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SHORT-RANGE ORDER IN SPIN DENSITY WAVE ANTIFERROMAGNETS WITH CHEMICAL DIMERIZATION

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Tthe spin density wave model in a quasi-one-dimensional itinerant antiferromagnet with staggered potential at finite temperature is studied. Only short-range ordering exists in this system above the Néel temperature. The local-band theory of spin fluctuations is developed to calculate the spin density wave amplitude and the effective exchange integral. The one-electron spectrum and magnon spectrum are obtained in the short-range ordering regime.

1. INTRODUCTION

In the modern theory of itinerant magnetism it is assumed that the destruction of long-range magnetic order with increasing temperature is mainly due to spin density fluctuations [1], which determine the phase transition temperature, changes in magnetic structure parameters below the transition point and short-range order. One of the most physically illustrative methods to account for spin fluctuations, known as the local band theory [2, 3], was developed for itinerant ferromagnets. In this theory, the magnetic moment of the unit cell is formed at a temperature considerably higher than the temperature for the onset of long-range order. Amplitude excitations of the spin density have characteristic frequencies of the order of the Stoner exchange splitting, and do not determine the temperature of the phase transition. Accordingly, transverse long-wavelength fluctuations of the spin density with low (of order of the spin-wave) frequencies play the dominant role in the production of ferromagnetic order. Thus, both the exchange (Stoner) splitting of electronic subbands and short-range ferromagnetic order (but not long-range) are conserved above the transition point.

In Ref. [4] local band theory was applied to investigate the thermodynamics of itinerant antiferromagnets with spin density waves (SDW). In the vicinity of the Néel point T_N, the thermally excited state of an antiferromagnet is formed by the electronic Bloch states with energies within $\sim T_N$ of the Fermi level ε_F, where $T_N \ll \Delta$ (Δ is the SDW amplitude). This assumption strongly reduces the configuration field of spin fluctuations, i.e., the wave packets are formed by Bloch functions with wave vectors $\mathbf{K}$ close to $\mathbf{G}/2$ ($\mathbf{G}$ being the reciprocal lattice vectors). As a result, long-wavelength transverse fluctuations of the magnetization with wave vectors $\mathbf{q}$ close to the vector of antiferromagnetic structure $\mathbf{Q} = \mathbf{G}/2$ (that is, the transverse spin density waves) will be the most relevant. Nevertheless, short-range order band structure similar (but not identical) to the long-range order structure is preserved. The quasimomentum and

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spin of a quasiparticle are «almost good» quantum numbers, at least as long as $|\mathbf{K}-\mathbf{G}/2|l > 1$, where l is the characteristic correlation length of SDW fluctuations ($l \to \infty$, when $T \to T_N$).

It is well known that band structure properties play an important role in the formation and properties of SDW antiferromagnets [5]. In nesting-type models [6] the first well-known mechanism what leads to the suppression of SDW in the ground state is doping. Indeed, in this case, when particles are added to (or removed from) the system, the perfect nesting of the Fermi surface at the wave vector $\mathbf{Q} = \mathbf{G}/2$, of the antiferromagnetic structure, is spoiled. Another band structure mechanism responsible for the destruction of the SDW state is associated with the deformation of the electronic spectrum as a consequence of the onset of a charge density wave. It may be shown that in the absence of doping, spin and charge density waves can not coexist.

However, a SDW state can exist in an external staggered potential introduced into the system as so-called «chemical dimerization» [7]. This system is of great interest, as it describes some real physical situations. For example, this is the case for reconstructed Si (111) and C (111) surfaces in which the crystal field of the bulk induces chemical dimerization at the surface, and SDW ordering appears in the surface band of itinerant electrons along the so-called π-chain [8].

The ground-state properties of the SDW system with chemical dimerization are investigated in Ref. [7]. Below we consider the thermodynamics of such a system in the short-range ordering (SRO) regime. We examine the influence of a staggered potential on the parameters of effective exchange, correlation length, electronic spectrum, and collective excitations of SDW phase with short-range order.

In Sec. 2 we introduce the model and briefly recall some results of Ref. [7] about the phase diagram of the system in the ground state. In Sec. 3 we introduce the techniques of the «local-band» spin-fluctuation theory specialized to the problem of itinerant antiferromagnets.

In Sec. 4 we calculate the effective exchange integral and the Néel temperature for our model. In Sec. 5 we develop the single-particle Green's function approach to calculate the electronic spectrum and renormalization of the SDW amplitude in the SRO state.

In Sec. 6 we develop the two-particle Green's function approach to calculate the dynamical transverse susceptibility of the system.

In Sec. 7 we calculate the spectrum of low-frequency excitations (paramagnons) in the SRO state. Concluding remarks are found in Sec. 8.

2. SELF-CONSISTENCY EQUATION FOR THE SDW AMPLITUDE IN THE GROUND STATE IN THE HARTREE–FOCK APPROXIMATION

We consider the single-band model with Hamiltonian

$$H = H_0 + H_{int}, \tag{1}$$

$$H_0 = \sum_{ij\sigma} t_{ij} C^+_{i\sigma} C_{j\sigma} + I \sum_{j\sigma} \exp(i\mathbf{Q}\mathbf{R}_j) n_{j\sigma}, \tag{2}$$

$$H_{int} = U \sum_j \left(n_{j\uparrow} - \frac{\overline{n}_j}{2}\right)\left(n_{j\downarrow} - \frac{\overline{n}_j}{2}\right), \tag{3}$$

where $C^+_{i\sigma}$, $C_{i\sigma}$ are fermionic operators, t_{ij} is the nearest-neighbor hopping parameter, I is the amplitude of a staggered local potential produced by the crystal field, $\mathbf{Q} = \mathbf{G}/2$, and $\mathbf{R}$, is a lattice site. This form of the interaction term H_{int} is discussed in Ref. [7]. Introducing the unit vector $\mathbf{e}_i$, which specifies the local orientation of the quantization axis at the i-th site, we rewrite the term H_{int} in the equivalent form:

$$H_{int} = U \sum_j \left[\left(\frac{n_j - \overline{n}_j}{2} \right)^2 - (\mathbf{e}_j \mathbf{S}_j)^2 \right], \tag{4}$$

where $n_j = n_{j\uparrow} + n_{j\downarrow}$ and $S_{jz} = (1/2)(n_{j\uparrow} - n_{j\downarrow})$ are the charge and spin densities, respectively. The representation (4) enables us, by means of the Hubbard–Stratonovich transformation, formally to reduce the initial many-particle problem (1) to a single-particle problem that involves the motion of an electron in the arbitrary scalar $x_j(\tau)$ and vector $\mathbf{y}_j(\tau) = \mathbf{e}_j(\tau) y_i(\tau)$ fields conjugate to the charge and spin densities, respectively [1]. In the «static» approximation, i.e., neglecting the dependence of x_i and y_i on the time τ, the partition function corresponding to the Hamiltonian (1) has the form

$$Z = Z_0 \int Dx\, dy \, \exp \left\{ -\pi \sum_j (x_j^2 + y_j^2) + \mathrm{Tr} \ln(1 - gV) \right\}, \tag{5}$$

where

$$g^{\sigma\sigma'}_{ij}(\omega) = \frac{1}{N} \sum_{\mathbf{k},\mathbf{p}} \exp\left(i(\mathbf{k}\mathbf{R}_i - \mathbf{p}\mathbf{R}_j) \right) \frac{(i\omega_n + \varepsilon_{\mathbf{k}})\delta_{\mathbf{kp}} + I\delta_{\mathbf{k},\mathbf{p}+\mathbf{Q}}}{(i\omega + \mu)^2 - E^2_{\mathbf{k}}} \delta_{\sigma\sigma'} \tag{6}$$

is the Green's function of the noninteracting electrons with dispersion $E_{\mathbf{k}} = \pm(\varepsilon^2_{\mathbf{k}} + I^2)^{1/2}$, $\mathbf{k}$ is the quasimomentum, $\omega_n = \pi T(2n + 1)$ is the frequency, μ is the chemical potential,

$$V_{j\sigma\sigma'} = (\pi TU)^{1/2}(i x_j \delta_{\sigma\sigma'} + \boldsymbol{\sigma}_{\sigma\sigma'} \mathbf{y}_j) \tag{7}$$

is a random potential, and Z_0 is the partition function of the noninteracting electrons. In expression (5) and in what follows, the symbol Tr denotes the sum over spin index j, and the frequency variable n.

We neglect fluctuations of the charge density x_j. In the saddle-point approximation for the variable x_j, one can obtain

$$\langle x_j \rangle \sim \langle n_j - \overline{n}_j \rangle = 0.$$

Thus, in the Hamiltonian (1), there is no renormalization of the chemical potential μ and the staggered potential I (see Ref. [7]).

