

Collective excitations in banded antiferromagnets with short-range order

V. N. Men'shov and V. V. Tugushev

Russian Scientific Center "Kurchatov Institute," 123182 Moscow, Russia

(Submitted 20 January 1995)

Zh. Éksp. Teor. Fiz. **108**, 303–323 (July 1995)

The dynamic susceptibility of a banded antiferromagnet with a spin density wave is calculated above the Néel point. Spin-fluctuation theory is used, which assumes the presence of orientational short-range order of the spin density with amplitude close to its maximum value, and the variations of the single-electron spectrum and spin density amplitude due to thermodynamic magnetic disorder are found. The properties of the low-frequency transverse excitations of the spin density are analyzed: for pulses $\delta \gg \delta_{cr}$ the excitation has the form of a magnon with weak decay; for $\delta < \delta_{cr}$ the excitation has a purely diffusive character. The vector δ is reckoned from the wave vector of the antiferromagnetic structure, and the quantity δ_{cr}^{-1} is proportional to the correlation length of the short-range magnetic order. The applicability of the results of this study to an analysis of the magnetic properties of a reconstructed (111)-(2×1) diamond or silicon surface is discussed. © 1995 American Institute of Physics.

1. INTRODUCTION

In contemporary theories of banded magnetism it is usually assumed that the breakdown of long-range magnetic order in crystals with increase of temperature is chiefly due to the collective excitations—fluctuations of the spin density.¹ They determine the phase transition temperature T_c , the changes in the magnetic structure parameters below T_c , and also the radius of short-range order and its temperature region above T_c . There is no universal method for calculating the influence of spin fluctuations on the properties of banded magnets, which underlies the variety of approaches to the construction of their thermodynamics.

One of the most physically intuitive of such approaches is the method² which has acquired the name "local band theory" and is used for "strong" (saturated) banded ferromagnets with spin density amplitude near maximum.³ In this theory the magnetic moment of a unit cell of the crystal is formed at temperatures significantly greater than the temperature at which long-range order arises. Amplitude spin density excitations have frequencies on the order of the Stoner exchange splitting and do not determine the phase transition temperature. The main role in the formation of ferromagnetic order according to Refs. 2 is played by the transverse long-wave spin density fluctuations with low frequencies (of the order of the spin-wave frequencies). Thus, above the transition point the exchange (Stoner) splitting of the subbands is preserved, along with the short-range (but not long-range) ferromagnetic order. It is clear that the method of Refs. 2 and 3 somewhat overestimate the role of transverse fluctuations in a three-dimensional system in comparison with the longitudinal; however, in systems with lower dimension the applicability of this method is much better justified. In Ref. 4 we employed "local band theory" to study the thermodynamics of banded antiferromagnets for which a spin density wave (SDW) has doubled (Néel) structure in the ground state. Let us briefly review the main features of the development of Ref. 4.

In the vicinity of the Néel point T_N a thermally excited state of an antiferromagnet is formed by electronic Bloch states with energies lying in a band $\sim T_N$ near the Fermi level ε_F , where $T_N \ll \Delta$ (Δ is the amplitude of the spin density wave). This assumption substantially narrows the configuration field of actual spin fluctuations: the wave packets are made up from the Bloch functions with wave vectors \mathbf{k} near $\pm \mathbf{G}/2$ (\mathbf{G} is the inverse lattice vector of the crystal). Consequently, the most probable fluctuations are large-scale transverse fluctuations of the magnetization at the wave vector \mathbf{q} near the antiferromagnetic structure vector $\mathbf{Q} = \mathbf{G}/2$, i.e., transverse spin density waves. Above the Néel point, thanks to the presence of short-range order, the idea of banded crystal structure remains meaningful. This structure is similar, but not identical, to the structure connected with pure period doubling in the ground state. The quasimomentum \mathbf{k} and the spin σ of the quasiparticle are "almost good" quantum numbers at least for $|\mathbf{k} - \mathbf{G}/2|l > 1$, where l is the characteristic scale of the SDW fluctuations ($l \rightarrow \infty$ as $T \rightarrow T_N$). An energy gap of almost the same magnitude, 2Δ , as in the ground state is preserved in the density of states.

In Ref. 4 we also emphasized the fundamental role of thermodynamic SDW fluctuations for the very existence of long-range order in banded antiferromagnets with lower dimension, in particular, quasi-two-dimensional. In such systems the temperature interval of the phase of the short-range order is substantially extended (in relation to the isotropic three-dimensional situation) toward lower temperatures, and the Néel temperature is lowered, vanishing (in the absence of magnetic anisotropy) in the strictly two-dimensional case. Thus, one can assume that low-dimensional banded antiferromagnets exist with anomalously low Néel temperatures, and also those in which there is no mean magnetization of the sublattices at all for $T > 0$. In our opinion, such objects include with a high probability atomically pure (111)-(2×1) surfaces of diamond-like conductors.⁵ This question will be discussed in more detail in the Conclusion of this paper.

In this paper we will extend the study of banded antifer-

romagnets with spin density waves in the region of orientational short-range order begun in Ref. 4. Two problems will be solved: 1) renormalization of the SDW amplitude due to thermodynamic spin fluctuations, 2) calculation of the transverse susceptibility and collective excitations—paramagnons—in the absence of long-range order. We will use the results of these calculations to explain some features of the band structure and the magnetic properties of the semiconducting (111)–(2×1) faces of Si (or C) according to the π -bonded chain model.⁶

2. TRANSVERSE SDW FLUCTUATIONS AND THE LOCAL BAND METHOD

Before going on to what is new in this paper, let us note briefly a number of well known techniques of the spin-fluctuation theory of banded magnetism,^{2,3} used in Ref. 4 to model antiferromagnets with spin density waves. We consider the single-band Hubbard model with Hamiltonian

$$H = H_0 + H_{\text{int}}, \quad H_0 = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma}, \quad (1)$$

$$H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where all of the notation is standard.

Introducing the unit vector \mathbf{e}_i prescribing the local orientation of the quantization axis at the i th node, we rewrite the term H_{int} in the equivalent form

$$H_{\text{int}} = U \sum_i \left[\frac{1}{4} n_i^2 - (\mathbf{e}_i \mathbf{S}_i)^2 \right], \quad (2)$$

where

$$n_i = n_{i\uparrow} + n_{i\downarrow}, \quad S_{iz} = \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})$$

are the charge and spin densities, respectively. Representation (2) allows us, by means of the Hubbard-Stratonovich transformation, formally to reduce the initial many-particle problem (1) to a single-particle problem involving the motion of an electron in the arbitrarily fluctuating (in space and in time) scalar $x_i(\tau)$ and vector $\mathbf{y}_i(\tau) = \mathbf{e}_i(\tau) \cdot \mathbf{y}_i(t)$ fields, conjugate to the charge and spin densities, respectively. In the “static” approximation, i.e., neglecting the dependence of the fields x_i and \mathbf{y}_i on τ , the partition function corresponding to Hamiltonian (1) has the form

$$Z = Z_0 \int D\mathbf{x} D\mathbf{y} \exp \left[-\pi \sum_i (x_i^2 + y_i^2) + \text{Tr} \ln(1 - gV) \right], \quad (3)$$

where

$$g_{ijn} = \frac{1}{N} \sum_{\mathbf{k}} \frac{\exp i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)}{i\omega_n + \mu_0 - \varepsilon_{\mathbf{k}}} \quad (4)$$

is the Green’s function of the noninteracting electrons with dispersion

$$\varepsilon_{\mathbf{k}} = \frac{1}{N} \sum_{i,j} t_{ij} \exp[-i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)],$$

\mathbf{k} is the quasi-momentum, \mathbf{r}_i is the position vector of the i th node, $\omega_n = \pi T(2n + 1)$ is the frequency, μ_0 is the chemical potential,

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

is a random potential, σ is the Pauli matrix, and Z_0 is the partition function of the noninteracting electrons.

In expression (3) and in what follows, the symbol Tr (the trace) denotes the sum of the diagonal matrix elements over spin index σ , node index i , and the frequency variable n .

The saddle-point approximation in the variable x_i (i.e., neglecting fluctuations of the charge density) gives the following renormalization of the chemical potential:

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

where \bar{x} is the crossover point.

