigma}^{+} c_{i\sigma}, \qquad (1)$$
$$H_{int}=U\sum_i n_{i\uparrow} n_{i\downarrow},$$

where

$$n_{i\sigma}=c_{i\sigma}^{+} c_{i\sigma},$$

$c_{i\sigma}$ is a Fermi operator in the site representation, U is the intra-atomic Coulomb repulsion, and t_{ij} is the hopping integral, which we shall assume to be nonzero only for nearest neighbors.

The partition function for the Hamiltonian (1)

$$Z=\mathrm{Sp}\left[\exp\left(-\frac{1}{T}(H-\mu_0 N)\right)\right]$$

can be expressed in the form of a functional integral, with imaginary time τ, over the anticommuting "classical" variable $c_{i\sigma}(\tau)$:

$$Z=\mathrm{const}\int \mathcal{D}[c,c^{*}]\exp(-S[c,c^{*}]), \qquad (2)$$
$$S=\int_0^{1/T} d\tau\left(\sum_{i\sigma} c_{i\sigma}^{*}\frac{\partial}{\partial\tau}c_{i\sigma}+H-\mu_0 N\right),$$

where μ_0 is the chemical potential of the system, and

$$N=\sum_{i\sigma} n_{i\sigma}.$$

By means of the identity

$$n_{i\uparrow}n_{i\downarrow}={}^1/_4(n_{i\uparrow}+n_{i\downarrow})^2-{}^1/_4(n_{i\uparrow}-n_{i\downarrow})^2 \qquad (3)$$

we can rewrite the interaction Hamiltonian in terms of the charge density n_i and spin density S_{iz}:

$$n_i=n_{i\uparrow}+n_{i\downarrow}, \quad S_{iz}={}^1/_2(n_{i\uparrow}-n_{i\downarrow}).$$

Assuming that the unit vector $\mathbf{e}_i$ that specifies the local orientation of the quantization axis at site i makes an arbitrary angle with respect to the crystallographic axes, we write the Hubbard term in the form

$$H_{int}=U\sum_i[{}^1/_4 n_i^2-(\mathbf{e}_i\mathbf{S}_i)^2]. \qquad (4)$$

The representation (4) of the interaction Hamiltonian permits us to make use of the Hubbard–Stratonovich representation:

$$\exp\left[-\int_0^{1/T} d\tau H_{int}\right]=\int \mathcal{D}x\,\mathcal{D}\mathbf{y}$$
$$\times\exp\left[-\pi T\int_0^{1/T} d\tau\sum_i (x_i^2(\tau)+\mathbf{y}_i^2(\tau))\right]$$
$$\times\exp\left[-i(\pi UT)^{1/2}\int_0^{1/T} d\tau x_i(\tau) n_i(\tau)\right.$$
$$\left.-2(\pi UT)^{1/2}\int_0^{1/T} d\tau(\mathbf{y}_i(\tau)\mathbf{S}_i(\tau))\right]. \qquad (5)$$

By means of this representation the initial many-particle problem (1) is replaced by the one-particle problem of the motion of an electron in a scalar field $x_i(\tau)$ and a vector field

$$y_i(\tau)=\mathbf{e}_i(\tau)\,y_i(\tau)$$

that fluctuate arbitrarily in space and time. We note that the configuration integration in (5) over all possible orientations of the vector $\mathbf{e}_i$ restores the rotational invariance of the system. We shall perform the subsequent calculations with neglect of the dependence of the fluctuations on the "time" variable τ, i.e., we assume that the static approximation gives the principal contribution to the integral (5) [in fact, this is equivalent to the high-temperature approximation in the integral (5)].

The electron variables can be eliminated in a straightforward manner by writing them first in the form of the series

$$c_i(\tau)=T\sum_n\frac{1}{N^{1/2}}\sum_{\mathbf{k}}\exp(-i\mathbf{k}\mathbf{r}_i-i\omega_n\tau)\,c_{\mathbf{k}n}, \qquad (6)$$

where the frequencies

$$\omega_n=\pi T(2n+1), \quad n=0, \pm 1, \pm 2, \ldots .$$

$\mathbf{k}$ is the quasimomentum, $\mathbf{r}_i$ is the coordinate of the ith site, and N is the total number of atoms in the crystal. Substituting the expansion (6) into the action S and then integrating over the Fourier components $c_{\mathbf{k}n}$ and $c^*_{\mathbf{k}n}$, we obtain a partition function of the following form:

$$Z=Z_0 \int \mathcal{D}x\, \mathcal{D}y \exp\left\{-\pi \sum_i (x_i^2+y_i^2)+\mathrm{Sp}\ln(1-gV)\right\}, \quad (7)$$

where

$$g_{ijn}=\frac{1}{N}\sum_{\mathbf{k}} g_{n\mathbf{k}} \exp i\mathbf{k}(\mathbf{r}_i-\mathbf{r}_j),$$
$$g_{n\mathbf{k}}=(i\omega_n+\mu_0-\varepsilon_{\mathbf{k}})^{-1} \quad (8)$$

is the Green function of the noninteracting electrons, with dispersion

$$\varepsilon_{\mathbf{k}}=\sum_i t_i \exp(-i\mathbf{k}\mathbf{r}_i), \quad (9)$$

$$V_{i\sigma\sigma'}=\pi UT(ix_i\delta_{\sigma\sigma'}+\boldsymbol{\sigma}_{\sigma\sigma'}\mathbf{y}_i)$$

is the random potential, σ are the Pauli matrices, and Z_0 is the partition function of the noninteracting particles.