We now turn to the problem of SDW antiferromagnetism in the model (1). We propose that the ground state of the system has a Néel structure. For $I = 0$ we assume that the electronic spectrum has the «nesting» property:

$$\varepsilon_{\mathbf{k}} = -\varepsilon_{\mathbf{k}+\mathbf{Q}}. \tag{8}$$

We distinguish two alternating magnetic sublattices, for one of these we take the local quantization axis $\mathbf{e}_j$ to coincide in direction with the local magnetization of the site $\mathbf{S}_j$, while for the other we assume that the vectors $\mathbf{e}_j$ and $\mathbf{S}_j$, are antiparallel.

Thus,

$$\mathbf{e}_j \mathbf{S}_j = S_{jz} \exp(i\mathbf{Q}\mathbf{R}_j).$$

The vector field $\mathbf{y}_j$ is normalized in energy units:

$$\mathbf{\Delta}_j = (\pi UT)^{1/2} \mathbf{y}_j \exp(i\mathbf{Q}\mathbf{R}_j) = U\mathbf{S}_j \exp(i\mathbf{Q}\mathbf{R}_j). \tag{9}$$

In the Hartree–Fock approximation we can write the standard expression for the one-particle Green's function in the lineary polarized SWD structure $\mathbf{\Delta}_i = \Delta \mathbf{e}_z$:

$$\overset{0}{G}{}^{\sigma\sigma'}_{\mathbf{kp}}(\omega_n) = \frac{(i\omega_n + \varepsilon_{\mathbf{k}} + \mu)\delta_{\mathbf{k},\mathbf{p}} + (\Delta\sigma^z_{\sigma\sigma'} + I\delta_{\sigma\sigma'})\delta_{\mathbf{k},\mathbf{p}+\mathbf{Q}}}{(i\omega_n + \mu)^2 - E^2_{\mathbf{k}\sigma}}. \tag{10}$$

The spectrum of one-particle excitations has the form

$$\omega^\sigma = \pm E_{\mathbf{k}\sigma}, \quad E_{\mathbf{k}\sigma} = \left[\varepsilon^2_{\mathbf{k}} + (I + \sigma\Delta)^2\right]^{1/2}. \tag{11}$$

It consists of four branches which-differ in their band indices ($\pm$ sign on the radical in (11)) and their spin projection σ along the vector $\mathbf{e}_z$.

The self-consistency equation for the spin density amplitude is found as a saddle-point condition for the field $\mathbf{y}_i$, and has the standard form:

$$\Delta = \frac{U}{2} T \sum_n \frac{1}{N} \sum_{\mathbf{k}} \sum_{\sigma\sigma'} \sigma^z_{\sigma\sigma'} G^{\sigma\sigma'}_{\mathbf{k},\mathbf{k}-\mathbf{Q}}(\omega_n). \tag{12}$$

We analyze Eq. (12) at zero temperature and in the absence of doping ($\mu = 0$). We restrict attention to the case of a one-dimensional chain, for which $\varepsilon_{\mathbf{k}} = -2t\cos(ka)$ (a is the chain period). We can then rewrite (12):

$$\frac{\Delta}{U} = \frac{1}{4\pi t} \sum_{\sigma=\pm1} \sigma k_\sigma K(k_\sigma)(I + \sigma\Delta), \tag{13}$$

where $K(k_\sigma)$ is the complete elleptic integral of the first kind with modulus

$$k_\sigma(\Delta) = \frac{2t}{\sqrt{(2t)^2 + (I + \sigma\Delta)^2}}. \tag{14}$$

Integrating Eq. (13) with respect to Δ, one can obtain the thermodynamic potential $\Omega(\Delta)$ per site. The energy difference between the antiferromagnetic and paramagnetic phase (per lattice site) is

$$E(\Delta) = \Omega(\Delta) - \Omega(\Delta = 0) = \frac{\Delta^2}{U} - \frac{2t}{\pi} \sum_{\sigma=\pm1} \frac{E(k_\sigma)}{k_\sigma} + \frac{4t}{\pi} \frac{E(k_0)}{k_0}, \tag{15}$$

where $E(k_\sigma)$ is the complete elliptic integral of the second kind, and $k_0 = k_\sigma(\Delta = 0)$.

In the weak-coupling limit ($I^2, \Delta^2 \ll (2t)^2$), we can use the well-known expansions of the functions $K(k_\sigma)$ and $E(k_\sigma)$ near $k_\sigma = 1$ (the so-called logarithmic approximations). For $I \ll \Delta_0$, where

$$\Delta_0 = \Delta(I = 0) = 8t\exp[-2\pi t/U],$$

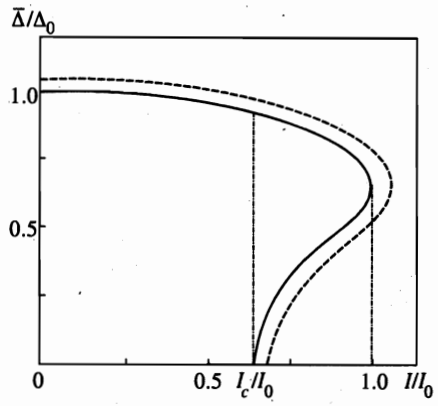

Fig. 1. $\bar{\Delta}(I)$ dependence for large (solid line) and short (dashed line) range order phases; limits of stability region $I_c < I < I_0$ (dash-dotted lines)

we obtain that

$$(\Delta(I) - \Delta_0)/\Delta_0 = -(I/\Delta_0)^2.$$

It can easily be shown that for $I < I_c = \Delta_0/e$, there exists only one nontrivial solution of Eq. (9), wilich is a decreasing function of I. However, for $I > I_c$ a second solution appears, which increases with I. In the vicinity of I_c the dependence $\Delta(I)$ is given by

$$\Delta^2(I) = 6I_c(I - I_c).$$

The numerical solution of Eq. (13) is obtained in Ref. [7] and plotted in Fig. 1 (solid line). It is clear that two nonzero solutions of Eq. (13) exist in the interval $I_c < I < I_0$, the first corresponding to a local minimum of the thermodynamic potential, and the second to a local maximum. The point $I = I_{eq}$ is the AFM-PM phase equilibrium point in the first-order phase transition, and I_0 and I_c are «superheating» and «supercooling» points for the AFM state.

Some analytic relations can be also obtained in the strong-coupling regime ($I, U \gg t$), when $k_\sigma \to 0$, as well numerical calculations for $\Delta(I)$ (see Ref. [7]). Thus, mean field analysis showes that in a dimerized chain with a staggered potential, the transition to the AFM phase is of first order in both the weak-coupling and strong-coupling limits.

3. TRANSVERSE SDW FLUCTUATIONS AND THE EFFECTIVE HAMILTONIAN OF THE SHORT RANGE ORDER ANTIFERROMAGNET

According to current ideas in the theory of itinerant magnetism based on the spin-fluctuation approach, the temperature T_N^0 determined by Eq. (12) is not the actual temperature at which antiferromagnetic long-range order is established (the Néel point). The quantity T_N^0 gives some nominal upper bound on the temperature below which long wave length SDW fluctuations with amplitude weakly dependent on T are formed. Long-range order (i.e., the onset of mean magnetization of the sublattices) is described not by Eq. (12), but by other relations that can be derived in the context of the spin-fluctuation approach for $T < T_N^0$. Below we will be oriented to the simply and physically visual scheme [2, 3], in which the formation and breakdown of long-range order are associated mainly with transverse long wave length thermodynamic fluctuations.

Let us briefly recall a familiar series of techniques from the theory of spin fluctuations in itinerant antiferromagnets. These constitute a «local band» method used earlier [4,9] for antiferromagnets. 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 SDW configurations $\{\Delta_i\}$ of Eq. (9) for which $\Delta_i = \mathbf{e}_i\Delta$, and the vector $\mathbf{e}_i$ changes direction slightly between nearest-neighbor sites of the lattice I and j: $|\mathbf{e}_i - \mathbf{e}_j| \ll 1$. We introduce a local coordinate system defined by the angles $\{\theta_i, \Phi_i\}$, which specify the direction of the local quantization axis $\mathbf{e}_i$ relative to the laboratory quantization axis. We introduce also the angle b_i, which describes the rotation of the spin-density vector about the $\mathbf{e}_i$ axis.