Let us now turn our attention specifically to the problem of an antiferromagnet with spin density waves, whereby we will consider only the situation in which the spin density waves in the ground state have doubled the Néel structure. We take the “nesting” condition for the electron spectrum

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

to be fulfilled, where $\mathbf{Q} = \mathbf{G}/2$. We distinguish two magnetic sublattices; for one of these we choose the local quantization axis \mathbf{e}_i to be aligned with the direction of local magnetization \mathbf{S}_i , and for the other we take the vectors \mathbf{e}_i and \mathbf{S}_i to be antiparallel, i.e.,

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

Next we normalize the vector field \mathbf{y}_i in energy units

$$\Delta_i = (\pi UT)^{1/2} \mathbf{y}_i \exp(i\mathbf{Q}\mathbf{r}_i) = U \mathbf{S}_i \exp(i\mathbf{Q}\mathbf{r}_i). \quad (5)$$

In the mean-field approximation it is possible to find the SDW amplitude Δ_i . For a linearly polarized spin density wave the quantity $\Delta_i = \Delta$ is given by the well-known self-consistency equation

$$-\frac{\Delta}{U} = \frac{T}{N} \sum_{n,k} \frac{\Delta}{(i\omega_n - \mu)^2 - E_{\mathbf{k}}^2}, \quad (6)$$

$$E_{\mathbf{k}} = (\varepsilon_{\mathbf{k}}^2 + \Delta^2)^{1/2}.$$

Equation (6) has a nontrivial solution in the temperature region $T < T_N^0$. In weak magnets for $U/t \ll 1$ (t is of the order of the width of the allowed band) the temperature T_N^0 is related to U/t by a formula of the BCS form, and for $U/t \gg 1$ (“strong” magnets) the formal solution of Eq. (6) gives $T_N^0 \sim U$. For $T \ll T_N^0$ it is possible to obtain from Eq. (6) the standard expression for the SDW amplitude $\Delta(U/t, T, \mu)$, which depends weakly on temperature.

A calculation of the renormalization of the SDW amplitude due to quantum fluctuations was carried out in Ref. 7 in the non-self-consistent random-phase approximation (RPA) for $T \ll T_N^0$. It was shown that these fluctuations give a smaller value of Δ than that given by Eq. (6), and the more strongly, the larger is the ratio U/t . The authors of Ref. 8

proposed a self-consistent approach for taking account of quantum spin fluctuations which preserves the invariance of the system with respect to rotations in spin space. In the approach of Ref. 8 the parameter Δ acquires a dependence on the frequency ω , the SDW amplitude is governed by the high-frequency limit of $\Delta(\omega)$, and the gap in the spectrum of single-particle excitations is governed by its low-frequency limit. Below we will consider the effect of quantum fluctuations on the magnitude of Δ , restricting ourselves, for simplicity, to the static approximation. Classical thermodynamic fluctuations of the spin density, leading to a renormalization of the SDW amplitude, will be taken into consideration within the framework of the "local band" method, which is worth going into in more detail.

According to current ideas in the band theory of magnetism based on the spin-fluctuation approach, the temperature T_N^0 is not the actual temperature at which antiferromagnetic long-range order is established (the Néel temperature). Rather, the quantity T_N^0 is some nominal upper bound on the temperature, below which are formed long-wave SDW fluctuations whose amplitude weakly depends on T . Long-range order (i.e., the Néel temperature T_N and the appearance of a mean magnetization of the sublattices) is described not by Eq. (6), but by other relations which can be obtained by spin-fluctuation approaches for $T \ll T_N^0$. Below we will be guided by the simply and physically intuitive approach of local band theory,² in which the formation and breakdown of long-range order are associated mainly with the transverse long-wave thermodynamic fluctuations of the spin density waves. We assume that for $T_N < T \ll T_N^0$ short-range order is present in the system, and the main contribution to the partition function comes from the SDW configurations $\{\Delta_i\}$ of Eq. (5) for which $\Delta_i = \mathbf{e}_i \Delta$, and the vector \mathbf{e}_i changes its direction slightly between neighboring nodes i and j of the lattice: $|\mathbf{e}_i - \mathbf{e}_j| \ll 1$. We will introduce a local coordinate system, defined by the angles $\{\Theta_i, \Phi_{ij}\}$, which define the direction of the local quantization axis \mathbf{e}_i relative to the laboratory quantization axis, and the angle b_i , which describes the rotation of the spin density vector about the \mathbf{e}_i axis.

In the local system of coordinates the Hamiltonian (1) is written as²

$$H_{\text{loc}} = H_0 + H_1 + H_2 + H_{\text{int}}, \quad (7)$$

$$H_1 = -i \sum_{i,j} \sum_{\sigma,\sigma'} t_{ij} (c_{i\sigma}^+ \sigma_{\sigma\sigma'}^+ c_{j\sigma'} a_{ij}^* + c_{i\sigma}^+ \sigma_{\sigma\sigma'}^- c_{j\sigma'} a_{ij} - c_{i\sigma}^+ \sigma_{\sigma\sigma'}^z c_{j\sigma'} g_{ij}), \quad (8)$$

$$H_2 = \sum_{i,j} \sum_{\sigma} t_{ij} d_{ij} c_{i\sigma}^+ c_{j\sigma}, \quad (9)$$

$$a_{ij} \approx \frac{1}{2} \exp(-i\bar{b}_{ij}) (\Phi_{ij} \sin \bar{\Theta}_{ij} - i\Theta_{ij}), \quad (10)$$

$$g_{ij} \approx \frac{1}{2} (b_{ij} + \Phi_{ij} \cos \bar{\Theta}_{ij}), \quad (11)$$

$$d_{ij} \approx -\frac{1}{2} (|a_{ij}|^2 + g_{ij}^2), \quad (12)$$

where

$$\Theta_{ij} = \Theta_i - \Theta_j, \quad \bar{\Theta}_{ij} = \frac{1}{2} (\Theta_i + \Theta_j),$$

and analogously for the angles Φ_i and b_i . In formulas (7)–(9) it is understood that the operators c_i and c_i^+ act in the local coordinate system, and the Hamiltonians H_0 and H_{int} have the same form as in the original representation (1). The matrix elements (10)–(12) as written take account of the condition $|\mathbf{e}_i - \mathbf{e}_j| \ll 1$ for nearest neighbors. In the local coordinate system the free energy of the system

$$F = -T \ln \text{Tr} \exp(-H_{\text{loc}}/T) \quad (13)$$

is easily represented in additive form

$$F = F_0[\Delta] + F_{\text{SF}}[\Delta, \{\mathbf{e}_i\}],$$

where the functional $F_0[\Delta]$, which can be reconstructed by integrating the self-consistency equation (6) over Δ , is the energy of a homogeneous spin density wave and is independent of the direction \mathbf{e}_i . The term $F_{\text{SF}}[\Delta, \mathbf{e}_i]$ is an additional exchange energy of the antiferromagnet, associated with thermodynamic orientational disorder.

For the case of large-scale configurations $\{\mathbf{e}_i\}$ the density of the spin-fluctuation part of the functional F can be represented as an expansion in powers of the difference angles Θ_{ij} , Φ_{ij} , and b_{ij} . We obtained an explicit expression for the functional $F_{\text{SF}}[a_{ij}, g_{ij}]$ to second order in H_1 and H_2 in our previous paper.⁴ As was discussed in detail in Refs. 2, the structure of the term g_{ij} (11) is such that it leads to contributions to the energy F_{SF} which are fourth-order and higher in Φ_{ij} . In the long-wave limit the first nonvanishing terms of the expansion of the energy F_{SF} are second-order in Φ_{ij} and Θ_{ij} and are proportional to $a_{ij}^* \cdot a_{lm}$. In accordance with formula (10) this quantity is equal to

$$a_{ij}^* a_{lm} = \frac{1}{4} (\mathbf{e}_i - \mathbf{e}_j)(\mathbf{e}_l - \mathbf{e}_m) \quad (14)$$

and the spin-fluctuation contribution to the free energy of the magnet acquires the form of an effective Heisenberg Hamiltonian for the classical spins $S=1$:

$$F_{\text{SF}} = - \sum_{i,j} J_{ij} \mathbf{e}_i \mathbf{e}_j. \quad (15)$$

An expression for the exchange integral J_{ij} in terms of the microscopic parameters of an antiferromagnet with spin density waves was also obtained in Ref. 4. Thus, the calculation of the partition function (3) reduces to an integration over the orientations of the random vector $\mathbf{e} = \{\mathbf{e}_i\}$, $|\mathbf{e}|=1$:

$$Z = Z_0 \exp(-F_0/T) Z_{\text{SF}},$$

$$Z_{\text{SF}} = \int D\mathbf{e} \exp(-F_{\text{SF}}/T), \quad (16)$$

where the energy F_{SF} is given in the form (15).

To find any physical characteristic of a banded antiferromagnet in the region of short-range order, it is necessary to average over the equilibrium ensemble of SDW fluctuations, restricted in our approach by the set of configurations $\{\mathbf{e}_i\}$. If

the quantity $A[\{e_i\}]$ corresponds to a specific configuration $\{e_i\}$ taken from this set, then the thermodynamic average $\langle A \rangle$ is calculated as a functional integral

$$\langle A \rangle = Z_{\text{SF}}^{-1} \int D\mathbf{e} A[\mathbf{e}] \exp(-F_{\text{SF}}[\mathbf{e}]/T). \quad (17)$$

We will perform the calculation of $\langle A \rangle$ in the Gaussian approximation for the distribution of orientation vectors \mathbf{e}_i , whose effective Hamiltonian is of the quadratic form (15). In this approximation all even spin correlators decouple into products of pairwise correlators $\langle \mathbf{e}_i \dots \mathbf{e}_j \rangle \rightarrow \langle \mathbf{e}_i \mathbf{e}_j \rangle \dots \langle \mathbf{e}_m \mathbf{e}_j \rangle$, and all odd, into products of pairwise correlators and mean values $\langle \mathbf{e}_i \rangle$. In what follows we will restrict the discussion to the paramagnetic phase, for which $\langle \mathbf{e}_i \rangle = 0$ holds and all odd correlators vanish.