In the expression (7) and henceforth, the symbol Tr denotes a sum of the diagonal matrix elements over the spin indices σ and site indices i and over the frequency variable n.

The integration over the charge variables x_i can be performed in the simplest, stationary-phase approximation, which is equivalent to neglecting the charge-density fluctuations (the characteristic frequency of which is of the order of the plasma frequency), and this determines their small contribution to (7) in temperature range of interest to us. As a result, we obtain in (7) the renormalization of the chemical potential

$$\mu_0 \to \mu=\mu_0-i(\pi UT)^{1/2}\bar{x}.$$

where $\bar{x}$ is the saddle point.

Now, after giving an account of this necessary information, we turn specifically to the problem of an antiferromagnet with SDW. For simplicity we shall consider a situation with a doubled (Néel) SDW structure in the ground state, without touching upon the interesting question of the thermodynamics of more-complicated structures with a modulated SDW amplitude. We shall assume that for the electron spectrum the "nesting" condition

$$\varepsilon_{\mathbf{k}}=-\varepsilon_{\mathbf{k}+\mathbf{Q}}$$

is fulfilled, where $\mathbf{Q}=\pm\mathbf{G}/2$, $\mathbf{G}$ being a reciprocal-lattice vector of the crystal. We distinguish two alternating magnetic sublattices, shifted by half a lattice constant: For one of these we shall take the local quantization axis $\mathbf{e}_i$ to coincide in direction with the local site magnetization $\mathbf{S}_i$, while for the other we shall assume that the vectors $\mathbf{e}_i$ and $\mathbf{S}_i$ are antiparallel. Thus,

$$\mathbf{e}_i\mathbf{S}_i=S_{iz}\exp(i\mathbf{Q}\mathbf{r}_i).$$

We shall also apply the stationary-phase method to determine the vector-field amplitude $\mathbf{y}_i$, which, below, we shall measure in energy units:

$$\Delta_i=(\pi UT)^{1/2}\mathbf{y}_i\exp(i\mathbf{Q}\mathbf{r}_i)=U\mathbf{S}_i\exp(i\mathbf{Q}\mathbf{r}_i). \quad (10)$$

The effective free-energy functional has the form

$$F[\Delta_i]=\sum_i \frac{\Delta_i^2}{U}+T\,\mathrm{Sp}\ln(1-g\bar{V}), \quad (11)$$

where

$$\bar{V}_i=\Delta_i\sigma\exp(-i\mathbf{Q}\mathbf{r}_i).$$

Assuming that, in the absence of fluctuations, a doubled SDW phase is realized ($\Delta_i=\Delta=\mathrm{const}$, $\mathbf{Q}=\mathbf{G}/2$), we find, by varying the functional (11), the Hartree–Fock self-consistency condition for Δ:

$$-\frac{\Delta}{U}=\frac{T}{N}\sum_{n\mathbf{k}}\frac{\Delta}{\mathrm{Det}_{n\mathbf{k}}},$$

$$\mathrm{Det}_{n\mathbf{k}}=(i\omega_n-\mu)^2-E_{\mathbf{k}}^2, \quad E_k=(\varepsilon_k^2+\Delta^2)^{1/2}. \quad (12)$$

In the following calculations we shall need the Green function of the quasiparticle in the SDW exchange field:

$$(G^0)^{-1}=g^{-1}-\bar{V}.$$

We write it in explicit form:

$$(G^0_{\mathbf{k}p\sigma\sigma'})^{-1}=\delta_{\mathbf{k},\mathbf{p}}\delta_{\sigma\sigma'}(-i\omega_n+\mu+\varepsilon_{\mathbf{k}})+\delta_{\mathbf{k},\mathbf{p}+\mathbf{Q}}\sigma^z_{\sigma\sigma'}\Delta. \quad (13)$$

where $\delta_{\mathbf{k},\mathbf{p}}=1$ if $\mathbf{k}=\mathbf{p}$, and $\delta_{\mathbf{k},\mathbf{p}}=0$ if $\mathbf{k}\neq\mathbf{p}$.

Allowance for the SDW fluctuations about the saddle point given by Eq. (12) requires certain assumptions about the character of these fluctuations. Generally speaking, Eq. (12) has a nontrivial solution in the range of temperatures $T<T_N^0$, but the identification of T_N^0 with the Néel temperature is by no means obvious. In "weak" magnets, with $U/t\ll 1$ (t is the width of the forbidden band), the quantity T_N^0 is related to U/t by a relation of the BCS type, but is exponentially small. For $U/t>1$ ("strong" magnets), formal solution of (12) gives $T_N^0\sim U$, and in the physically real temperature range $T\ll t$ the amplitude Δ is practically fixed, and depends only weakly on T. A calculation of the renormalization of the SDW amplitude on account of quantum (principally, longitudinal) fluctuations for a two-dimensional system with SDW has been performed recently by Schrieffer *et al.*[13] in the random-phase approximation for $T\ll T_N^0$.