In the local coordinate system, the Hamiltonian (1) can be rewritten in the form [2]

$$H_{loc} = H_0 + H_1 + H_2 + H_{int}, \tag{16}$$

$$H_1 = -i\sum_{ij}\sum_{\sigma\sigma'} \tilde{t}_{ij}^{\sigma\sigma'} C_{i\sigma}^{+} C_{j\sigma'}, \tag{17}$$

$$\tilde{t}_{ij}^{\sigma\sigma'} = t_{ij}\left[\sigma_{\sigma\sigma'}^{+} a_{ij}^{*} + \sigma_{\sigma\sigma'}^{-} a_{ij} - \sigma_{\sigma\sigma'}^{z} g_{ij}\right], \tag{18}$$

$$H_2 = \sum \overset{\approx}{t}{}_{ij}^{\sigma\sigma'} C_{i\sigma}^{+} C_{j\sigma'}, \tag{19}$$

$$\overset{\approx}{t}{}_{ij}^{\sigma\sigma'} = t_{ij} d_{ij} \delta_{\sigma\sigma'}. \tag{20}$$

The matrix elements a_{ij}, g_{ij} and d_{ij} can be written in the form

$$a_{ij} \approx \frac{1}{2}\exp(-i\bar{b}_{ij})\left(\Phi_{ij}\sin\left(\bar{\Theta}_{ij} - i\Theta_{ij}\right)\right), \tag{21}$$

$$g_{ij} \approx \frac{1}{2}\left(b_{ij} + \Phi_{ij}\cos\bar{\Theta}_{ij}\right), \tag{22}$$

$$d_{ij} \approx -\frac{1}{2}\left(|a_{ij}|^2 + g_{ij}^2\right), \tag{23}$$

where $\Theta_{ij} = \Theta_i - \Theta_j$, $\bar{\Theta}_{ij} = (1/2)(\Theta_i + \Theta_j)$, and analogously for the angles Φ_i and b_i. In Eqs. (16)–(20), it is assumed that the operators $C_{i\sigma}$ and $C_{i\sigma}^{+}$ act in the local coordinate system, and the Hamiltonians H_0 and H_{int} have the same form as in (1). The matrix elements (21)–(23) have been written with allowance for the condition $|\mathbf{e}_i - \mathbf{e}_j| \ll 1$ for nearest nighbours. In the local coordinate system, the free energy of the system F can easily be represented as

$$F = -T\ln \mathrm{Tr}\exp\left(-\frac{1}{T}H_{loc}\right) = F_0[\bar{\Delta}] + F_{SF}\left[\bar{\Delta}, \{\mathbf{e}_j\}\right], \tag{24}$$

where the functional $F_0[\bar{\Delta}]$ can be reconstructed by integrating the self-consistency equation for the mean SDW amplitude $\Delta = \bar{\Delta}$. It is formally independent of the $\{\mathbf{e}_i\}$ directions, so $F_0[\bar{A}]$ is the free energy of the homogeneous SDW with some amplitude $\bar{\Delta}$. The term $F_{SF}[\bar{\Delta}, \mathbf{e}_i]$ is an additional exchange energy of the antiferromagnet, associated with thermodynamic orientational disorder. The large-scale SDW configurations $\{\mathbf{e}_i\}$ in the functional F_{SF} can

be represented as an expansion in the angles Θ_{ij}, Φ_{ij}, b_{ij}. Let us write the explicit expression for the functional F_{SF} to second order in H_1 and H_2:

$$F_{SF} = F_\perp + F_\parallel, \tag{25}$$

$$F_\perp = -\frac{1}{4} T \sum_n \left[\sum_{ij} \sum_\sigma \overset{0}{G}{}^{\sigma\sigma'}_{ij} \; t_{ij} |a_{ij}|^2 + \sum_{ijlm} \sum_{\sigma\alpha\beta\gamma} \overset{0}{G}{}^{\sigma\alpha}_{ij} \times \right.$$

$$\left. \times \; t_{jl} \left(\sigma^+_{\alpha\beta} a^*_{jl} + \sigma^-_{\alpha\beta} a_{jl} \right) \overset{0}{G}{}^{\beta\gamma}_{lm} \; t_{mi} \left(\sigma^+_{\gamma\sigma} a^*_{mi} + \sigma^-_{\gamma\sigma} a_{mi} \right) \right], \tag{26}$$

$$F_\parallel = -\frac{1}{4} T \sum_n \left[\sum_{ij} \sum_\sigma \overset{0}{G}{}^{\sigma\sigma}_{ij} \; t_{ij} g^2_{ij} + \sum_{ijlm} \sum_{\sigma\alpha\beta\gamma} \overset{0}{G}{}^{\sigma\alpha}_{ij} \; t_{jl} \sigma^z_{\alpha\beta} g_{ij} \; \overset{0}{G}{}^{\beta\gamma}_{lm} \; t_{mi} \sigma^z_{\gamma\sigma} g_{mi} \right], \tag{27}$$

where $\overset{0}{G}$ is the Green function (10), but $\overline{\Delta}$ is not defined by Eq. (12) (see Sec. 5 below). It is noted in Ref. [2] that the structure of the term g_{ij} (22) is such that it leads to contributions to the energy F_{SF} of fourth and higher order in Φ_{ij}. In the long-wave limit, the first nonvanishing terms in the energy expansion of F_{SF} are of second order in Φ_{ij} and Θ_{ij} and are proportional to $a^*_{ij} a_{lm}$. We now take into account that in accordance with (21),

$$a^*_{ij} a_{lm} = \frac{1}{4} (\mathbf{e}_i - \mathbf{e}_j)(\mathbf{e}_l - \mathbf{e}_m). \tag{28}$$

Thus, in this limit the spin-fluctuation contribution to the free energy of the itinerant antiferromagnet has the form of the effective Heisenberg Hamiltonian for classical spins $S = 1$,

$$F_{SF} = -\sum_{ij} J_{ij} \mathbf{e}_i \mathbf{e}_j. \tag{29}$$

In the next section, we analyze in detail the structure of the exchange integral J_{ij}. Here we emphasize that the calculation of the partition function reduces to an integration over the orientations of the random vector field $\{\mathbf{e}_i\}$, $|\mathbf{e}_i| = 1$:

$$Z = Z_0 \exp\left(-E_0/T\right) Z_{SF}, \tag{30}$$

$$Z_{SF} = \int \exp\left(-F_{SF}/T\right) D\{\mathbf{e}_i\}, \tag{31}$$

where F_{SF} is given in the form (29).

To find any pliysical characteristic of an itinerant antiferromagnet in the SRO region, it is necessary to average over the ensemble of SDW fluctuations, restricted in our approach to the set of configurations $\{\mathbf{e}_i\}$. If the quantity $A[\{\mathbf{e}_i\}]$ corresponds to any configuration $\{\mathbf{e}_i\}$, then the thermodynamic average $\langle A \rangle$ is calculated as a functional integral,

$$\langle A \rangle = Z^{-1}_{SF} \int A\left[\{\mathbf{e}_i\}\right] \exp\left(-F_{SF}\left[\overline{\Delta}, \{\mathbf{e}_i\}\right]/T\right) D\{\mathbf{e}_i\}. \tag{32}$$

We calculate $\langle A\rangle$ in the ordinary Gaussian approximation for the distribution $\{\mathbf{e}_i\}$ of the vector orientation, whose effective Hamiltonian is of the quadratic form (29). In this approximation, all even spin correlators decouple into products of the pairwise correlators $\langle \mathbf{e}_i \dots \mathbf{e}_j\rangle \to \langle \mathbf{e}_i\mathbf{e}_l\rangle \dots \langle \mathbf{e}_m\mathbf{e}_j\rangle$, and all odd correlators into products of pairwise correlators and mean values $\langle \mathbf{e}_i\rangle$. In what follows we restrict our discussion solely to 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 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 by obtained on the basis of general assumptions about the spatial and temperature dependence of f_{ij}. Thus, it is natural to assume that in the short-range order regime, with $T_N < T \ll T_N^0$, the Fourier component $f_{\mathbf{q}}$ has a sharp maximum at small values of the wave vectors $q \ll a^{-1}$, corresponding to the maximum of the spin correlator $\langle \mathbf{S}_{\mathbf{q}}\mathbf{S}_{-\mathbf{q}}\rangle$ at wave vectors $\mathbf{q}$ near the antiferromagnetic structure vector $\mathbf{Q} = \mathbf{G}/2$. The spin correlation radius $l(T)$ and the temperature dependence of $f_{\mathbf{q}}(T)$ can be estimated [4] on the basis of well-known results for the classical Heisenberg Hamiltonian.