To calculate any average $\langle A \rangle$, it is thus necessary to determine the amplitude Δ and the pairwise correlator $f_{ij} = \langle \mathbf{e}_i \mathbf{e}_j \rangle$, and it is necessary, strictly speaking, to have a system of self-consistency equations for these quantities. Many qualitative results, however, can be obtained on the basis of general considerations about the shape of the spatial and temperature dependence of f_{ij} . Thus, it is natural to assume that in the region of short-range order for $T_N < T \ll T_N^0$ the Fourier component $f_{\mathbf{q}}$ has a sharp maximum at small values of the wave vector $q \ll a^{-1}$, which corresponds to a maximum of the spin density correlator $\langle S_{\mathbf{q}} S_{-\mathbf{q}} \rangle$ at values of \mathbf{q} near the antiferromagnetism vector $\mathbf{Q} = \mathbf{G}/2$. The spin correlation radius $l(T)$ and the shape of the temperature dependence of $f_{\mathbf{q}}(T)$ can be estimated, as in Ref. 4, on the basis of well-known results for the classical Heisenberg Hamiltonian.

3. SINGLE-PARTICLE EXCITATIONS AND RENORMALIZATION OF THE SDW AMPLITUDE

Scattering of band electrons by a typical SDW fluctuation $\{e_i\}$ above the Néel point is characterized by the single-particle temporal Green's function $G_{ij\sigma\sigma'}(\{e_i\}, t)$, the equation for which we write in symbolic form as

$$\langle G_{\mathbf{k}\rho\sigma\sigma'}(\omega) \rangle = -N \frac{\delta_{\mathbf{k},\rho} \delta_{\sigma\sigma'} [(\omega + \varepsilon_{\mathbf{k}} + \nu_{\mathbf{k}})(\omega^2 - E_{\mathbf{k}}^2) - (\omega - \varepsilon_{\mathbf{k}})F_{\mathbf{k}}^2] + \delta_{\mathbf{k},\rho+\mathbf{Q}} \sigma_{\sigma\sigma'}^z \Delta (\omega^2 - E_{\mathbf{k}}^2 + F_{\mathbf{k}}^2)}{(\omega^2 - (\omega_{\mathbf{k}}^+)^2)(\omega^2 - (\omega_{\mathbf{k}}^-)^2)} \quad (22)$$

The poles of the function (22) determine the spectrum of single-electron excitations in the phase with antiferromagnetic order:

$$(\omega_{\mathbf{k}}^{\pm})^2 = E_{\mathbf{k}}^2 + F_{\mathbf{k}}^2 + \nu_{\mathbf{k}}^2/2 + \varepsilon_{\mathbf{k}} \nu_{\mathbf{k}} \pm [4E_{\mathbf{k}}^2 F_{\mathbf{k}}^2 + F_{\mathbf{k}}^2(\nu_{\mathbf{k}}^2 + 4\varepsilon_{\mathbf{k}} \nu_{\mathbf{k}}) + (\varepsilon_{\mathbf{k}} \nu_{\mathbf{k}} + \nu_{\mathbf{k}}^2/2)^2]^{1/2}, \quad (23)$$

where

$$F_{\mathbf{k}}^2 = \frac{1}{4} \sum_{\alpha} \left(\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{\alpha}} \right)^2 l_{\alpha}^{-2}, \quad (24)$$

$$[(G^0)^{-1} - H_1 - H_2]G = 1. \quad (18)$$

Orientational disorder enters into Eq. (18) through the Hamiltonians H_1 (8) and H_2 (9). The quasiparticle Green's function in the exchange field of the spin density wave in the ground (Néel) state has the form

$$(G_{\mathbf{k}\rho\sigma\sigma'}^0(\omega))^{-1} = \delta_{\mathbf{k},\rho} \delta_{\sigma\sigma'} (-\omega + \varepsilon_{\mathbf{k}}) + \delta_{\mathbf{k},\rho+\mathbf{Q}} \sigma_{\sigma\sigma'}^z \Delta, \quad (19)$$

where ω is the frequency and $\delta_{\mathbf{k},\rho} = 1$ for $\mathbf{k} = \rho$ and $\delta_{\mathbf{k},\rho} = 0$ for $\mathbf{k} \neq \rho$.

The procedure outlined above, of configurational integration makes it possible to express the $\{e_i\}$ ensemble-averaged propagator $\langle G_{\mathbf{k},\rho\sigma\sigma'}(\{e_i\}, \omega) \rangle$ in terms of the correlation function $f_{\mathbf{q}}$:

$$\langle G \rangle^{-1} = (G^0)^{-1} - \Sigma, \quad \Sigma = \langle H_2 \rangle + \langle H_1 G^0 H_1 \rangle. \quad (20)$$

The eigenenergy part Σ is equal to

$$\Sigma_{\mathbf{k}\rho\sigma\sigma'} = -\frac{1}{4} \left[\delta_{\mathbf{k},\rho} \delta_{\sigma\sigma'} \sum_{\mathbf{q}} (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}}) f_{\mathbf{q}} + \delta_{\mathbf{k},\rho} \delta_{\sigma\sigma'} \sum_{\mathbf{q}} A_{\mathbf{k}-\mathbf{q}} f_{\mathbf{q}} (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 f_{\mathbf{q}} + \delta_{\mathbf{k},\rho+\mathbf{Q}} \sigma_{\sigma\sigma'}^z \sum_{\mathbf{q}} B_{\mathbf{k}-\mathbf{q}} f_{\mathbf{q}} (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 f_{\mathbf{q}} \right], \quad (21)$$

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

Since the structure factor of the spin correlations $f_{\mathbf{q}}$ is assumed to be nonzero in the small interval of quasimomenta near $\mathbf{q} = 0$, the slowly varying (in comparison to $f_{\mathbf{q}}$) factors standing under the summation signs on the right-hand side of Eq. (21) can be expanded in series about the point $\mathbf{q} = 0$. Retaining the lowest-order terms of this expansion in \mathbf{q} , we obtain an expression for the averaged Green's function:

$$\nu_{\mathbf{k}} = -\frac{1}{8} \sum_{\alpha} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_{\alpha}^2} l_{\alpha}^{-2},$$

$$l_{\alpha}^{-2} = \frac{1}{N} \sum_{\mathbf{q}} f_{\mathbf{q}} q_{\alpha}^2, \quad (25)$$

\mathbf{q}_{α} are the components of the vector \mathbf{q} , $\alpha = 1, \dots, d$, where d is the dimension of the system. It is natural to treat the quantity l_{α} as the correlation length of magnetic short-range order in the α -th direction.

Near the point where long-range order arises (where $(k_F l_{\alpha})^{-1} \ll 1$) the correlation length l_{α} grows significantly,

and to the first nonvanishing terms in $\nu_{\mathbf{k}}$ we obtain

$$(\omega_{\mathbf{k}}^{\pm})^2 = (E_{\mathbf{k}} \pm F_{\mathbf{k}})^2 + \varepsilon_{\mathbf{k}} \nu_{\mathbf{k}}. \quad (26)$$

Relation (26) allows us to elucidate the physical meaning of the doubling of the number of dispersion branches $\omega_{\mathbf{k}} \rightarrow \omega_{\mathbf{k}}^{\pm}$ in comparison with the case of long-range antiferromagnetic order, when $l_{\alpha} = \infty$ and $\omega_{\mathbf{k}} = \pm E_{\mathbf{k}}$. It is not hard to convince oneself that the energy parameter $F_{\mathbf{k}}$ (24) associated with the Hamiltonian H_1 given by Eq. (8) corresponds to scattering of a quasiparticle by a spin fluctuation with spin flip; respectively, the parameter $\nu_{\mathbf{k}}$ (25) associated with the Hamiltonian H_2 of Eq. (9) corresponds to scattering without spin flip. Thus, in the phase with short-range order electron motion with the "right" or "wrong" spin direction is possible in each of the two antiferromagnetic sublattices if they are oriented slightly differently.

The doubling of the number of dispersion branches was noted in Ref. 4. The authors of Ref. 4 calculated the renormalization of the density of single-electron states due to scattering of carriers by fluctuations of the direction of the SDW vector specifically for the case of a two-dimensional system (a square lattice) and showed that narrowing of the antiferromagnetic gap occurs.