It was shown that fluctuations decrease the amplitude Δ given by Eq. (12), the more strongly the greater the ratio U/t. Here, for simplicity, we shall not take into account quantum corrections in the self-consistency condition (12) for the SDW amplitude. Next, we assume that the analysis is performed in the region $T\ll T_N$ and the quantity Δ does not depend on T. We shall assume that the decisive role in the destruction of the long-range order is played by the transverse long-wavelength components of the spin fluctuations, which lead to vanishing of the coherence in the orientation of the spin density $\mathbf{S}_i$ for the alternating sublattices, with maintenance of an almost constant value of the SDW amplitude. This picture corresponds to the ideas of the "local-band theory" that has already been mentioned above.[4,5] Here, the temperature T_N^0 specifies only the limit of applicability of our approximation of constancy of the amplitude Δ, but does not have the meaning of the Néel temperature.

Thus, we assume that the main contribution to the par-

tition function of the system is made by SDW configurations for which

$$\Delta_i = \mathbf{e}_i \Delta,$$

where $\mathbf{e}_i$ is a unit vector that is varying slowly in space ($|\mathbf{e}_i|^2 = 1$, and $|\mathbf{e}_i - \mathbf{e}_j| < 1$ for neighboring lattice sites). We introduce a local coordinate system, specified by three angles θ_i, Φ_i, and b_i. The angles θ_i and Φ_i specify, in spherical coordinates, the directin of the local quantization axis $\mathbf{e}_i$ with respect to the laboratory quantization axis, and the angle b_i describes the rotation of the spin-density vector about the axis $\mathbf{e}_i$.

In the local coordinate system the Hamiltonian (1) can be rewritten in the form

$$H_{loc} = H_0 + H_1 + H_2 + H_{int}, \tag{14}$$

$$H_1 = -i \sum_{ij} \sum_{\sigma\sigma'} t_{ij} (c_{i\sigma}^{+} \sigma_{\sigma\sigma'} c_{j\sigma'} a_{ij}^{*} + c_{i\sigma}^{+} \sigma_{\sigma\sigma'}^{z} c_{j\sigma'} g_{ij}). \tag{15}$$

$$H_2 = \sum_{ij} \sum_{\sigma} t_{ij} d_{ij} c_{i\sigma}^{+} c_{j\sigma}, \tag{16}$$

$$a_{ij} \approx {}^1/_2 \exp(-i\bar{b}_{ij}) (\Phi_{ij} \sin \bar{\theta}_{ij} - i\theta_{ij}), \tag{17}$$

$$g_{ij} \approx {}^1/_2 (b_{ij} + \Phi_{ij} \cos \bar{\theta}_{ij}), \tag{18}$$

$$d_{ij} \approx -{}^1/_2 (|a_{ij}|^2 + g_{ij}^2), \tag{19}$$

where

$$\theta_{ij} = \theta_i - \theta_j, \quad \bar{\theta}_{ij} = {}^1/_2 (\theta_i + \theta_j)$$

and analogously for the angles b_i and Φ_i. In Eqs. (14)–(16) it is to be understood that the operators c_i and c_i^{+} act in the local coordinate system, and the Hamiltonians H_0 and H_{int} do not change their form when we go from the laboratory to the local coordinate system. The expressions (17)–(19) have been written with allowance for the condition

$$|\mathbf{e}_i - \mathbf{e}_j| \ll 1$$

for nearest neighbors. After going over to the local coordinate system we can calculate the free energy

$$F = -T \ln \operatorname{Sp} \exp\left(-\frac{1}{T} H_{loc}\right) \tag{20}$$

under the assumption that the orientation of the vector $\mathbf{\Delta}_i$ is slowly varying from site to site, with a fixed modulus $|\mathbf{\Delta}_i|$. In second order in H_1 and H_2 we obtain

$$F = F_0 + F_{SF}, \quad F_{SF} = F_{\perp} + F_{\parallel},$$

where $F_0 = F[\Delta]$ (see Ref. 11),

$$F_{\perp} = -{}^1/_4 T \sum_{n} \Big[\sum_{ij} \sum_{\sigma} G_{ij\sigma\sigma}^{0} t_{ij} |a_{ji}|^2 + \sum_{ijlm} \sum_{\alpha\beta\gamma} G_{ij\alpha}^{0} t_{jl} (\sigma_{\alpha\beta}^{+} a_{jl}^{*} + \sigma_{\alpha\beta}^{-} a_{jl}) \times G_{lm\beta\gamma}^{0} t_{mi} (\sigma_{\gamma\sigma}^{+} a_{mi}^{*} + \sigma_{\gamma\sigma}^{-} a_{mi}) \Big], \tag{21}$$

$$F_{\parallel} = -{}^1/_4 T \sum_{n} \Big[\sum_{ij} \sum_{\sigma} G_{ij\sigma\sigma}^{0} t_{ji} g_{ji}^2 + \sum_{ijlm} \sum_{\alpha\beta\gamma} G_{ij\sigma\alpha}^{0} t_{jl} \sigma_{\alpha\beta}^{z} g_{jl} G_{lm\beta\gamma}^{0} t_{mi} \sigma_{\gamma\delta}^{z} g_{mi} \Big], \tag{22}$$

and $\mathring{G}_{ij\sigma\alpha}$ is the Green function (13) in the site representation.