4. EFFECTIVE EXCHANGE INTEGRAL AND THE NÉEL POINT

The exchange integral in (29) is given by

$$J_{ij} = \frac{1}{N^2}\sum_{\mathbf{pp}'} J_{\mathbf{pp}'} \exp\left(i\left(\mathbf{pR}_i - \mathbf{p}'\mathbf{R}_j\right)\right), \tag{33}$$

$$J_{\mathbf{pp}'} = I_{\mathbf{p}}\delta_{\mathbf{pp}'} + K_{\mathbf{p}}\delta_{\mathbf{p},\mathbf{p}'+\mathbf{Q}}, \tag{34}$$

$$I_{\mathbf{p}} = -\frac{T}{8N}\sum_{n\mathbf{k}}\left[\varepsilon_{\mathbf{k}-\mathbf{p}}\left(A_{\mathbf{k}}^{\uparrow} + A_{\mathbf{k}}^{\downarrow}\right) + (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{p}})^2\left(A_{\mathbf{k}}^{\uparrow}A_{\mathbf{k}-\mathbf{p}}^{\downarrow} - B_{\mathbf{k}}^{\uparrow}B_{\mathbf{k}-\mathbf{p}}^{\downarrow}\right)\right], \tag{35}$$

$$K_{\mathbf{p}} = -\frac{T}{8N}\sum_{n\mathbf{k}}\left[\varepsilon_{\mathbf{k}-\mathbf{p}}\left(B_{\mathbf{k}}^{\uparrow} + B_{\mathbf{k}}^{\downarrow}\right) + (\varepsilon_{\mathbf{k}}^2 - \varepsilon_{\mathbf{k}-\mathbf{p}}^2)^2\left(A_{\mathbf{k}}^{\uparrow}B_{\mathbf{k}-\mathbf{p}}^{\downarrow} - B_{\mathbf{k}}^{\uparrow}A_{\mathbf{k}-\mathbf{p}}^{\downarrow}\right)\right], \tag{36}$$

$$A_{\mathbf{k}}^{\sigma} = \frac{i\omega_n + \mu + \varepsilon_{\mathbf{k}}}{(i\omega_n + \mu)^2 - E_{\mathbf{k}\sigma}^2}, \quad B_{\mathbf{k}}^{\sigma} = \frac{I + \sigma\Delta}{(i\omega_n + \mu)^2 - E_{\mathbf{k}\sigma}^2}. \tag{37}$$

Below, we analyze only the case $T = 0$ and $\mu = 0$ to obtain explicit expressions for J_{ij}. We also assume that to zeroth order in $(a/l)^{-1} \ll 1$, $\overline{\Delta} \approx \Delta$ from Eq. (12) and $(\Delta \pm I)^2 \gg (a/l)^2 t^2$. In this case we can convince ourselves that the ferromagnetic component $K_{\mathbf{p}} = 0$ (since $\mu = 0$), and that to calculate the Néel temperature we need the quantity $M_{\mathbf{p}} = I_{\mathbf{p}=0} - I_{\mathbf{p}}$. After some transformations, the latter can be written in the form

$$M_{\mathbf{p}} = \frac{\Delta^2}{8N}\sum_{\mathbf{k}}\frac{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{p}})^2}{E_{\mathbf{k}\uparrow}E_{\mathbf{k}-\mathbf{p}\downarrow}(E_{\mathbf{k}\uparrow} + E_{\mathbf{k}-\mathbf{p}\downarrow})}, \tag{38}$$

where the summation over the wave vector $\mathbf{k}$ extends over the first Brillouin zone. For the classical Heisenberg model with $S = 1$, mean-field theory yields the phase-transition temperature

$$T_N^{MF} = \frac{2}{3}\frac{1}{N}\sum_{\mathbf{p}} M_{\mathbf{p}}. \tag{39}$$

The self-consistent contribution of magnetization fluctuations, evaluated by means of the spin Green's functions method, reduces the Néel temperature in comparison with (39):

$$T_N^{SF} = \frac{2}{3}\left(\frac{1}{N}\sum_{\mathbf{p}} M_{\mathbf{p}}^{-1}\right)^{-1}. \tag{40}$$

Eq. (40) was derived previously (for example, see Refs. [10] and [11]). The difference between T_N^{MF} and T_N^{SF} becomes sizable in low-dimensional systems. To illustrate this fact, we specify the dispersion relation in the form

$$\varepsilon_{\mathbf{k}} = -\sum_{\alpha} 2t_\alpha \cos(k_\alpha a_\alpha), \quad \alpha = x, y, z.$$

Above all, we consider the formal limit of strong interaction: $U, I \gg t$. If $(\Delta - I)^2 \gg (2t)^2$, the reduced exchange integral acquires the simple form

$$M_{\mathbf{p}} = \frac{\Delta}{2(\Delta^2 - I^2)}\sum_{\alpha} t_\alpha^2 \sin^2\left(\frac{p_\alpha a_\alpha}{2}\right). \tag{41}$$

The Néel temperture in the mean-field approximation is

$$T_N^{MF} = \frac{\Delta}{6(\Delta^2 - I^2)}\sum_{\alpha} t_\alpha^2 \tag{42}$$

and remains finite for all effective dimensions of the electronic system. Thermodynamic fluctuations lead to different behaviour of the Néel point. For example, if $(t_y/t_x)^2 \ll 1$, $(t_z/t_y)^2 \ll 1$, we obtain

$$T_N^{SF} = T_N^{MF}\pi\frac{t_y}{t_x}\left(\ln\frac{8t_y}{t_z}\right)^{-1}. \tag{43}$$

Recall that for an isotropic situation ($t_x = t_y = t_z$), $T_N^{SF} = T_N^{MF}/1.51$. The dependence of the temperature T_N^{SF} on the anisotropy parameter for a quasi-two-dimensional itinerant antiferromagnet was calculated in [4] in the case $t_y \equiv t_x \gg t_z$ (see Eq. (43)). In the limit $t/U \ll 1$, the temperature at which of the SDW amplitude Δ appears (given by Eq. (12)) is formally $T_N^0 \sim U$, i.e., much higher than T_N^{SF}. Thus, over a wide range of temperatures above the Néel point, short-range magnetic order can be described by a model with fixed (independent of T) SDW amplitude ($T_N^{SF} < T \ll T_N^0$). This order is characterized by the correlation length $l(T)$ of transverse fluctuations of the spin density. For the classical Heisenberg Hamiltonian in the one-dimensional case, the expression for $l(T)$ can be obtained by means of the renormalization-group method. For $T \ll J$,

$$l(T) \simeq aJ/T.$$

In the strong-coupling regime $(\Delta \pm I)^2 \gg (2t)^2$, the exchange integral is

$$J \sim \frac{\Delta t^2}{|\Delta^2 - I^2|} \sim \frac{t^2}{U} \ll t. \tag{44}$$

For $t \ll I \ll U$ we can write the explicit expression

$$J(I) = J_0 + \frac{8t^2 I^2}{U^3}, \quad J_0 = \frac{2t^2}{U}.$$

Thus, the staggered potential leads to an increase in correlation length. When the ratio U/t is not large, calculation of the function $M_{\mathbf{p}}$ is very complicated. However, only the behaviour of the exchange integral at small values of $\mathbf{p}$ ($p_\alpha a_\alpha \ll 1$) is of importance. Therefore, to estimate the transition temperature, we make use of a piecewise linear approximation to the function $M_{\mathbf{p}}$. For the one-dimensional chain we take

$$M_{\mathbf{p}}^{(1)} = \begin{cases} M(p_x a_x)^2, & |p_x| < p_0, \\ \tilde{M}, & |p_x| > p_0, \end{cases} \tag{45}$$

where

$$M = -\frac{\Delta t_x}{8\pi I} \sum_\sigma \sigma \frac{K(k_\sigma) - E(k_\sigma)}{k_\sigma}, \tag{46}$$

$$\tilde{M} = -\frac{\Delta t_x}{2\pi I} \sum_\sigma \sigma \frac{E(k_\sigma) - (1 - k_\sigma)^2 K(k_\sigma)}{k_\sigma}, \tag{47}$$

$$(p_0 a)^2 = \tilde{M}/M \ll 1.$$

For the quasi-one-dimensional case, up to the first-order terms in the overlap integral between chains, for which $\Delta^2, t_x^2 \gg t_y^2 \gg t_z^2$, we have

$$M_{\mathbf{p}}^{(2)} = M_{\mathbf{p}}^{(1)} + \frac{t_y^2 \sin^2(p_y a_y/2) + t_z^2 \sin^2(p_z a_z/2)}{8t_x^2} \left(\tilde{M} + 4M\right). \tag{48}$$