Let us examine the influence of spin fluctuations on the SDW amplitude. Since the order parameter $\Delta(T)$ due to the quasiparticle statistics is varies negligibly in the investigated temperature range $T_N < T \leq T_N^0$, we will use the self-consistency condition in which the Fermi function is replaced by the step

$$\Delta = \frac{U}{2} \int \frac{d\omega}{2\pi i} \frac{1}{N^2} \sum_{\mathbf{k}, \mathbf{p}} \sum_{\sigma, \sigma'} \sigma_{\sigma\sigma'}^2 \langle G_{\mathbf{k}, \mathbf{p} + \mathbf{Q}\sigma\sigma'}(\omega) \rangle. \quad (27)$$

The amplitude $\Delta(T)$ acquires a temperature dependence only because of the orientational disorder with correlator $f_{\mathbf{q}}(T)$. We substitute the averaged Green's function (22) in Eq. (27) and close the integration contour in the complex variable ω in the upper half-plane. As a result, we obtain to second order in the inverse correlation length the following equation for the mean amplitude of the spin density:

$$\Delta = \Delta U \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}} \left(1 - \frac{\varepsilon_{\mathbf{k}} \nu_{\mathbf{k}}}{E_{\mathbf{k}}^2} \right). \quad (28)$$

In the absence of disorder ($l_{\alpha}^{-2} \rightarrow 0$) this equation reduces to the Hartree-Fock equation (6) for $\mu = T = 0$. As can be seen from Eq. (28), in the implemented approximation the SDW amplitude changes only as a result of scattering processes without spin flip. The temperature dependence of $\Delta(T)$ is governed by the corresponding behavior of the correlation length $l_{\alpha}(T)$.

To carry out specific calculations, we assign the following form to the dispersion law of the free electrons $\varepsilon_{\mathbf{k}}$, which satisfies a "nesting" condition:

$$\varepsilon_{\mathbf{k}} = -2t \sum_{\alpha} \cos k_{\alpha} a. \quad (29)$$

According to the exchange approximation for the inter-electron interaction, which we have used here, the character-

istic scales of the orientational correlations of the spin density in any of the directions α coincide, i.e., $l_{\alpha} = l$. We therefore have

$$\nu_{\mathbf{k}} = \frac{\varepsilon_{\mathbf{k}}}{8} \left(\frac{a}{l} \right)^2, \quad F_{\mathbf{k}}^2 = \frac{\eta_{\mathbf{k}}^2}{8} \left(\frac{a}{l} \right)^2, \\ \eta_{\mathbf{k}}^2 = 2(2t)^2 \sum_{\alpha} \sin^2 k_{\alpha} a, \quad (30)$$

where naturally we assume that $l/a \gg 1$.

In the mean field model of banded antiferromagnetism in the absence of impurity scattering the SDW amplitude $\Delta = \Delta_0$ coincides with the half-width of the dielectric gap in the Néel phase $E_g = 2\Delta_0$. In the region of short-range order such a coincidence does not take place, and it follows from relations (26) and (30) that near the Néel point ($T \gtrsim T_N$) the width of the forbidden band for single-particle excitations is equal to

$$E_g = 2 \left(\Delta_0 - \frac{at\sqrt{d}}{l} \right). \quad (31)$$

Note that the narrowing of E_g is due exclusively to fluctuational scattering with spin flip.

We substitute the quantity $\nu_{\mathbf{k}}$ from formula (30) into Eq. (28) and estimate the magnitude of the change of the spin density at a node due to partial orientational disorder. For example, if we have $t/U \ll 1$, then

$$\Delta = \Delta_0 + \frac{(2t)^2 d}{2U} \left(\frac{a}{l} \right)^2. \quad (32)$$

In the weak interaction limit ($U/t \ll 1$) the influence of transverse SDW fluctuations is manifested in the renormalization of the effective potential U :

$$\Delta = \frac{\Delta \tilde{U}}{2N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}}, \quad \tilde{U} = U \left(1 + \frac{1}{8} \left(\frac{a}{l} \right)^2 \right). \quad (33)$$

This result coincides qualitatively with the renormalization of the potential U due to quantum fluctuations of the spin density, obtained in Ref. 8.

4. TRANSVERSE DYNAMIC SUSCEPTIBILITY

Capellmann and Vieira⁹ developed a general theory of dynamic susceptibility of banded ferromagnets with strong short-range order above the Curie point. They proposed a calculation scheme (the so-called "random phase approximation with exchange"), within which they drew some qualitative conclusions about the nature of the response. We propose a method for calculating the dynamic susceptibility which is somewhat different from theirs,⁹ based on the spin-fluctuation approach^{2,3} and on our previous work,⁴ to calculate the two-particle Green's function. In this approach it is possible to describe explicitly the low-frequency spin dynamics of banded antiferromagnets with spin density waves above the Néel temperature, as is required for the problem at hand.

According to Refs. 2, in the "local band" method one introduces a spin density correlator for each individual fluctuation $\{e_i\}$

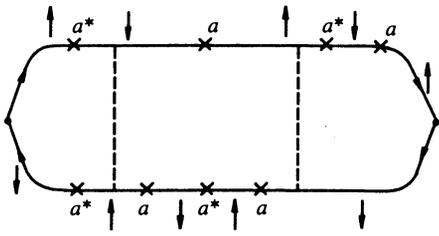


FIG. 1.

$$\chi_{\mathbf{q},\mathbf{q}'}^{\alpha\beta}(t, \{\mathbf{e}_i\}) = \frac{i}{2N} \left(TS_{\mathbf{q}}^{\alpha}(t) S_{-\mathbf{q}'}^{\beta}(0) \right)_{\{\mathbf{e}_i\}}. \quad (34)$$

The parentheses on the right-hand side of Eq. (34) denote averaging over quantum states for fixed set of vectors $\{\mathbf{e}_i\}$ giving the configuration of the spin density wave; the symbol T stands for time-ordering in t . The complete response to an external variable magnetic field (the magnetic susceptibility at the frequency Ω) is defined as the average over the SDW configurations [in the sense of (16)]:

$$\chi_{\mathbf{q},\mathbf{q}'}^{\alpha\beta}(\Omega) = \int_0^{\infty} dt \exp(i\Omega t) \langle \chi_{\mathbf{q},\mathbf{q}'}^{\alpha\beta}(t, \{\mathbf{e}_i\}) \rangle. \quad (35)$$

Let us dwell in detail on the question of the calculation of the averages (34) and (35).

The two-particle Green's function of the system with fluctuating spin density in the graphical representation can be depicted as an infinite series of "ladder" diagrams taking account of scattering by the randomly oriented moments at its nodes. By way of illustration, Figure 1 shows one of the simplest diagrams: the solid line denotes the unperturbed function G^0 given by (19), the dashed line denotes the Coulomb repulsion of particles with opposite spins U , the cross represents the matrix element a_{ij} for processes with spin flip H_1 (8), and the arrows \downarrow and \uparrow correspond to the projections of the electron spin. Let us turn our attention to the alternation in the arrangement of terms a_{ij} and a_{ij}^* and the spin indices. In the language of diagrams the averaging procedure (35) can be thought of as taking into account all possible variants of the pairwise joining of crosses by wavy lines. The graphical element consisting of a pair of crosses joined by a wavy line corresponds to the spin correlator f_{ij} . Figure 2 displays some typical diagrams which contribute to the averaged two-particle Green's function to first order in U and to fourth order in the disorder a_{ij} . Below we will consider only diagrams of type (a), assuming that diagrams (b), (c), and (d) have already been taken into account in the renormalization of the interaction U . In passing, it may be noted

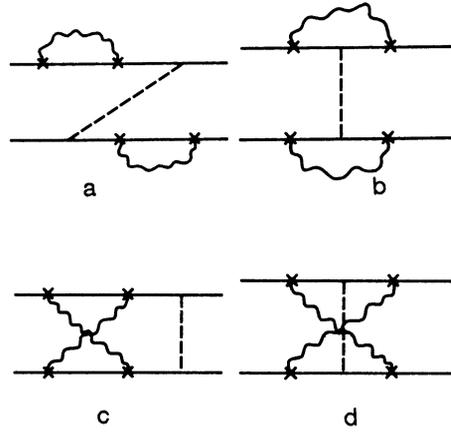


FIG. 2.

that we have intentionally omitted processes without spin flip [corresponding to H_2 of (9)] since their direct average $\langle |a_{ij}|^2 \rangle$ in the single-particle channel is not needed in any of the additional explanations that are to follow.

Thus, the calculation of the susceptibility of a magnet in the phase with strong thermal short-range order reduces to a modified random phase approximation with "dressed" quasiparticles (i.e., dressed by the disorder), in other words, to the sum of the infinite sequence of "ladder" diagrams shown in Fig. 3, where the double line represents the single-particle Green's function averaged over the space of orientational fluctuations. The expression for the latter is well known and is given by formulas (20)–(26).