Thus, the calculation of the partition function of the system has reduced to the problem of integrating over the orientations of the random vector field $\mathbf{e} = \{\mathbf{e}_i\}$:

$$Z = Z_0 \exp\left(-\frac{F_0}{T}\right) \int \mathcal{D}\mathbf{e} \exp\left(-\frac{1}{T} F_{SF}\right). \tag{23}$$

3. EFFECTIVE SDW HAMILTONIAN IN THE PHASE OF SHORT-RANGE ORDER

The analysis of the expressions (21)–(23) still remains rather complicated. Introducting further simplifying assumptions, we require that all four vectors $\mathbf{e}_i$ appearing in (21) and (22) be close in direction for neighboring sites, and write the simplified relation

$$a_{ij}^{*} a_{lm} = {}^1/_4 (\mathbf{e}_i - \mathbf{e}_j)(\mathbf{e}_l - \mathbf{e}_m). \tag{24}$$

After this replacement the spin-fluctuation contribution F_{SF} acquires the simple form

$$F_{SF} = -\sum_{ij} J_{ij} \mathbf{e}_i \mathbf{e}_j, \tag{25}$$

i.e., has the form of the Heisenberg Hamiltonian for classical spins $S = 1$ with exchange integral

$$J_{ij} = \frac{1}{N^2} \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k},\mathbf{k}'} \exp(i\mathbf{k}\mathbf{r}_i - i\mathbf{k}'\mathbf{r}_j), \tag{26}$$

$$J_{\mathbf{k}\mathbf{k}'} = I_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}'} + K_{\mathbf{k}} \delta_{\mathbf{k},\mathbf{k}'+\mathbf{Q}},$$

$$I_{\mathbf{k}} = -\frac{T}{8N} \sum_{n\mathbf{p}} [2\varepsilon_{\mathbf{k}+\mathbf{p}} A_{\mathbf{p}} + (\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{k}})^2 (A_{\mathbf{p}} A_{\mathbf{p}+\mathbf{k}} + B_{\mathbf{p}} B_{\mathbf{p}+\mathbf{k}})], \tag{27}$$

$$K_{\mathbf{k}} = \frac{T}{8N} \sum_{n\mathbf{p}} (\varepsilon_{\mathbf{p}}^2 - \varepsilon_{\mathbf{p}+\mathbf{k}}^2)(A_{\mathbf{p}} B_{\mathbf{p}+\mathbf{k}} + B_{\mathbf{p}} A_{\mathbf{p}+\mathbf{k}}), \tag{28}$$

$$A_{\mathbf{p}} = \frac{i\omega_n - \mu + \varepsilon_{\mathbf{p}}}{\operatorname{Det}_{n\mathbf{p}}}, \quad B_{\mathbf{p}} = -\frac{\Delta}{\operatorname{Det}_{n\mathbf{p}}}.$$

Up to now we have not made explicit use of the special form of the spectrum $\varepsilon(\mathbf{k})$ in the model with "nesting," so that Eqs. (27)–(28) have a rather general form. When the condition

$$\varepsilon(\mathbf{k}) = -\varepsilon(\mathbf{k}+\mathbf{Q})$$

is rigorously fulfilled, we can convince ourselves that the "ferromagnetic" component of the exchange integral

$$K_{\mathbf{k}} = 0.$$

To calculate the Néel temperature we shall need the quantity

$$M_{\mathbf{k}} = I_{\mathbf{k}=0} - I_{\mathbf{k}},$$

which, after certain transformations, can be written in the form

$$M_{\mathbf{k}} = \frac{\Delta^2 T}{4N} \sum_{n\mathbf{p}} \frac{\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{p}+\mathbf{k}}}{\varepsilon_{\mathbf{p}} + \varepsilon_{\mathbf{p}+\mathbf{k}}} \left[\frac{1}{(i\omega_n - \mu)^2 - E_{\mathbf{p}}^2} - \frac{1}{(i\omega_n - \mu)^2 - E_{\mathbf{p}+\mathbf{k}}^2} \right], \tag{29}$$

where the summation over the wave vector $\mathbf{p}$ is bounded by the first Brillouin zone. For the classical Heisenberg model

with $S=1$, mean-field theory gives the following phase-transition temperature:

$$T_N^{MF}=\frac{2}{3}\frac{1}{N}\sum_{\mathbf{k}} M_{\mathbf{k}}, \tag{30}$$

while the method of spin Green functions[14] gives

$$T_N^{SF}=\frac{2}{3}\left(\frac{1}{N}\sum_{\mathbf{k}} M_{\mathbf{k}}^{-1}\right)^{-1}. \tag{31}$$

The summation in (30) and (31) runs over the first Brillouin zone. For an explicit calculation of (31) we specify the following form of dispersion law $\varepsilon_{\mathbf{p}}$, satisfying the "nesting" condition:

$$\varepsilon_{\mathbf{p}}=-2t(\cos p_x a+\cos p_y a)-2t_\perp \cos p_z c. \tag{32}$$

where a is the lattice constant in the x and y directions, and c is the lattice constant in the z direction. By varying the spectral-anisotropy constant

$$\gamma=t_\perp/t,$$

we can calculate the dependence of the Néel temperature on the effective dimensionality of the electorn subsystem of the crystal.