In the weak-coupling limit, where $|I \pm \Delta|^2 \ll (2t)^2$, one can obtain

$$T_N^{MF} = \frac{\Delta^2}{3\pi t} \ln \frac{8t}{\sqrt{|\Delta^2 - I^2|}}, \quad t = t_x, \tag{49}$$

$$T_N^{SF} = \left[(T_N^{MF})^{-1} + \frac{12\sqrt{2} I \ln(8t_y/t_z)}{\Delta t_y \ln|(\Delta + I)/(\Delta - I)|} \right]^{-1}. \tag{50}$$

Thus, long-range antiferromagnetic order appears at the temperature T_N^{SF}. With increasing temperature ($T_N^{SF} < T < T_N^0$), the system passes over the region of short-range order with the correlation length $l(T) \sim aJ/T$, where for the weak-coupling case ($U \ll t$) we can estimate

$$J \sim \frac{\Delta^2}{t} \ln \frac{8t}{\sqrt{|\Delta - I||\Delta + I|}} \sim \frac{\Delta^2}{U} \ll \Delta. \tag{51}$$

This estimate holds for all $I < I_c$ in the stability region of the phase diagram (see Fig. 1 and Ref. [7]), where $1 \gg |\Delta \pm I|/t \gg a/l$. Note that $T_N^0 \ll U$ for weak-coupling case, and T_N^{MF} and T_N^{SF} are also small compared with T_N^0. The situation $I_c < I < I_0$ (the metastable region) is more difficult to analyze, since the ratio $|\Delta - I|/t$ may be of order a/l. Thus, the renormalization of $\bar{\Delta}(T)$ takes an important role in this case, and a $J(T)$ dependence arises. We are not interested here in the detailed expressions for $J(T)$ and T_N^{SF} in this special case. For $I \ll \Delta_0$ can easily obtain from (51) the dependence of J on the staggered potential I:

$$J(I) = J_0 - \frac{4\pi}{U} I^2, \quad J_0 = \frac{4\pi\Delta_0^2}{U}.$$

Thus, the correlation length $l(I)$ decreases witli increasing I.

5. SINGLE-PARTICLE EXCITATIONS AND RENORMALIZATION OF SDW AMPLITUDE IN THE LOCAL HARTREE–FOCK APPROXIMATION

The scattering of itinerant eliectrons by a certain SDW fluctuation $\{\mathbf{e}_i\}$ above the Néel point $T_N \simeq T_N^{SF}$ is characterized by the single-particle Green's function $G_{ij}^{\sigma\sigma'}(\{\mathbf{e}_i\}, t)$:

$$G = \overset{0}{G} + \overset{0}{G}\,(H_1 + H_2)G. \tag{52}$$

Thermodynamic disorder enters into Eq. (52) through the Hamiltonians H_1 and H_2, and $\overset{0}{G}$ has the form (10).

The foregoing configurational integration procedure makes it possible to express the propagator $\langle G_{\mathbf{kp}}^{\sigma\sigma}(\{\mathbf{e}\}, \omega)\rangle$ averaged over the $\{\mathbf{e}_i\}$ configurations; in the lowest order of perturbation theory,

$$\langle G^{-1}\rangle = \langle \overset{0}{G}{}^{-1}\rangle - \Sigma, \quad \Sigma = \langle H_2\rangle + \langle H_1 \overset{0}{G} H_1\rangle. \tag{53}$$

The self-energy part Σ is

$$\Sigma_{\mathbf{kp}}^{\sigma\sigma} = -\frac{1}{4}\delta_{\sigma\sigma'} \times$$
$$\times \left\{ \delta_{\mathbf{kp}} \sum_{\mathbf{q}} \left[f_{\mathbf{q}}(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}}) + f_{\mathbf{q}}(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 A_{\mathbf{k}-\mathbf{q}}^{\sigma} \right] - \delta_{\mathbf{k},\mathbf{p}+\mathbf{Q}} \sum_{\mathbf{q}} f_{\mathbf{q}}(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 B_{\mathbf{k}-\mathbf{p}}^{-\sigma} \right\}. \tag{54}$$

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 factors (in comparison to $f_{\mathbf{q}}$) on the right-hand side of Eq. (54) can be expanded in series near the point $\mathbf{q} = 0$. Retaining the lowest-order terms in this expansion in $\mathbf{q}$, we obtain an expression for the averaged Green's function:

$$\langle G_{\mathbf{kp}}^{\sigma\sigma'}(\omega)\rangle = \left\{ \delta_{\mathbf{kp}}\delta_{\sigma\sigma'} \left[\omega + \varepsilon_{\mathbf{k}} - \nu_{\mathbf{k}} - F_{\mathbf{k}}^2 A_{\mathbf{k}+\mathbf{Q}}^{\sigma} \right] + \delta_{\mathbf{k},\mathbf{p}+\mathbf{Q}}\delta_{\sigma\sigma'} \left[\left(\overline{\Delta}\sigma + I\right) - F_{\mathbf{k}}^2 B_{\mathbf{k}}^{-\sigma} \right] \right\} / D_{\mathbf{k}}^{\sigma}(\omega), \tag{55}$$

$$D_{\mathbf{k}}^{\sigma}(\omega) = \left[\omega - \varepsilon_{\mathbf{k}} + \nu_{\mathbf{k}} - F_{\mathbf{k}}^2 A_{\mathbf{k}}^{\sigma} \right] \left[\omega + \varepsilon_{\mathbf{k}} - \nu_{\mathbf{k}} - F_{\mathbf{k}}^2 A_{\mathbf{k}+\mathbf{Q}}^2 \right] - \left[\left(\overline{\Delta}\sigma + I\right) - F_{\mathbf{k}}^2 B_{\mathbf{k}}^{-\sigma} \right]^2, \tag{56}$$

where

$$\nu_{\mathbf{k}} = -\frac{1}{8} \sum_{\alpha} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial^2 k_{\alpha}^2} l_{\alpha}^{-2}, \tag{57}$$

$$F_{\mathbf{k}}^2 = \frac{1}{4} \sum_{\alpha} \left(\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{\alpha}} \right)^2 l_{\alpha}^{-2}, \tag{58}$$

and l_{α} is the transverse correlation length of the spin-density fluctuations in the α-th direction. The poles of the averaged Green's function $\langle G\rangle$ determine the spectrum of single-particle excitations in a short-range-order antiferromagnet.

The zeroes of the denonimator (56) of the function (55) are given by the dispersion relation

$$(\omega^2 - E_{k\sigma}^2)^3 + (2\varepsilon_k\nu_k - 2F_k^2 - \nu_k^2)(\omega^2 - E_{k\sigma}^2)^2 + \\ + F_k^2(F_k^2 - 4E_{k\sigma}^2 + 2\varepsilon_k\nu_k + 4I^2 + 4I\sigma\bar{\Delta})(\omega^2 - E_{k\sigma}^2) + 4I\sigma\bar{\Delta}E_{k\sigma}^4 = 0. \quad (59)$$

Thus, there are twelve branches of energy dispersion. To order $(a/l)^2$, we see that

$$(\omega_0^\sigma)^2 = E_{k\sigma}^2 + \frac{\sigma\bar{\Delta}IF_k^2}{E_{k\sigma}^2 - I(I + \sigma\bar{\Delta})}, \quad (60)$$

$$(\omega_{1,2}^\sigma)^2 = E_{k\sigma}^2 \pm \left[4F_k^2\left(E_{k\sigma}^2 - I\left(I + \sigma\bar{\Delta}\right)\right)\right]^{1/2} + F_k^2 - \varepsilon_k\nu_k - \frac{\sigma\bar{\Delta}IF_k^2}{2(E_{k\sigma}^2 - I(I + \sigma\bar{\Delta}))}. \quad (61)$$

Note that to first order in a/l, with $(\omega_0^\sigma)^2 = E_{k\sigma}^2$, only eight new branches $\pm\omega_{1,2}^\sigma$ found. It is not hard to show that the parameter F_k associated with the Hamiltonian H_1 (19) corresponds to the scattering of a quasiparticle by a spin fluctuation with spin flip. Thus, in the short-range-order phase, the motion of an electron with «right» or «wrong» spin direction is possible in each of the two antiferromagnetic sublattices if they are in part randomly oriented. As a consequence, the dispersion branches are «split» and the gap for single-particle excitations is reduced. For example, (see Fig. 2),

$$E_g \approx 2\left(|I - \bar{\Delta}| - \frac{a}{l}t\left(\frac{\bar{\Delta}}{|I - \bar{\Delta}|}\right)^{1/2}\right) \quad (62)$$

for the one-dimensional system. Note that the reduction in E_g and the spin amplitude $\bar{\Delta}$, as compared with the long-range-order state ($a/l = 0$), is due exclusively to the spin-flip scattering Hamiltonian H_1. The scattering process without spin flip is described by the Hamiltonian H_2 and the corresponding parameter ν_k. This process leads to effective narrowing of the energetic band $\tilde{\varepsilon}_k = \varepsilon_k - \nu_k$, where

$$\tilde{\varepsilon}_k = -\sum_\alpha 2t_\alpha\left[1 - \frac{1}{8}\left(\frac{a_\alpha}{l_\alpha}\right)^2\right]\cos(k_\alpha a_\alpha). \quad (63)$$