Let us translate the graphical expressions into the language of analytical relations. The first diagram in the series (Fig. 3, not explicitly containing the interaction U or the analogous elementary electron-hole loop in the system of free electrons) corresponds to the following function of the two quasimomenta:

$$\bar{\chi}_{\mathbf{q},\mathbf{q}'}^{+-}(\Omega) = \frac{1}{N^2} \int \frac{d\omega}{2\pi i} \sum_{\mathbf{k},\mathbf{k}'} \langle G_{\mathbf{k},\mathbf{k}'}^{\downarrow\downarrow}(\omega) \rangle \times \langle G_{\mathbf{k}',\mathbf{k}+\mathbf{q}}^{\uparrow\uparrow}(\omega - \Omega) \rangle. \quad (36)$$

Thus, like the function $\langle G \rangle$ in (22), the expression for the response $\bar{\chi}^{+-}$ contains both a diagonal and a nondiagonal (in the quasimomenta) contribution, each of which depends on one quasimomentum:

$$\bar{\chi}_{\mathbf{q},\mathbf{q}'}^{+-}(\Omega) = \delta_{\mathbf{q},\mathbf{q}'} \chi_0^{+-}(\mathbf{q}, \Omega) + \delta_{\mathbf{q},\mathbf{q}'+\mathbf{Q}} \chi_{\mathbf{Q}}^{+-}(\mathbf{q}, \Omega). \quad (37)$$

Summing the geometric progression in Fig. 3 (in fact, solving the Dyson equation), we obtain the total response function in general form:

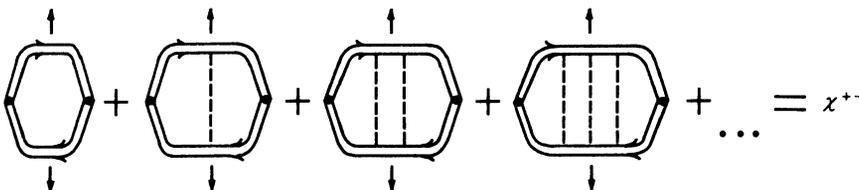


FIG. 3.

$$\chi_{\mathbf{q},\mathbf{q}'}^{+-}(\Omega) = \sum_{\mathbf{q}_1} \bar{\chi}_{\mathbf{q},\mathbf{q}_1}^{+-}(\Omega) [1 - U \bar{\chi}_{\mathbf{q}_1,\mathbf{q}'}^{+-}(\Omega)]^{-1}, \quad (38)$$

where

$$[1 - U \bar{\chi}_{\mathbf{q},\mathbf{q}'}^{+-}(\Omega)]^{-1} = \frac{[1 - U \chi_0^{+-}(\mathbf{q} + \mathbf{Q}, \Omega)] \delta_{\mathbf{q},\mathbf{q}'} + U \chi_0^{+-}(\mathbf{q}, \Omega) \delta_{\mathbf{q},\mathbf{q}' - \mathbf{Q}}}{[1 - U \chi_0^{+-}(\mathbf{q}, \Omega)] [1 - U \chi_0^{+-}(\mathbf{q} + \mathbf{Q}, \Omega)] - [U \chi_0^{+-}(\mathbf{q}, \Omega)]^2}. \quad (39)$$

The structure of the denominator of the transverse dynamic susceptibility (38), (39), with the equation of state (28) taken into account, determines the spectrum of the natural oscillations of the spin density of a banded antiferromagnet in the phase with short-range order. Let us proceed to some concrete calculations.

First we will calculate the susceptibility $\bar{\chi}_{\mathbf{q},\mathbf{q}'}(\Omega)$ (36)–(37), for which we substitute function (22) in expression (36), sum over the quasimomentum \mathbf{k}' and integrate over the frequency ω . We restrict ourselves to lower-order terms in the orientational fluctuations, i.e., terms of order $(a/l)^2$. Omitting the long chain of involved algebraic transformations, especially for the case of the electron spectrum (29), we obtain formulas (A1) and (A2) in Appendix A, also cumbersome, for the diagonal and nondiagonal components of the function $\bar{\chi}_{\mathbf{q},\mathbf{q}'}(\Omega)$. These formulas coincide in the limit $(a/l)^2 \rightarrow 0$ with the expressions obtained in Ref. 7 for the ground state of an antiferromagnet with spin density waves.

In order to determine the spectrum of the low-frequency long-wave excitations, we expand the functions (A1) and (A2) entering into the expression for the total susceptibility (38), (39) in the frequency Ω ($|\Omega| \ll \Delta$) and the quasimomentum $\delta = \mathbf{q} - \mathbf{Q}$ ($\delta a \ll 1, \delta \Delta \ll \Delta$) and drop the corrections generated by the disorder $\sim (a/l) \cdot \Omega^{2m}$ ($m > 0$). However, in this case we must keep the last term in the expression for $\bar{\chi}_0^{+-}(q, \Omega)$ (A1), which is proportional to

$$\Theta(\delta, \Omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}} \frac{\Omega^2}{\Omega^2 - \frac{\varepsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} \left(\sum_{\alpha} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{\alpha}} \delta_{\alpha} \right)^2}. \quad (40)$$

The summand in Eq. (40) possesses a singularity, the nature of which depends on the dimensionality and shape of the electron spectrum of the system. As we shall see below, it is precisely the function $\Theta(\delta, \Omega)$ that determines the analytical properties of the response $\bar{\chi}_{\mathbf{q},\mathbf{q}'}(\Omega)$. In contrast to the diagonal component of the (null) response, the nondiagonal component $\bar{\chi}_0^{+-}(\mathbf{q}, \Omega)$ of (A2) does not contain any term like the summand on the right-hand side of Eq. (40).

In the indicated region of frequencies and quasimomenta, with allowance for the equation for the mean amplitude of the spin density waves (28), we obtain the dynamic susceptibility

$$\chi_{\mathbf{q},\mathbf{q}'}^{+-}(\Omega) = \frac{\delta_{\mathbf{q},\mathbf{q}'}}{\text{Det}(\delta, \Omega)}, \quad (41)$$

$$- \frac{4}{U^2} \text{Det}(\delta, \Omega) = \Omega^2 \varphi_3 \frac{\varphi_1 + 3\Delta^2 \varphi_3}{\varphi_1 - \Delta^2 \varphi_3} - \Psi(\delta)$$

$$+ \frac{1}{2} \left(\frac{a}{l} \right)^2 (\rho + b \Theta(\delta, \Omega)), \quad (42)$$

where we have introduced the notation

$$\varphi_n = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}^n}, \quad (43)$$

$$\Psi(\delta) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}^3} \left[\frac{2\Delta^2 - \varepsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} \left(\sum_{\alpha} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{\alpha}} \delta_{\alpha} \right)^2 + \varepsilon_{\mathbf{k}} \sum_{\alpha} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_{\alpha}^2} \delta_{\alpha}^2 \right], \quad (44)$$

$$\rho = \frac{1}{2N} \sum_{\mathbf{k}} \frac{\eta_{\mathbf{k}}^2}{E_{\mathbf{k}}^3}. \quad (45)$$

Note that the parameters φ_n , ρ , and Ψ and the coefficient of Ω^2 in Eq. (42) are positive definite, while the function $\Theta(\delta, \Omega)$ is, generally speaking, complex.

The poles of the response (41) determine the paramagnon spectrum $\Omega(\delta)$. Its main features can be understood from the general form of the denominator $\text{Det}(\delta, \Omega)$ of (42). Collective excitations of the system with wave vectors δ that are so large that the magnitude of the fluctuation term $\sim (a/l)^2$ in relation (42) is negligibly small in comparison with $\Psi(\delta)$ are of a general spin-wave nature $\Omega = v \delta$. In the opposite limit of strong magnetic disorder the diffusion mode is excited: as $\delta \rightarrow 0$, the susceptibility (41) has a purely imaginary pole. Thus, in an antiferromagnet with delocalized spin density in the phase with short-range order there exists a singular wave vector δ_{cr} , upon passage through which the nature of the propagation of the magnetic excitations changes over from wavelike (oscillatory) to relaxational. Analogous behavior of the paramagnon branch of the spin oscillations was predicted by Capellmann and Vieira⁹ for a banded ferromagnet.

Let us analyze in detail the dependence $\Omega(\delta)$. As the parameter Δ in expression (41) we use its mean-field value Δ_0 , at which the equality $1 = U \varphi_1$ reduces to an identity. The equation $\text{Det}(\delta, \Omega) = 0$, generally speaking, can be solved only numerically. Nevertheless, a number of important results can be obtained in the one-dimensional case without resorting to numerical calculations. For $d=1$ the dispersion relation can be expressed exactly in terms of complete elliptical integrals [for details, see Appendix B, formulas (B3)–(B5)]:

$$\frac{\Lambda + 3}{\Lambda - 1} \tilde{\Omega}^2 + \left(\frac{1}{2(l\delta)^2} - 1 \right) (1 - k'^2 \Lambda)$$

$$+ \frac{1}{2(l\delta)^2} \frac{k'^2}{1+k'} \frac{1}{E(k)} \Pi\left(\frac{(1-k')^2}{\tilde{\Omega}^2}, \frac{1-k'}{1+k'}\right) b = 0,$$

$$k = \frac{2t}{((2t)^2 + \Delta^2)^{1/2}}, \quad k' = (1-k^2)^{1/2}, \quad \tilde{\Omega} = \frac{\Omega k}{2t\delta a},$$

$$\Lambda = \frac{K(k)}{E(k)}. \quad (46)$$

The main complication in solving Eq. (46) is the integral term, which arises as a result of the fluctuational disorder: the quantity $\tilde{\Omega}$ enters into the Schrodinger integral (B2) as a parameter. Employing the estimates made in Appendix B, we have shown the dependence $\Omega(\delta)$ in the situations that are the most important from a physical point of view.