First of all we shall consider the formal limit of strong interaction $U\gg t$, when the spin density is localized at the lattice sites. For purely half filling of the band, we obtain from Eqs. (12) and (29) in this limit

$$\Delta=U/2$$

and the exchange integral

$$M_{\mathbf{k}}=\frac{t^2}{U}(2+\gamma^2-\cos k_x a-\cos k_y a-\gamma^2\cos k_z c). \tag{33}$$

The mean-field phase-transition temperature (30) is equal to

$$T_N^{MF}=\frac{2}{3}\frac{t^2}{U}(2+\gamma^2)$$

and remains finite for the two-dimensional case, when $\gamma\to 0$. More correct allowance for thermodynamic fluctuations, which leads to the relation (31), gives, for small γ,

$$T_N^{SF}=\frac{4\pi}{3}\frac{t^2}{U}\left(\ln\frac{8}{\gamma^2}\right)^{-1}\approx T_N^{MF}\pi\left(\ln\frac{8}{\gamma^2}\right)^{-1}. \tag{34}$$

The Néel temperature T_N (34) tends to zero as $\gamma\to 0$, although giving the system a small degree of three-dimensionality leads to a sharp increase of $T_N(\gamma)$. For an isotropic system, with $\gamma=1$ (a simple cubic lattice), we have

$$T_N^{MF}=2\frac{t^2}{U},\quad T_N^{SF}=\frac{T_N^{MF}}{1{,}51}.$$

A dependence of the Néel temperature on the anisotropy parameter analogous to (34) was obtained in Ref. 15 for a phenomenological model of an anisotropic Heisenberg antiferromagnet.

Formally, the "temperature of the appearnce of the SDW amplitude," which is given by the expression (12) (and which is essentially the characteristic temperature for the excitation of SDW amplitude fluctuations), amounts in the limit $t/U\ll 1$ to $T_N^0\sim U$, i.e., is certainly greater than (30) and (31). Thus, in the entire range of temperatures above the Néel point the phase of short-range order can be described by the above-considered model with a fixed SDW amplitude. In a three-dimensional system the correlation length $\zeta(T)$ of the spin fluctuations in this phase has the standard square-root behavior

$$\zeta(T)\sim\left(\frac{T-T_N^{SF}}{T_N^{SF}}\right)^{-1/2}.$$

In a quasi-two-dimensional system there is a regime of crossover from high-temperature two-dimensional behavior at $T\gg T_N^{SF}$, when

$$\zeta(T)\sim\exp\left(\frac{2\pi}{T}\frac{4t^2}{U}\right),$$

to three-dimensional behavior at $T\to T_N^{SF}$. This result can be obtained using the technique of Ref. 16 for investigating a two-dimensional chiral model in the continuum approximation with a small coupling constant, and we shall not focus attention on it here.

Let us consider in more detail the limit of delocalized spin density (the case of weak interaction $t\gg U$). For a two-dimensional system, with $\gamma=0$ and half filling ($\mu=0$), the temperature of formation of the SDW amplitude is, as follows from (12),

$$T_N^0\propto t\exp[-2^{1/2}\pi(t/U)^{1/2}]. \tag{35}$$

The region of critical amplitude fluctuations is small, and can be estimated as

$$(\delta T)_A\propto (T_N^0)^2/t\ll T_N^0.$$

For $T<T_N$ the dependence $\Delta(T)$ reaches saturation, and the thermodynamics of the system is determined by the low-energy transverse SDW fluctuations. We shall confine ourselves to the case of half filling ($\mu=0$) and to the quasi-two-dimensionality condition $\gamma\ll 1$ in the calculation of the exchange integral (29), since the calculation of $M_{\mathbf{k}}$ in general form is extremely cumbersome. Allowance for the strong dependence of $M_{\mathbf{k}}$ on the quasimomentum $\mathbf{k}$ in the region of small values of $\mathbf{k}$ (we have in mind the region $(ka)^2\ll 1$) is of fundamental importance. Integration over the frequencies and internal momenta in (29) for

$$(ka)^2\ll(\Delta/t)^2$$

gives for the case $\gamma=0$

$$M_k^<=\frac{t(ka)^2}{\pi}. \tag{36}$$

For

$$(ka)^2\gg\left(\frac{\Delta}{t}\right)^2$$

and $\gamma=0$, to within corrections of higher order in $(\Delta/t)^2$, we obtain

$$M_k^>=\frac{\Delta^2}{(2\pi)^2 t}\left(\ln\frac{\Delta}{t}\right)^2\approx\frac{t^2}{2U}\exp\left[-4\pi\left(\frac{t}{2U}\right)^{1/2}\right]=\bar{M}, \tag{37}$$

i.e., the dependence on $\mathbf{k}$ reaches saturation.