We now address the influence of spin fluctuations on the mean SDW amplitude $\bar{\Delta}$. Since the order parameter $\bar{\Delta}(T)$ has very weak temperature dependence in the temperature range

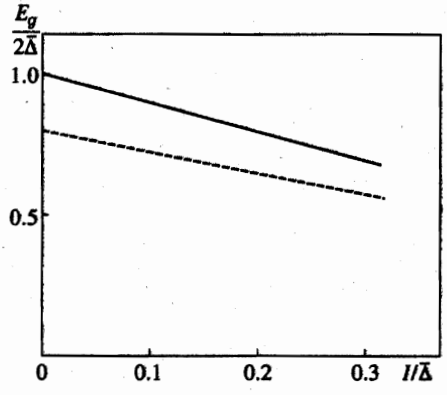

Fig. 2. $E_g(I)$ dependence for large (solid line) and short (dashed line) range order phases

$T_N < T \ll T_N^0$ due to the Fermi statistics of the quasiparticles, we use the self-consistency equation (local Hartree–Fock approximation), in which the Fermi function is replaced by the step function:

$$\bar{\Delta} = \frac{U}{2} \int \frac{d\omega}{2\pi i} \frac{1}{N^2} \sum_{\mathbf{kp}} \sum_{\sigma\sigma'} \sigma^z_{\sigma\sigma'} \langle G^{\sigma\sigma'}_{\mathbf{k},\mathbf{p}+\mathbf{Q}} \rangle. \tag{64}$$

The amplitude is temperature-dependent only bacause of the transverse spin fluctuations with correlation length $\{l_\alpha(T)\}$. We substitute the average Green's function (55) into Eq. (64), and after some manipulations we obtain the following equation to second order in a/l:

$$\bar{\Delta} = \frac{U}{4N} \sum_{\mathbf{k}} \sum_{\sigma} \frac{\sigma}{E_{\mathbf{k}\sigma}} \left[\left(I + \sigma\bar{\Delta}\right) \left(1 + \frac{\varepsilon_{\mathbf{k}} \nu_{\mathbf{k}}}{E^2_{\mathbf{k}\sigma}}\right) + \frac{I F^2_{\mathbf{k}}}{E^2_{\mathbf{k}\sigma}} \left(1 - \frac{3\left(I + \sigma\bar{\Delta}\right)^2}{2E^2_{\mathbf{k}\sigma}}\right)\right]. \tag{65}$$

Note that in the absence of a staggered potential ($I = 0$), renormalization of the SDW amplitude is due to the process without spin flip ($\nu_{\mathbf{k}}$), since the term proportional to $F^2_{\mathbf{k}}$ vanishes on the right-hand side of (65). As a consequence of the above mentioned narrowing of the band $\varepsilon_{\mathbf{k}}$ (63) the resulting change in the mean spin density per site $\bar{\Delta}$ is positive, i.e, it increases compared with Δ. For a one-dimensional chain one can take Eq. (65) in the form

$$\bar{\Delta} = \frac{U}{4\pi t} \sum_{\sigma} k_\sigma \left[\sigma K(k_\sigma) \left(I + \sigma\bar{\Delta}\right) + \frac{\bar{\Delta}}{8} \left(\frac{a}{l}\right)^2 \left[K(k_\sigma) - E(k_\sigma)\right]\right], \quad k_\sigma = k_\sigma\left(\bar{\Delta}\right). \tag{66}$$

The temperature dependence of $\bar{\Delta}$ is due only to the dependence of $l(T)$. If, in agreement with our estimates in Sec. 3, we express the correlation length $l(T)$ in terms of the model parameters, it becomes clear that the contribution of transverse spin fluctuations to the renormalization of the SDW amplitude significantly exceeds the corresponding contribution arising from the temperature dependence of the Fermi function. It can be shown from (66) that $\bar{\Delta}(T) - \Delta \sim [a/l(T)]^2$, but to calculate the exchange integrals J_{ij} in Sec. 3 it was assumed for simplicity that $\bar{\Delta}(T) \approx \Delta$, where Δ is defined by Eq. (13). An explicit expression for $\bar{\Delta}$ can be obtained in the limit $I \ll \Delta$:

$$\begin{aligned} &\bar{\Delta}(I) \approx \tilde{\Delta}_0 \left(1 - \tilde{I}^2/\tilde{\Delta}_0^2\right), \\ &\tilde{\Delta}_0 = 8t \exp\left[-\frac{2\pi t}{U(1+\lambda)}\right], \\ &\tilde{I}^2 = \frac{I^2}{1+\lambda}, \quad \lambda = \frac{1}{8}(a/l)^2. \end{aligned} \tag{67}$$

Omitting the detailed analysis of Eq. (66) we note that in the phase diagram $\Delta(I)$, the metastable region ($I_c < I < I_0$) is shifted to the right as compared with the case $a/l = 0$. This tendency is shown qualitatively in Fig. 1 by the dashed line.

6. TRANSVERSE DYNAMICAL SUSCEPTIBILITY IN RANDOM-PHASE APPROXIMATION

A general theory of the dynamical susceptibility of itinerant magnets with short-range order was developed in Ref. [12]. A calculation scheme (the socalled «RPA with exchange») was

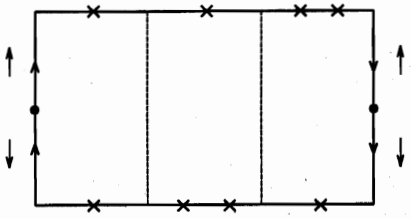

Рис. 3

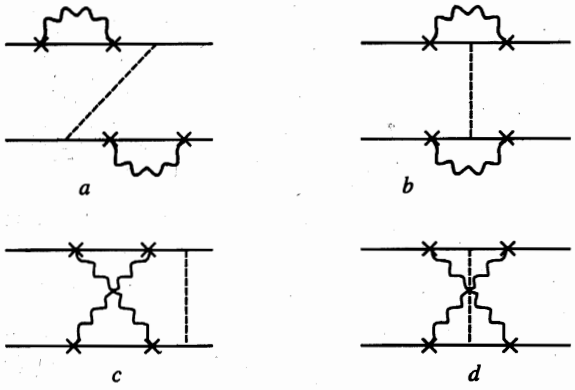

Рис. 4

Fig. 3. Diagram for process with spin flip H_1

Fig. 4. Diagrams for average two-particle Green's function to fourth order in a_{ij}

proposed to draw some qualitative conclusions about the nature of the response to an external magnetic field. In Ref. [13], a method for the calculation of the dynamical susceptibility that is somewhat different from Ref. [12] was proposed, based on the spin-fluctuation approach [2, 3]. The two-particle Green's function for itinerant antiferromagnets without a staggered potential was calculated [9, 13]. This method enables one to describe SDW antiferromagnets above the Néel point.

According to Ref. [12] one introduces a spin-density correlator for each fluctuation $\{\mathbf{e}_i\}$:

$$\chi^{\alpha\beta}_{\mathbf{q}\mathbf{q}'}\left(t, \{\mathbf{e}_i\}\right) = \frac{i}{2N}\left(TS^{\alpha}_{\mathbf{q}}(t)S^{\beta}_{-\mathbf{q}'}(0)\right)_{\{\mathbf{e}_i\}}. \tag{68}$$

Parentheses on the right-hand side of Eq. (68) denote averaging over quantum states for the fixed set of vectors $\{\mathbf{e}_i\}$ that specify the SDW configuration: the symbol T denotes time ordering in t. The complete response to an external variable magnetic field (the magnetic susceptibility at frequency Ω) is defined as the average over the SDW configurations:

$$\chi^{\alpha\beta}_{\mathbf{q}\mathbf{q}'}(\Omega) = \int_0^{\infty} \exp(i\Omega t)\langle\chi^{\alpha\beta}_{\mathbf{q}\mathbf{q}'}\left(t, \{\mathbf{e}_i\}\right)\rangle dt. \tag{69}$$

We now discuss the calculation of the averages in (69). The two-particle Green's function of the system with fluctuating spin density can be usefully represented as an infinite series of «ladder» diagrams that take into account electron scattering by randomly oriented magnetic moments at sites. One of the simplest diagrams is shown in Fig. 3. The solid line denotes the unperturbed function $\overset{0}{G}$ given by Eq. (10), 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, and the arrows $\downarrow$ and $\uparrow$ correspond to the projections of electron spin.