Suppose $|\tilde{\Omega}| \ll 1$. Then relation (B4) is valid, and Eq. (46) reduces to a quadratic equation in Ω , analogous to the equation for small oscillations of a pendulum with damping. The solution of this equation has the form

$$\tilde{\Omega}_{\pm} = -\frac{1}{2} \frac{\Lambda-1}{\Lambda+3} \left\{ \frac{i\pi b}{2(l\delta)^2 E(k)} \left(\frac{k'}{k}\right)^2 \pm \left[4 \frac{\Lambda+3}{\Lambda-1} \times \left(1 - \frac{1}{2(l\delta)^2}\right) (1-k'^2\Lambda) - \left(\frac{\pi b}{E(k)}\right)^2 \frac{1}{4(l\delta)^4} \left(\frac{k'}{k}\right)^4 \right]^{1/2} \right\}. \quad (47)$$

This solution describes the dynamics of the paramagnons in the vicinity of the crossover point δ_{cr} . The value of δ_{cr} is found by setting to zero the expression standing under the radical in Eq. (47):

$$(l\delta_{cr})^{-2} = 4\lambda(\sqrt{1+\lambda^{-1}}-1),$$

$$\lambda = \left(\frac{E(k)}{\pi b}\right)^2 \left(\frac{k}{k'}\right)^4 \frac{\Lambda+3}{\Lambda-1} (1-k'^2\Lambda). \quad (48)$$

The limits of variation of δ_{cr} (48) and of the damping rate of the excitation at the critical point $|\Omega_{cr}| = |\Omega_{\pm} \delta_{cr}|$ with variation of k are for:

$$U \ll t$$

$$2(l\delta_{cr})^2 = 1 + \left(\frac{\pi b}{2}\right)^2 \left(\frac{\Delta}{2t}\right)^4, \quad |\Omega_{cr}| = \frac{\pi \sqrt{2} a \Delta^2}{8l t} b, \quad (49)$$

for $U \gg t$

$$l\delta_{cr} = \frac{U}{8t} \sqrt{b}, \quad |\Omega_{cr}| = \frac{ta}{4l}. \quad (50)$$

For comparatively small wave vectors $\delta < \delta_{cr}$, Eq. (46) has only purely imaginary solutions, $\text{Re } \Omega = 0$. And, in the interval $\delta_{cr} > \delta > (\sqrt{2}l)^{-1}$ a pair of relaxational modes Ω_{\pm} is present, and below the resonance point $\delta = (\sqrt{2}l)^{-1}$ (the point at which the spatial scales of the spin fluctuations and the external magnetic field coincide) only one of them, Ω_{+} , is preserved. As δ approaches the resonant point $(\sqrt{2}l)^{-1}$ from above, the Ω_{-} mode vanishes as

$$|\tilde{\Omega}_{-}| = \frac{E(k)}{\pi b} \left(\frac{k}{k'}\right)^2 (1-k'^2\Lambda)(2(l\delta)^2-1). \quad (51)$$

In the limit of strong disorder, when $(l\delta)^2 \ll 1$ holds, the frequency Ω_{+} approaches the limiting value

$$\Omega_{+} = -i \left(\frac{(2t)^2 + \Delta^2}{2} \frac{\Lambda-1}{\Lambda+3} \right)^{1/2} \frac{a}{l}. \quad (52)$$

For wave vectors $\delta > \delta_{cr}$ superposed on short-range antiferromagnetic ordering, a paramagnon is excited with characteristic lifetime $\tau \sim |\Omega_{\text{Im}}|^{-1}$, where

$$\left| \frac{\Omega_{\text{Im}}}{\Omega_{\text{cr}}} \right| = \frac{\delta_{cr}}{\delta}.$$

In this case the real part of the frequency vanishes like the square root:

$$\Omega_{\text{Re}} = \Omega_0 (\delta^2 - \delta_{cr}^2)^{1/2} a, \quad (53)$$

where we have $\Omega_0 = 2t$ for $U \ll t$, and $\Omega_0 = 2t^2/\Delta$ in the opposite case $U \gg t$.

The parameter $l\delta$ is, in essence, the ratio of the dimension of a typical magnetically ordered domain to the dimension of the region from which the response is (collected) ("gathered"). On a scale less than the radius of the orientational correlations, the magnetic disorder is assumed to be weak: $(l\delta)^{-2} \ll 1$. This case can be described analytically for the two limiting cases of the parameter k by making use of the estimates derived in Appendix B.

In the case of a weak Coulomb interaction $U \ll t$ (or $k' \ll 1$), we will use the approximation (B7)–(B8) for the integral (B5) and the standard expansions for $K(k)$ and $E(k)$.¹⁰ Substituting them in Eq. (46) and keeping only the lowest-order terms in k' , we obtain Eq. (B9). Expanding Eq. (B9) in the small parameter $(l\delta)^{-2}$ near the point $\tilde{\Omega} = 1$ and discarding terms of order $(k'/l\delta)^2$ and higher, we obtain this simple dependence:

$$\Omega = 2t\delta a \left[1 - \frac{1}{4(l\delta)^2} - \frac{\pi i}{2} \frac{b}{2(l\delta)^2 + (2t/\Delta)^2} \right]. \quad (54)$$

Formula (54) describes, on the one hand, the small shift of the peak of the magnetic susceptibility (41) in the disordered phase relative to its spin-wave position ($\Omega = 2t\delta a$) in the ground state and, on the other, the weak fluctuational broadening of this peak. These conclusions, of course, are also valid in the case $U \gg t$ (or $k \ll 1$).

The dependence of the frequency of the spin wave on the momentum

$$\Omega = \frac{t^2 \delta a}{\Delta} \left[1 - \frac{1}{4(l\delta)^2} - \frac{ib}{\sqrt{3} 2(l\delta)^2} \left(\frac{\Delta}{2t}\right)^2 \right] \quad (55)$$

was obtained from Eq. (B8) by expanding near the unperturbed value $\Omega = t^2 \delta a / \Delta$ (the value unperturbed by the disorder).

It would be interesting to draw a parallel between the picture of the dispersion of SDW paramagnons presented in Fig. 4 over the entire range of δl and the picture of the natural oscillations of a classical oscillator with damping. In the latter case there also exist two-dimensional (depending on the magnitude of the damping coefficient Γ) temporal

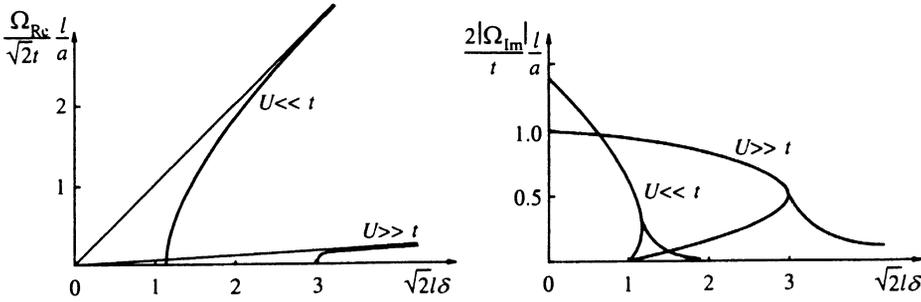


FIG. 4.

regimes of small oscillations $u(t)$ (Ref. 11): either $u(t) = A \exp(i\Omega_{\text{Re}} - \Omega_{\text{Im}})t$ for relatively small Γ , or $u(t) = A_+ \exp(-\Omega_+ t) + A_- \exp(-\Omega_- t)$ (for large Γ), where the coefficients A_{\pm} are determined by the initial conditions. It is possible, in principle, to reconstruct the effective Lagrangian $\mathcal{L}[\partial\Delta/\partial t, \partial\Delta/\partial x_\alpha]$ of the low-frequency transversely-polarized spin-density oscillations for an antiferromagnet with spin density waves from (42).

In the one-dimensional case, in the low-frequency region $|\tilde{\Omega}| \ll 1$ this Lagrangian \mathcal{L} is similar to the Lagrangian of a pendulum with damping. The term $(a/l)^2 \Theta(\delta, \Omega)$ in expression (42) is responsible for dissipation processes when spin excitations propagate in a medium with short-range antiferromagnetic order. The quantity $\Theta(\delta, \Omega)$ was obtained by means of an appropriate microscopic consideration. The correlation length l in our approach is a phenomenological parameter. We use the relation

$$l \approx a \frac{J}{T}, \quad (56)$$

which can be obtained for $T \ll J$ and $d=1$ from the classical Hamiltonian (16) by the renormalization group method. Employing results obtained earlier,⁴ we adduce estimates for the exchange integral

$$J \sim \frac{t^2}{U} \quad (57)$$

for $t \ll U$, and

$$J \sim \frac{\Delta^2}{t} \ln \frac{t}{\Delta} \quad (58)$$

for $t \gg U$. Taking (56)–(58) into consideration, it is possible to estimate the temperature dependence of the spectral characteristics of the paramagnons.