We have not succeeded in obtaining an exact analytical expression for the function $M_{\mathbf{k}}$, and therefore, to estimate the transition temperature, we shall make use of the piecewise-linear approximation

$$M_k=\begin{cases} M_k^< & \text{for } k<k_0, \\ M_k^> & \text{for } k>k_0, \end{cases}$$

where

$$k_0 a=\left(\frac{\pi T}{2U}\right)^{1/2}\exp\left[-2\pi\left(\frac{t}{2U}\right)^{1/2}\right].$$

After this, the "mean-field" Néel temperature can be estimated as

$$T_N^{MF}\approx{}^2/_3\bar{M}\sim(T_N^0)^2/U\ll T_N^0. \tag{38}$$

To calculate the "true" Néel temperature in the spin-fluctuation approach for a quasi-two-dimensional system we shall calculate $M_{\mathbf{k}}$ in lowest order in $t_\perp$. Assuming that

$$\Delta^2\gg\gamma^2 t^2,$$

we obtain

$$M_{\mathbf{k}}(\gamma)=M_{\mathbf{k}}(0)+\frac{t}{\pi}\gamma^2\left(\frac{t}{2U}\right)^{1/2}\sin^2\frac{k_z c}{2}.$$

Substituting this expression into (31), after integration over $\mathbf{k}$ we obtain

$$T_N^{SF}=T_N^{MF}\left[1+\frac{3}{2}\frac{T_N^{MF}}{t}\ln\left(\pi\left(\frac{t}{U}\right)^{1/2}\frac{\Delta^2}{t_\perp^2}\right)\right]^{-1}. \tag{39}$$

For small values $\gamma\to 0$, when $T_N^{\mathrm{SF}}<T_N^{\mathrm{MF}}$, just as in the case of the limit of local moments, crossover from the three-dimensional (near T_N^{SF}) to the two-dimensional regime becomes possible. The latter regime, characterized by an exponential dependence of $\zeta(T)$ on the temperature:

$$\zeta(T)\propto a\exp\left(\frac{2\pi}{T}\bar{M}\right),$$

is bounded from above, however, by the requirement $T\ll T_N^0$, while the latter is itself bounded by $T_N^0\ll t, U$. The region of temperatures

$$T_N^{MF}<T<T_N^0$$

may conventionally be called the region of two-dimensional short-range order, while the region

$$T_N^{MF}<T<T_N^{SF}$$

may be called the region of three-dimensional short-range order.

4. DENSITY OF STATES IN THE PHASE OF SHORT-RANGE ORDER

To determine the one-electron characteristics of a system with short-range antiferromagnetic order it is necessary to specify a procedure for averaging over the SDW-fluctuation ensemble, specified in our approach by the set of vectors $\{\mathbf{e}_i\}$, for the corresponding one-particle Green functions.

Considering the Hamiltonian H_1+H_2 as a perturbation with a given SDW configuration in the system of band electrons, we write for the "configuration" Green function the symbolic relation

$$G=G^0+G^0(H_1+H_2)G, \tag{40}$$

where G is the one-electron Green function (13) of the ground (Néel) state. We shall determine the averaged (over the orientations $\{\mathbf{e}_i\}$) Green function $\langle G\rangle_{\mathrm{SF}}$ in the simplest, Gaussian approximation for the distribution of the spin fluctuations, the effective Hamiltonian of which is specified by the quadratic form (25). In this approximation all even spin correlators are decoupled into pair correlators ($\langle\mathbf{e}_i\ldots\mathbf{e}_j\rangle-\langle\mathbf{e}_i\mathbf{e}_l\rangle\ldots\langle\mathbf{e}_m\mathbf{e}_j\rangle$), and all odd correlators are decoupled into products of pair correlators and averages $\langle\mathbf{e}_i\rangle$. We shall confine ourselves to considering only phases with short-range order, when all $\langle\mathbf{e}_i\rangle=0$ and the odd correlators vanish upon summation over the spin indices. Making in (13) the replacement

$$i\omega_n+M\to\omega,$$

we write for the temporal Green functions averaged over the ensemble of configurations $\{\mathbf{e}_i\}$ the relation

$$\langle G\rangle^{-1}=(G^0)^{-1}-\Sigma,\quad \Sigma=\langle H_2\rangle+\langle H_1 G^0 H_1\rangle. \tag{41}$$

We write out the self-energy part in explicit form:

$$\begin{aligned}\Sigma_{\mathbf{k}p\sigma\sigma'}=&-\delta_{\sigma\sigma'}\delta_{\mathbf{k},\mathbf{p}}{}^1/_4\sum_{\mathbf{q}}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}-\mathbf{q}})f_{\mathbf{q}}\\ &-\delta_{\sigma\sigma'}\delta_{\mathbf{k},\mathbf{p}}{}^1/_4\sum_{\mathbf{q}}A_{k-q}(\varepsilon_{\mathbf{k}-\mathbf{q}}-\varepsilon_{\mathbf{k}})^2 f_{\mathbf{q}}\\ &-\sigma_{\sigma\sigma'}{}^z\delta_{\mathbf{k},\mathbf{p}+\mathbf{Q}}{}^1/_4\sum_{\mathbf{q}}B_{\mathbf{k}-\mathbf{q}}(\varepsilon_{\mathbf{k}-\mathbf{q}}-\varepsilon_{\mathbf{k}})^2 f_{\mathbf{q}},\end{aligned} \tag{42}$$

where

$$A_{\mathbf{k}}=\frac{\omega+\varepsilon_{\mathbf{k}}}{\omega^2-E_{\mathbf{k}}{}^2},\qquad B_{\mathbf{k}}=\frac{\Delta}{\omega^2-E_{\mathbf{k}}{}^2}.$$