Let us turn our attention to the alternation in the arrangement of matrix elements a_{ij}, a^*_{ij} and spin indices. In the diagrammatic language, the averaging procedure (69) amounts

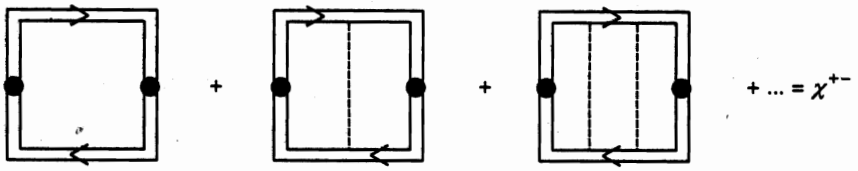

Fig. 5. Ladder diagrams to calculate the transverse susceptibility

to taking into account all the possible ways of joining the crosses pairwise by wavy lines. A graphical element consisting of a pair of crosses joined by a wavy line corresponds to the spin correlator f_{ij}. Figure 4 displays some typical diagrams that contribute to the average two-particle Green's function to first order in U, and to fourth order in the disorder a_{ij}. Below we 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. Note that U is not renormalized to second order in a_{ij}. In Fig. 3 and 4, processes without spin flip corresponding to H_2 are omitted, since their direct average $\langle |a_{ij}^2| \rangle$ in the single-particle channel is not needed in any additional explanations.

Thus, calculation of the suspectibility of an antiferromagnet in the short-range-order phase reduces to the modified RPA with quasiparticles «dressed» by disorder. In other words, it reduces to summation of the infinite sequence of «ladder»-type diagrams shown in Fig. 5, where the double line represents the average single-particle Green's function. The first diagram in the series in Fig. 5, which does not explicitly contain the interaction U, corresponds to the following function of the two quasimomenta:

$$\overline{\chi}^{+-}_{\mathbf{q}\mathbf{q}'}(\Omega) = \frac{1}{N^2} \int \sum_{\mathbf{k}\mathbf{k}'} \langle G^{\downarrow\downarrow}_{\mathbf{k},\mathbf{k}-\mathbf{q}'}(\omega) \rangle \langle G^{\uparrow\uparrow}_{\mathbf{k},\mathbf{k}+\mathbf{q}}(\omega - \Omega) \rangle \frac{d\omega}{2\pi i}. \tag{70}$$

Apart from the function $\langle G \rangle$, the expression for the response $\overline{\chi}^{+-}$ contains boths diagonal and off-diagonal contributions in the quasimomentum space, each of which depends on just one quasimomentum:

$$\overline{\chi}^{+-}_{\mathbf{q}\mathbf{q}'}(\Omega) = \delta_{\mathbf{q}\mathbf{q}'} \overline{\chi}^{+-}_0(\mathbf{q}, \Omega) + \delta_{\mathbf{q},\mathbf{q}'+\mathbf{Q}} \overline{\chi}^{+-}_{\mathbf{Q}}(\mathbf{q}, \Omega). \tag{71}$$

Summing the geometric series in Fig. 5 (in fact, solving the Dyson equation), we obtain the response function

$$\overline{\chi}^{+-}_{\mathbf{q}\mathbf{q}'}(\Omega) = \sum_{\mathbf{q}_1} \overline{\chi}^{+-}_{\mathbf{q},\mathbf{q}_1}(\Omega) \left[1 - U \overline{\chi}^{+-}_{\mathbf{q}_1,\mathbf{q}'}(\Omega) \right]^{-1}, \tag{72}$$

where

$$\left[1 - U \overline{\chi}^{+-}_{\mathbf{q}\mathbf{q}'}(\Omega) \right]^{-1} = \frac{\left[1 - U \overline{\chi}^{+-}_0(\mathbf{q}+\mathbf{Q}, \Omega) \right] \delta_{\mathbf{q}\mathbf{q}'} + U \overline{\chi}^{+-}_{\mathbf{Q}}(\mathbf{q}, \Omega) \delta_{\mathbf{q},\mathbf{q}'-\mathbf{Q}}}{\mathrm{Det}(\mathbf{q}, \Omega)}, \tag{73}$$

$$\mathrm{Det}(\mathbf{q}, \Omega) = \left[1 - U \overline{\chi}^{+-}_0(\mathbf{q}, \Omega) \right] \left[1 - U \overline{\chi}^{+-}_0(\mathbf{q}+\mathbf{Q}, \Omega) \right] - U^2 \overline{\chi}^{+-}_{\mathbf{Q}}(\mathbf{q}, \Omega) \overline{\chi}^{+-}_{\mathbf{Q}}(\mathbf{q}+\mathbf{Q}, \Omega). \tag{74}$$

The structure of the denominator of the transverse dynamical susceptibility (72) determines the spectrum of magnetic excitations of the system. We now proceed to some detailed calculations.

7. SPECTRUM OF LOW-FREQUENCY EXCITATIONS

We first calculate the irreducible susceptibility $\overline{\chi}_{qq'}(\Omega)$. We substitute the function $\langle G\rangle$ (55) into Eq. (70) sum over the quasimomentum $\mathbf{k}'$, and integrate over frequency ω. We restrict ourselves to lowest-order terms in the fluctuations, i.e., terms of order of $(a/l)^2$.

To determine the spectrum of the long-wave length and low-frequency excitations, we expand function that enter into the expression for the susceptibility (72) in low frequencies Ω ($|\Omega| \ll \overline{\Delta}$) and the quasimomenta $\boldsymbol{\delta} = \mathbf{q} - \mathbf{Q}$ ($\delta a \ll 1$, $\delta a \ll \overline{\Delta}/t$). We also drop corrections generated by terms of order $(a/l)^2(\Omega/\overline{\Delta})^2$ or $(a/l)^2(\delta a)^2$. Omitting some lengthy algebraic transformations, we write the series expansions for the irreducible components of the responses $\overline{\chi}_0^{+-}(\mathbf{q},\Omega)$ and $\overline{\chi}_{\mathbf{Q}}^{+-}(\mathbf{q},\Omega)$ for the one-dimensional case:

$$\overline{\chi}_0^{+-}(0,0) = \chi, \tag{75}$$

$$\overline{\chi}_0^{+-}(\mathbf{Q}+\delta,\Omega) = \frac{1}{U} + \alpha\left(\frac{\Omega}{2\Delta}\right)^2 - B\left(\frac{\delta a}{2\Delta}\right)^2 + \left(\frac{a}{l}\right)^2\gamma, \tag{76}$$

$$\overline{\chi}_{\mathbf{Q}}^{+-}(0,\Omega) = \overline{\chi}_{\mathbf{Q}}^{+-}(\mathbf{Q},\Omega) = \frac{\Omega}{2\Delta}\alpha, \tag{77}$$

where

$$\chi = \frac{1}{2N}\sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}^{\uparrow} + E_{\mathbf{k}}^{\downarrow}}\left(1 - \frac{\varepsilon_{\mathbf{k}}^2 + I^2 - \Delta^2}{E_{\mathbf{k}}^{\uparrow}E_{\mathbf{k}}^{\downarrow}}\right), \tag{78}$$

$$\alpha = \frac{1}{2N}\sum_{\mathbf{k}} \frac{2\Delta^2}{E_{\mathbf{k}}^{\uparrow}E_{\mathbf{k}}^{\downarrow}(E_{\mathbf{k}}^{\uparrow} + E_{\mathbf{k}}^{\downarrow})}\left(1 - \frac{4I^2}{(E_{\mathbf{k}}^{\uparrow} + E_{\mathbf{k}}^{\downarrow})^2}\right), \tag{79}$$

$$B = \frac{1}{2N}\sum_{\mathbf{k}} \frac{2(\varepsilon_{\mathbf{k}})^2 a^{-2}}{E_{\mathbf{k}}^{\uparrow}E_{\mathbf{k}}^{\downarrow}(E_{\mathbf{k}}^{\uparrow} + E_{\mathbf{k}}^{\downarrow})}\left[1 - \frac{4I^2\varepsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^{\uparrow}E_{\mathbf{k}}^{\downarrow}}\left(\frac{1}{E_{\mathbf{k}}^{\uparrow}E_{\mathbf{k}}^{\downarrow}} + \frac{1}{(E_{\mathbf{k}}^{\uparrow} + E_{\mathbf{k}}^{\downarrow})^2}\right)\right], \tag{80}$$

$$\gamma = \frac{1}{2N}\sum_{\mathbf{k}} \frac{(\varepsilon_{\mathbf{k}})^2 a^{-2}}{16\Delta^2}\left[\frac{\varepsilon_{\mathbf{k}}^2}{I\Delta}\left(\frac{1}{E_{\mathbf{k}}^{\uparrow}} - \frac{1}{E_{\mathbf{k}}^{\downarrow}}\right) + \frac{1}{E_{\mathbf{k}}^{\uparrow}} + \frac{1}{E_{\mathbf{k}}^{\downarrow}} - I\left(\frac{I+\Delta}{E_{\mathbf{k}}^{\uparrow 3}} + \frac{I-\Delta}{E_{\mathbf{k}}^{\downarrow 3}}\right)\right]. \tag{81}$$

In all of these expressions we assume $\overline{\Delta} \approx \Delta$ since we need only the second order in the a/l expansion. Note that the self-consistency equation (64) is taken into account to obtain (75)-(81), but only after this we can write $\overline{\Delta} \approx \Delta$, where Δ is given by Eq. (12).