If we substitute relations (56)–(58) in (32) and (33), it is not hard to show that the contribution of the transverse fluctuations to the renormalization of the SDW amplitude significantly exceeds the corresponding contribution arising from the temperature smearing of the Fermi distribution function for $T \ll \Delta$.

5. CONCLUSION

Having developed a general formalism in terms of the “local band” concept for describing spin density excitations in the disordered phase of a banded antiferromagnet, we have investigated the paramagnon spectrum in the greatest detail in the one-dimensional SDW model. The choice of such a

system is not arbitrary, since the results obtained with it can be used to interpret the magnetic properties of an atomically pure (111)–(2×1) surface of semiconductors with diamond structure. We may point out, for example, that experimental studies of Auger electron spectroscopy of a (111)–(2×1) surface of diamond (Ref. 12) indicate the presence of antiferromagnetic correlations of the spins at neighboring sites.

A free (111) face of a homeopolar crystal is subject to intrinsic atomic reconstruction (1×1)→(2×1). For example, this phenomenon is observed at room temperature on a freshly vacuum-cleaved silicon surface⁵ or on a diamond surface heated above 900 °C (the hydrogen desorption temperature). As a result, according to Pandey,⁶ the surface acquires a new relief in the form of alternating (with period twice its starting value in the (1×1) phase) parallel zigzag-shaped chains, at whose nodes the π -orbitals of the broken bonds, oriented along the normal to the (111) plane, are localized. The overlap of the valence orbitals leads to the formation of a half-filled metallic π -band of surface states with strong dispersion $t \sim 1$ eV in the longitudinal direction (along the chain) and with weak dispersion $t < 0.1$ eV in the transverse direction. This band structure is inherent to the ideal geometry of one of Pandey’s chains. In reality, the chain is dimerized, because its neighboring sites are located in the different chemical environment of the lower-lying layers.

On the other hand, it is well known that a low-dimensional metal with a half-filled band is unstable with respect to the appearance at temperatures $T < T_N^0 = 2t \exp(-U/t)$ of an antiferromagnetic phase with spin density waves even in the presence of a weak inter-electron interaction $U/t \ll 1$. Without going into the history of the question of banded antiferromagnetism on a (111) face of a semiconductor, we only briefly note that the most realistic situation for a (111)–(2×1) Si (C) surface is one in which the spin superstructure $\Delta_i = \Delta \exp iQx_i$ arises against a background of charge (chemical) corrugation $n_i = n \cos Qx_i$. Thus, Lannoo and Allan,¹⁴ using mean field theory (taking it, by the way, beyond its limits of applicability) showed that the ground state of a π -chain is antiferromagnetic. For a given amplitude of charge corrugation $V \sim n$ the antiferromagnetic mean value $\Delta \sim U \langle c_{i\alpha}^+ c_{\alpha\beta}^z c_{i\beta} \rangle$ is realized if the interaction constant U exceeds a certain threshold value $U_0(V)$. The quantity U_0 tends toward zero as $V \rightarrow 0$. In the “local band” picture which we have adopted, $T_N^0 \sim \Delta(T=0)$ serves as an estimate for the point of formation of spontaneous spin polarization at the site S_{i_z} . The estimate derived in Ref. 14 for the model of a (111)–(2×1) Si surface with parameters $U/2t=2$ and $V/2t$

$=0.2$ gives $S_{iz}=0.37$, i.e., here we are dealing with a magnet close to saturation.

From photoelectron spectroscopic data¹⁵ the Coulomb repulsion energy of the electrons in the orbital of a broken valence bond on a (111) Si face is of the order of $U \sim 1$ eV. In the parameter region $U/2t \sim 1$ the main contribution to the free energy of the magnet comes from spin density fluctuations. Moreover, the role of fluctuations is amplified in systems with diminished dimensionality. In our previous paper⁴ we showed that the orientational disorder in a banded antiferromagnet with a quasi-two-dimensional electron spectrum steeply decreased the true Néel point to values $T_N \ll T_N^0$. Therefore, for a (111)-(2×1) Si (C) surface, whose valence states are weakly coupled with the exchange states (and moreover, $t \gg t_\perp$), the problem of identifying the properties of the phase with short-range magnetic ordering is completely well posed. For a qualitative consideration of this problem it is reasonable to use the Hubbard model for a one-dimensional chain without charge doubling ($V/U \rightarrow 0$) when modeling the electron structure of the surface band. The results obtained above can be useful on the experimental plane.

Lannoo and Allan¹⁴ indicated the existence of four surface branches of the electron spectrum (of which the two lower are filled) when charge and spin doubling coexist in the π -chain:

$$E_k^2 = \varepsilon_k^2 + (\Delta \pm V)^2. \quad (59)$$

This result does not agree with the experimental results of Uhlberg *et al.*¹⁶ (photoelectron spectroscopy with angular resolution), which gave only one filled surface band for the (111) face of silicon. This discrepancy can be due to low experimental resolution in comparison with the "fine" structure of the surface states near the boundaries of the bands. Recall⁴ that in the short-range order regime the pseudogap (31) is preserved, but the singularities in the spectra near the boundaries are smeared out due to orientational disorder. For a (111)-(2×1) Si (C) surface, fluctuational smearing has the estimate $tT/J \sim 0.1$ eV, which is comparable to the splitting (59).

To analyze spin correlations on a (111)-(2×1) surface of C or Si, it would be conducive to carry out an inelastic neutron scattering study. The analysis which we have given of low-energy spin dynamics (see Fig. 4) allows us to predict the basic outlines of the corresponding spectral characteristics. For a fixed energy of the particles incident on the atomically pure face (at grazing angles), three different temperature regions should be observed. At low temperatures $T < T_{cr}$ the peak of the neutron energy losses should be found at the frequency of the spin waves. As temperature increases, this peak should broaden and shift toward the "red" end of the spectrum. In the interval $T_{cr} < T < T_l$ (T_{cr} is given by formula (48), T_l is found from the equality $\sqrt{2} \delta l(T) = 1$) an inhomogeneously broadened central peak should be observed, and for $T > T_l$ there should be a simple, broad, diffuse peak.

This work was partially supported by the Russian Federation Research Fund, Grant 94-02-03506 (No. 566).

APPENDIX 1

The diagonal component $\chi_0^{+-}(q, \Omega)$ of the susceptibility $\bar{\chi}_{q, q'}^{+-}(\Omega)$ has the form

$$\begin{aligned} \chi_0^{+-}(q, \Omega) = & \frac{1}{N} \sum_{\mathbf{k}} \frac{E_+ + E_-}{(E_+ + E_-)^2 - \Omega^2} \left(1 - \frac{\varepsilon_+ \varepsilon_- - \Delta^2}{E_+ E_-} \right) \\ & \times \left[1 - \frac{a^2}{8l^2} \left(1 - \frac{\eta_+^2 + \eta_-^2}{(E_+ + E_-)^2 - \Omega^2} - \frac{\Delta^2}{E_+ E_-} \right. \right. \\ & \times \left. \left. \left(1 + \frac{E_+^2 + E_-^2}{E_+ E_-} \right) \right) \right] - \frac{a^2}{8l^2} \\ & \times \frac{1}{N} \sum_{\mathbf{k}} \frac{\Delta^2}{E_+^2 E_-^2} \frac{(E_+ + E_-)^3}{(E_+ + E_-)^2 - \Omega^2} + \frac{a^2}{8l^2} \\ & \times \frac{1}{N} \sum_{\mathbf{k}} \frac{\Omega^2 (E_+ + E_-)}{((E_+ + E_-)^2 - \Omega^2)^2} \\ & \times \left[\frac{4(\eta_+^2 + \eta_-^2)}{(E_+ + E_-)^2 - \Omega^2} \right. \\ & \times \left(1 - \frac{\varepsilon_+ \varepsilon_- - \Delta^2}{E_+ E_-} \right) - 3 - \frac{\Delta^2}{E_+ E_-} \\ & \times \frac{(E_+^2 + E_-^2 - E_+ E_-)((E_+ - E_-)^2 - \Omega^2)}{4E_+^2 E_-^2} \\ & + \frac{(E_+ + E_-)^2 - \Omega^2}{4E_+ E_-} + 2 \frac{\Delta^2 - \varepsilon_+ \varepsilon_-}{E_+ E_-} \left(\frac{\Delta^2}{E_+ E_-} \right. \\ & \left. \left. - 1 \right) \right] - \frac{a^2}{8l^2} \frac{1}{N} \sum_{\mathbf{k}} \frac{\Omega^2 (E_+ + E_-)}{((E_+ + E_-)^2 - \Omega^2)^2} \\ & \times \frac{bE_+ E_-}{(E_+ - E_-)^2 - \Omega^2}. \quad (A1) \end{aligned}$$