In Eq. (42) the quantity $f_{\mathbf{q}}$ is a Fourier component of the pair correlation function $\langle\mathbf{e}_i\mathbf{e}_j\rangle$. To be specific, we shall consider the case of a purely two-dimensional system ($\gamma=0$) and perform the calculation in the long-wavelength approximation, assuming $f_{\mathbf{q}}$ to be nonzero in a small range of quasimomenta $q\ll 1/a$. We introduce the dimensionless quantity

$$\xi^{-2}=\frac{1}{16N}\sum_{\mathbf{q}}f_{\mathbf{q}}(qa)^2, \tag{43}$$

which is inversely proportional to the square of the correlation length of the short-range order.

Direct determination of the poles of the averaged Green function (41) leads to the dispersion relation

$$\begin{aligned}\omega_{\mathbf{k}}{}^2=&E_{\mathbf{k}}{}^2+\xi^{-2}(\eta_{\mathbf{k}}{}^2+\varepsilon_{\mathbf{k}}{}^2+{}^1/_2\varepsilon_{\mathbf{k}}{}^2\xi^{-2})\\ &\pm\xi^{-1}[4E_{\mathbf{k}}{}^2\eta_{\mathbf{k}}{}^2+\eta_{\mathbf{k}}{}^2\varepsilon_{\mathbf{k}}{}^2\xi^{-2}(\xi^{-2}+4)+\xi^{-2}\varepsilon_{\mathbf{k}}{}^4(1+{}^1/_2\xi^{-2})]^{1/2},\\ \eta_{\mathbf{k}}{}^2=&2(2t)^2(\sin^2 k_x a+\sin^2 k_y a).\end{aligned} \tag{44}$$

It can be seen from this relation that thermodynamic SDW fluctuations lead to a doubling of the number of dispersion branches in comparison with the case $T=0$, $\xi=\infty$, i.e., when there exists long-range AFM order with

$$\omega_{\mathbf{k}}=\pm E_{\mathbf{k}}.$$

The physical meaning of this doubling is related to the possibility of motion of an electron with the "right" and the "wrong" spin in each of the two antiferromagnetic sublattices when they are partially disoriented. For the case of ideal long-range order the branch with the "wrong" spin disappears (the corresponding residue in the Green function vanishes), and the short-range order leads to a redistribution of the population of the "right" and "wrong" branches.

Near the point of onset of long-range order ($\xi \to \infty$) the expression (44) is simplified:

$$\omega_{\mathbf{k}} = \pm (E_{\mathbf{k}} \pm \xi^{-1}\eta_{\mathbf{k}}). \tag{45}$$

Substituting (45) into the standard formula for the density of states $\rho(\omega)$, we obtain

$$\rho(\omega) = -\frac{1}{8\pi}\operatorname{Im}\frac{1}{N}\sum_{\mathbf{k}}\left(\omega - \varepsilon_{\mathbf{k}} - \frac{\omega+\varepsilon_{\mathbf{k}}}{\omega^2 - E_{\mathbf{k}}^2}\xi^{-2}\eta_{\mathbf{k}}^2\right)$$
$$\times\left[\left(\frac{1}{\omega} - \frac{1}{E_{\mathbf{k}}}\right)\left(\frac{1}{\omega + i0 + E_{\mathbf{k}} + \xi^{-1}\eta_{\mathbf{k}}} + \frac{1}{\omega + i0 + E_{\mathbf{k}} - \xi^{-1}\eta_{\mathbf{k}}}\right)\right.$$
$$\left. + \left(\frac{1}{\omega} + \frac{1}{E_{\mathbf{k}}}\right)\left(\frac{1}{\omega + i0 - E_{\mathbf{k}} - \xi^{-1}\eta_{\mathbf{k}}} + \frac{1}{\omega + i0 - E_{\mathbf{k}} + \xi^{-1}\eta_{\mathbf{k}}}\right)\right]. \tag{46}$$

The complexity in the exact calculation of the double integral in (46) is due to the differing symmetries in $\mathbf{k}$ of the functions $\varepsilon_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$; it is the function η_k that determines the behavior of the integrand near the Fermi surface. Simplifying the calculations, in (46) we replace the quantity $\eta_{\mathbf{k}}$ by its value on the Fermi surface, after which the double integral reduces to successive integration over the energy ε, reckoned from the Fermi level, and the polar angle ψ. Performing the first of these, we have

$$\rho(\omega) = \int_{-\pi/2}^{\pi/2}\frac{d\psi}{\pi}\rho^0(\omega + 4t\xi^{-1}\sin\psi), \tag{47}$$

where $\rho(\omega)$ is the density of states for a system with a uniform SDW on a square lattice:

$$\rho^0(\omega) = \frac{1}{\pi^2 t}\frac{|\omega|}{(\omega^2-\Delta^2)^{1/2}}K\left(\left(1 - \frac{\omega^2-\Delta^2}{(4t)^2}\right)^{1/2}\right),$$
$$(4t)^2 + \Delta^2 > \omega^2 > \Delta^2,$$
$$\rho^0(\omega) = 0, \quad \omega^2 < \Delta^2. \tag{48}$$