Inserting the expressions (75)-(81) into Eq. (72)–(74), we obtain the dynamical susceptibility in the low-frequency limit:

$$\overline{\chi}_{qq'}^{+-}(\Omega) = \delta_{qq'}/\mathrm{Det}(\delta,\Omega), \tag{82}$$

$$\mathrm{Det}(\delta,\Omega) = -U^2\left[\alpha\left(\frac{\Omega}{2\Delta}\right)^2\left(1 + \frac{\alpha}{1/U - \chi}\right) - B\left(\frac{\delta a}{2}\right)^2 + \frac{\gamma a^2}{l^2}\right]. \tag{83}$$

The poles of the response (82) determine the paramagnon spectrum $\Omega(\delta)$ in the short-range-order phase. The equation $\mathrm{Det}(\delta, \Omega) = 0$ can only be solved numerically, so we consider the case of a weakly-dimerized chain ($I \ll \Delta$) for qualitative analysis, where

$$\alpha = \chi = \Delta^2\varphi_3 - \frac{5\Delta^2 I^2}{2}(\varphi_5 - \Delta^2\varphi_7), \tag{84}$$

$$B = -\varphi_1 + \left[(2t)^2 + \Delta^2\right]\varphi_3 + \frac{I^2}{2}\left\{13\varphi_3 - 15\Delta^2\varphi_5 + \left[(2t)^2 + \Delta^2\right]\left[15\Delta^2\varphi_7 - 13\varphi_5\right]\right\}, \tag{85}$$

$$\frac{1}{U} = \varphi_1 - \frac{3I^2}{2}(\varphi_3 - \Delta^2\varphi_5), \tag{86}$$

$$8\gamma = -\varphi_1 + \left[(2t)^2 + \Delta^2\right]\varphi_3 + \frac{I^2}{2}\left[-\varphi_3 - 5\Delta^2\varphi_5 + \left[(2t)^2 + \Delta^2\right]\left[\varphi_5 + 5\Delta^2\varphi_7\right]\right], \tag{87}$$

$$\varphi_n(\Delta) = \frac{1}{2N}\sum_{\mathbf{k}} \frac{1}{(\varepsilon_{\mathbf{k}}^2 + \Delta^2)^{n+2}}. \tag{88}$$

Finally, after some calculations, we obtain the excitation spectrum of paramagnons, taking into account the dependence $\Delta(I)$ from Eq. (2). For $U \gg t$,

$$\Omega = \frac{(2t)^2}{U}\left[(a\delta)^2\left(1 - 2\left(\frac{2t}{U}\right)^2 + \frac{8I^2}{U^2}\right) - \frac{1}{2}\left(\frac{a}{l}\right)^2\left(1 - 2\left(\frac{2t}{U}\right)^2 + \frac{16I^2}{U^2}\right)\right]^{1/2}; \tag{89}$$

for $U \ll t$,

$$\Omega = 2t\left[(a\delta)^2\left(1 - \frac{U}{2\pi t} + \frac{1}{3}\left(\frac{I}{\Delta_0}\right)^2\frac{U}{2\pi t}\right) - \right.$$
$$\left. - \frac{1}{2}\left(\frac{a}{l}\right)^2\left(1 - \frac{U}{2\pi t} + \frac{1}{3}\left(\frac{I}{\Delta_0}\right)^2\left(6 - \frac{5U}{2\pi t}\right)\right)\right]^{1/2}. \tag{90}$$

Note that in the paramagnetic phase with finite correlation length, the collective excitations (89) and (90) have a very different character for $\delta < \delta_c$ and $\delta > \delta_c$, where δ_c is the critical quasimomentum (see Fig. 6). For $U \ll t$ (weak-coupling limit) the value of δ_c is determined qualitatively by the equation

$$\sqrt{2}\, l\delta_c \approx 1 + \left(\frac{I}{\Delta_0}\right)^2, \quad I \ll \Delta_0. \tag{91}$$

For $t \ll I \ll U$ (strong-coupling limit), the equation for δ_c has the form

$$\sqrt{2}\, l\delta_c \approx 1 + \left(\frac{I}{U}\right)^2. \tag{92}$$

When $\delta > \delta_c$, a weakly decaying spin-wave mode exists with a quasi-Goldstone spectrum $\Omega \approx v\delta$ for $(\delta l)^2 > 1$, where v is the spin-wave velocity. The decay of paramagnons results from

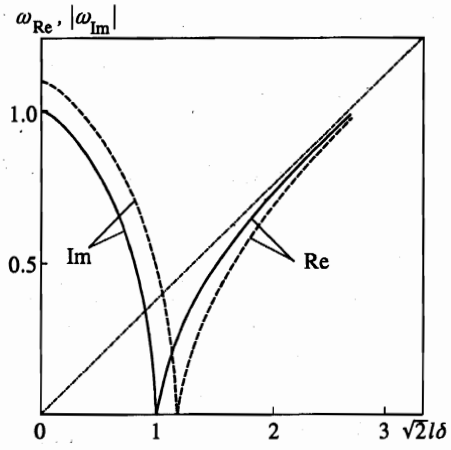

Fig. 6. Paramagnon spectrum $\omega_{Re} = (\Omega_{Re}/2t)(l/a)$, $\omega_{Im} = (2\Omega_{Im}/t)(l/a)$ for $I = 0$ (solid line) and $I \neq 0$ (dashed line)

thermal excitations of electrons through the antiferromagnetic gap ($\mathrm{Im}\,\Omega \sim \exp(-Eg/2T)$). Here we completely neglect this effect. In the region of strong magnetic disorder ($\delta < \delta_c$), a diffusive mode exists and the frequency Ω is imaginary. The effect of the staggered potential (at least in the case $I \ll \Delta$) on paramagnon dynamics amount to an increase in the critical quasimomentum δ_c, and in the spin-wave velocity v as compared with the case $I = 0$ (see Ref. [9]). The staggered potential also leads to an increase in diffusion frequency. In the case $\delta = 0$, Eqs. (89) and (90) yield

$$i\Omega(\delta = 0) = -\Omega_{Im} \approx \frac{(2t)^2}{U}\,\frac{a}{l}\,\frac{1}{\sqrt{2}}\left(1 + \frac{8I^2}{U^2}\right), \quad t \ll I \ll U, \tag{93}$$

$$i\Omega(\delta = 0) = -\Omega_{Im} \approx \frac{2t}{\sqrt{2}}\,\frac{a}{l}\left(1 + \frac{I^2}{\Delta_0^2}\right), \quad U \ll t, \quad I \ll \Delta_0. \tag{94}$$

Note also that the decrease in $l(T)$ in Eq. (94) (see Sec. 4) is very small ($\sim I^2/U$) as compared with the term I^2/Δ_0^2, since $U \gg \Delta_0$ in the weak-coupling limit.

Our analysis confirms the tendency of Ω_{Im} and δ_c to increase for all I in the stability region of the phase diagram $\Delta(I)$.

8. CONCLUSION

In the SDW model with a staggered potential, we have shown that short-range antiferromagnetic order exists in this system far above the Néel point. We have calculated the dependence of the SDW amplitude on correlation length $l(T)$ and the staggered potential I. We have also obtained the renormalization of the Néel temperature T_N and effective exchange integral J on $l(T)$ and I, which both increase with $l(T)^{-1}$ and I in the weak-coupling regime.

In the short-range-order regime, the dielectric type of electron spectrum is preserved and the singularities in the density of states are smeared out. There exist twelve branches of this spectrum $\varepsilon(I, l(T))$, and the energy gap E_g narrows with increasing I and $l(T)^{-1}$. Finally, we have obtained parameters of the magnon spectrum that depend on I and $l(T)$.

It would be very interesting to extend our analysis to other models of itinerant magnets, for example the $t - J$ model in the weak-coupling regime [14].

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