The nondiagonal component $X_Q^{+-}(q, \Omega)$ satisfies the condition

$$\chi_Q^{+-}(q, \Omega) = \chi_Q^{+-}(q \pm Q, \Omega)$$

and is equal to

$$\begin{aligned} \chi_Q^{+-}(q, \Omega) = & 2\Delta\Omega \frac{1}{N} \sum_{\mathbf{k}} \frac{E_+ + E_-}{E_+ E_- ((E_+ + E_-)^2 - \Omega^2)} \\ & \times \left[1 + \frac{a^2}{8l^2} \frac{\eta_+^2 + \eta_-^2}{(E_+ + E_-)^2 - \Omega^2} \right. \\ & \times \left(3 + \frac{4\Omega^2}{(E_+ + E_-)^2 - \Omega^2} \right) - \frac{a^2}{8l^2} \\ & \times \left(3 + \frac{2\Omega^2}{(E_+ + E_-)^2 - \Omega^2} - \frac{\Delta^2}{E_+^2 E_-^2} \right. \\ & \left. \left. \times \left(E_+^2 + E_-^2 + E_+ E_- + \frac{2\Omega^2 E_+ E_-}{(E_+ + E_-)^2 - \Omega^2} \right) \right) \right]. \quad (A2) \end{aligned}$$

where we have used the notation

$$E_{\pm} = (\varepsilon_{\pm}^2 + \Delta^2)^{1/2}, \quad \varepsilon_{\pm} = \varepsilon(\mathbf{k} \pm \mathbf{q}/2),$$

$$\eta_{\pm} = \eta(\mathbf{k} \pm \mathbf{q}/2), \quad b = \frac{(2t)^2}{\Delta T} \exp\left(-\frac{\Delta}{T}\right).$$

APPENDIX 2

In the one-dimensional case the quantities (40), (43)–(45) entering into the dispersion equation can be expressed exactly in terms of total elliptic integrals:

$$\varphi_1 = \frac{kK(k)}{2\pi t}, \quad \Delta^2 \varphi_3 = \frac{kE(k)}{2\pi t},$$

$$\rho = \frac{\Psi(\delta)}{\delta^2} = \frac{\Delta^2 \varphi_3}{k'^2} - \varphi_1, \quad (\text{A3})$$

where $K(k)$ and $E(k)$ are total elliptic integrals of the first and second kind with modulus $k = 2t/[(2t)^2 + \Delta^2]^{1/2}$, $k' = \sqrt{1-k^2}$ is the complementary modulus;¹⁰

$$\Theta(\delta, \Omega) = \frac{1}{2\pi t} \frac{k}{1+k'} \Pi\left(\frac{(1-k')^2}{\tilde{\Omega}^2}, \frac{1-k'}{1+k'}\right), \quad (\text{A4})$$

where

$$\Pi\left(\frac{(1-k')^2}{\tilde{\Omega}^2}, \frac{1-k'}{1+k'}\right) = 2(1+k') \int_0^{1-k'} \frac{dx}{\sqrt{(1-k')^2 - x^2} \sqrt{(1+k')^2 - x^2}} \frac{\tilde{\Omega}^2}{\tilde{\Omega}^2 - x^2} \quad (\text{A5})$$

is the total elliptic integral of the third kind.¹⁰

We obtain such a form of the fluctuational term $\Theta(\delta, \Omega)$ if after the usual transformation in Eq. (40) from a sum over quasimomenta k to an integral over energy E_k we introduce the new integration variable

$$x = \frac{(\tilde{E}^2 - k'^2)^{1/2}(1 - E^2)^{1/2}}{\tilde{E}}, \quad \tilde{E} = \frac{E}{\sqrt{(2t)^2 + \Delta^2}},$$

and we also define a dimensionless frequency $\tilde{\Omega} = \Omega k [2t \delta a]^{-1}$. Substituting (A3) and (A4) into Eq. (42), we obtain Eq. (46).

The integral (A3) is understood to be improper. It is uniquely determined by the following auxiliary condition: the real and imaginary parts of the frequency should have opposite signs, i.e., $\text{sgn}(\text{Re } \Omega \cdot \text{Im } \Omega) = -1$. We stress that in the given problem the condition $|\text{Re } \tilde{\Omega}| < 1 - k'$ is fulfilled; therefore, the function $\Theta(\delta, \Omega)$ (A4) and (A5) will always be complex.

We have made special use of the form (A4) for representing the function $\Theta(\delta, \Omega)$ in terms of an elliptic integral. Its explicit form (A5) allows one rather simply to obtain estimates for $\Theta(\delta, \Omega)$ in limiting cases. Thus, for example, for small values of the variable $|\tilde{\Omega}| \ll 1$ we have

$$\frac{2\tilde{\Omega}}{\tilde{\Omega}^2 - x^2} = i\pi \delta(x),$$

and the integral (A4) and (A5) substantially simplifies:

$$\Theta(\delta, \Omega) = \frac{i\tilde{\Omega}}{2tk}. \quad (\text{A6})$$

Two other estimates are related to the modulus of the Schrodre integral (A5). Thus, in the limit $k' \rightarrow 0$ we have

$$\Pi\left(\frac{(1-k')^2}{\tilde{\Omega}^2}, \frac{1-k'}{1+k'}\right) = \frac{2\tilde{\Omega}^2}{1-\tilde{\Omega}^2} \left[\int_0^1 \frac{dx}{\tilde{\Omega}^2 - x^2} - \frac{1}{2} \ln \frac{4}{k'} \right], \quad (\text{A7})$$

where

$$2\tilde{\Omega} \int_0^1 \frac{dx}{\tilde{\Omega}^2 - x^2} = 2 \tanh \frac{2 \text{Re } \tilde{\Omega}}{1 + |\tilde{\Omega}|^2} + i \left(\arctan \frac{2 \text{Im } \tilde{\Omega}}{1 - |\tilde{\Omega}|^2} + \pi h(1 - |\tilde{\Omega}|) \right). \quad (\text{A8})$$

The corresponding dispersion equation takes the form

$$\tilde{\Omega}^2 + \frac{1}{2(l\delta)^2} - 1 + \frac{k'^2}{(l\delta)^2} \frac{\tilde{\Omega}^2}{1 - \tilde{\Omega}^2} \times \left[\int_0^1 \frac{dx}{\tilde{\Omega}^2 - x^2} - \frac{1}{2} \ln \frac{4}{k'} \right] b = 0. \quad (\text{A9})$$

In the second limit, when $k \rightarrow 0$, we can neglect the variable $x^2 \ll (1+k')^2$ under one of the radicals in the integral (B5). The latter integral is then rather easily evaluated by quadratures, and Eq. (46) reduces to

$$\left(\frac{4\tilde{\Omega}}{k^2}\right)^2 + \frac{1}{2(l\delta)^2} - 1 - \frac{1}{2(l\delta k)^2} \left(\frac{4\tilde{\Omega}}{k^2}\right)^2 \times \left[\left(1 - \frac{1}{2} \left(\frac{4\tilde{\Omega}}{k^2}\right)^2\right)^2 - 1 \right]^{-1/2} b = 0. \quad (\text{A10})$$

¹T. Moriya, *Spin Fluctuations in Itinerant Electron Magnets*, Springer, Berlin (1988).

²V. Korenman, J. L. Murray, and R. E. Prange, *Phys. Rev. B* **16**, 4032 (1977); R. E. Prange and V. Korenman, *Phys. Rev. B* **19**, 4691 (1979).

³H. Capellmann and R. E. Prange, *Phys. Rev. B* **23**, 4709 (1981).

⁴V. N. Men'shov and V. V. Tugushev, *Zh. Éksp. Teor. Fiz.* **102**, 1637 (1992) [*Sov. Phys. JETP* **75**, 885 (1992)].

⁵B. A. Nesterenko and V. G. Lyapin, *Phase Transitions on Free Faces and Interphase Boundaries in Semiconductors* [in Russian], Naukova Dumka, Kiev (1990).

⁶K. C. Pendey, *Phys. Rev. Lett.* **47**, 1913 (1981).

⁷J. R. Schrieffer, X. C. Wen, and S. C. Zhang, *Phys. Rev. B* **39**, 11663 (1989).

⁸E. A. Zhukovskii and V. V. Tugushev, *Zh. Éksp. Teor. Fiz.* **103**, 568 (1993) [*Sov. Phys. JETP* **76**, 286 (1993)].

⁹H. Capellmann and V. Vieira, *Phys. Rev. B* **25**, 3333 (1982).

- ¹⁰M. A. Abramowitz and I. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, U.S. Government Printing Office, Washington, D.C. (1972).
- ¹¹K. Magnus, *Schwingungen* [in German], Mir, Moscow (1982). [Transl. as *Vibrations*, Blackie, London (1965)].
- ¹²D. E. Ramaker and F. L. Hutson, *Solid State Commun.* **63**, 335 (1987).
- ¹³P. G. Lurie and J. M. Wilson, *Surface Science* **65**, 453 (1977).

- ¹⁴M. Lannoo and G. Allan, *Solid State Commun.* **47**, 153 (1983).
- ¹⁵Y. J. Chabal, J. E. Rowe, and D. A. Zwemer, *Phys. Rev. Lett.* **46**, 600 (1981).
- ¹⁶R. I. G. Uhrberg, G. V. Hansson, J. M. Nicholls, and S. A. Flodström, *Phys. Rev. Lett.* **48**, 1032 (1982).

Translated by Paul F. Schippnick