Here, $K(k)$ is a complete elliptic integral of the first kind. For a qualitative estimate of the dependence $\rho(\omega)$ in the most interesting range of energies

$$|\omega^2/\Delta^2 - 1| \ll 1$$

we use in the integral (47) the simplifying approximation

$$\sin\psi \to \psi,$$

assuming that the quantity

$$4t\xi^{-1} = \beta \ll \Delta;$$

after this we obtain

$$\rho(\omega) = \frac{1}{4\pi^2 t^2 \xi^{-1}}\begin{cases}\Omega_+ - \Omega_- + \Omega_+ \ln\dfrac{16t}{\Omega_+} - \Omega_- \ln\dfrac{16t}{\Omega_-}, & \omega > \Delta + \beta,\\ \Omega_- \ln\dfrac{16t}{\Omega_+} + \Omega_+, & \Delta + \beta > \omega > \Delta - \beta,\\ 0, & \omega < \Delta - \beta,\end{cases}$$
$$\Omega_\pm = [(\omega \pm \beta)^2 - \Delta^2]^{1/2}, \quad \rho(\omega) = \rho(-\omega). \tag{49}$$

Thus, the transverse spin fluctuations smear out the density-of-states singularity at $\omega = \pm\Delta$ that would have occurred in the phase with ideal long-range order when

$$\xi^{-1} \to 0.$$

At the same time, the gap decreases to the value

$$2\tilde{\Delta} = 2(\Delta - \beta),$$

while the temperature dependence of $2\tilde{\Delta}(T)$ is determined by the corresponding behavior of the correlation length, which, in a two-dimensional system, is exponential in T. For a quasi-two-dimensional system near the Néel point the quantity $\tilde{\Delta}(T)$ can also have a part with a square-root temperature dependence.

5. CONCLUSION

Thus, a phase of short-range order can exist in systems with SDW in a wide range of temperatures above the Néel point, irrespective of the degree of saturation of the magnetic moment of the sublattice (i.e., both in the band limit and in the localized limit). Of course, throughout we have been concerned only with systems with weak magnetic anisotropy, and electron-electron interaction has been considered in the exchange approximation. The inclusion of relativistic terms (of the spin-orbit or magnetic-dipole type) can suppress orientational fluctuations for $W_{an} > T_N^{SF}$, where W_{an} is the magnetic-anisotropy energy, and for such systems the temperature T_N of the establishment of long-range order is $\sim T_{eV}$. It is apparently the latter situation that we encounter in Cr alloys for a 1**Q** state with a fixed axis of sublattice magnetization.[9] Nevertheless, a "tail" of a phase of short-range order above the Néel point has been observed both in pure Cr (Ref. 17) and in Cr–V alloys,[18] although in a substantially weakened form (the nominal root-mean-square amplitude of the SDW is reduced by a factor of approximately five in comparison with the maximum value in the phase with long-range order). It may be supposed that a phase of short-range antiferromagnetic order will be manifested more clearly in complex magnets. In particular, we would hope that the above approach will be applicable to systems of the type K_2NiF_4, La_2CuO_4, and similar systems (see the discussion in the review in Ref. 19).

In the framework of the standard SDW model we have shown that above the Néel point the dielectric type of electron spectrum is preserved and the square-root singularities in the density of states are smeared out. The edges of the pseudogap have been determined [see Eqs. (41)]. It should also be noted that allowance for the short-wavelength components of the SDW fluctuations, which, in view of their smallness, were discarded in our scheme, would lead to the appearance of an imaginary part in the poles of the averaged Green functions of the band electrons, and, as a consequence, to smearing out of the edges of the pseudogap by virtue of the attenuation.

An important queestion that has not been touched upon in the present paper is that of the description of dynamical SDW fluctuations in the phase of short-range order, and, in the first place, the construction of an effective Lagrangian

from a microscopic model. The solution of this question depends on the performance of correct averaging over the SDW configurations of the two-particle electron Green functions in the phase of short-range order. Such averaging is in no way trivial, even in the case of band ferromagnetism (see the similar paper Ref. 20) with a simple form of electron spectrum.

Of course, the "naive" approach with the introduction of an effective quantum Hamiltonian of the quasi-two-dimensional Heisenberg model with an antiferromagnetic exchange integral calculated in the static approximation cannot be used seriously in the situation of a band antiferromagnet with delocalized spin density. We hope that the solution of this problem in the framework of an approach analogous to that of Ref. 20 will make it possible to calculate the dynamic susceptibility, spectrum, and damping of the paramagnons, and other magnetic characteristics, in the phase of short-range order with SDW.

A further interesting problem is the construction of a model of short-range order in systems with SDW with other than half ($\mu = 0$) filling of the band, and the determination of the $T_N(\mu)$ phase diagram.

We must expect an increase of ferromagnetic fluctuations and an increase of the weight of the corresponding configurations in the partition function; structures with phase separation into "normal," "ferromagnetic," and "antiferromagnetic" droplets, and also structures with a modulated SDW amplitude, are possible.

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