Self-consistent theory of quantum spin fluctuations in antiferromagnets with a spin density wave

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A microscopic theory of quantum spin fluctuations in antiferromagnets with a spin density wave (SDW) is suggested. The resultive system of equations allows one to find, in a self-consistent way, both the single-particle Green's function and low-energy limit of the two-particle spin-spin correlator. Calculations are carried out for a three-dimensional isotropic system at $T = 0$ in the weak coupling limit. The energy dependence of the gap in the single-particle excitation spectrum is approximated by a steplike function. It is shown that the SDW amplitude is determined mainly by the high-frequency behavior of the gap, whereas both the absorption edge and the gap in the density of states are determined by the low-frequency behavior. The difference between these limits is connected with reduction of the coupling constant by spin fluctuations in the low-frequency range.

1. INTRODUCTION

The usual description of collective excitations of spin density (spin fluctuations) in band antiferromagnets with a SDW (spin density wave) is restricted to the random phase approximation,[1] which is not self-consistent. The SDW parameters and electron spectrum are calculated in the mean-field approximation without allowance for renormalization due to electron scattering by SDW fluctuations. This approach is asymptotically exact in the limit of a small coupling constant $U/t \ll 1$ (the so-called logarithmic approximation in the model with "nesting," where U is the electron-electron interaction potential and t is the bandwidth). The question of correct calculation of spin-fluctuation corrections in the logarithmic approximation, let alone the intermediate coupling regime ($U/t \sim 1$), remains open.

Meanwhile, as is well known,[2] spin fluctuations play an important role both in the thermodynamics of band magnets and in the renormalization of parameters pertaining to the magnetic structure of the ground state at $T = 0$. In the high-temperature region (greater than or on the order of the critical temperature) the methods most widely used today are those which allow for classical thermodynamic fluctuations of spin density against the background of a mean-field ground state.[2] The great majority of these methods do not allow for quantum fluctuations (or, in terms of functional approach, dynamic configurations of spin density). The only exception is the early theory of renormalized spin fluctuations,[3] whose range of validity, however, is quite indefinite ($U/t > 1$, but $U/t - 1 \ll 1$) and for which the correctness of the assumptions made is unverifiable.

In Ref. 4 an attempt was made to extend the method of Ref. 3 to the objects of interest—antiferromagnets with the SDW described by the "nesting" model. The simplest version of self-consistent (in the static limit) calculations of the SDW amplitude and pair spin-spin correlator was carried out, taking into account the renormalization of the self-energy part of the single-particle Green's function of band electrons. Though the qualitative result obtained—the decrease in the SDW amplitude in comparison with the mean-field value—does not arouse objections, the technique used, which can be shown, to violate invariance with respect to spin rotations[1)] of a system with purely exchange interaction, when one exceeds the limits of the mean field approximation, seems questionable.

Until recently, the problem of the self-consistency of spin fluctuations and SDW amplitude renormalization has been of interest only to a relatively narrow circle of specialists in the field of band magnetism. The situation has, however, changed due to intensive studies of magnetic properties of metal oxides having high-T_c superconductivity. The presence of highly developed spin fluctuations in these substances, as well as short- and long-range antiferromagnetic order, affects their normal and (probably) superconducting features.[5] In the latter case a particularly important role is played by low-temperature quantum spin fluctuations, which, in some of the models (see, e.g., Ref. 6), can cause Cooper pairing of band electrons.

The effect of quantum fluctuations on the decrease in the mean sublattice magnetization at $T = 0$ in the Heisenberg antiferromagnets has been investigated by Anderson[7] for $S \gg 1$ semiclassical spins in the spin-wave approximation. This effect is particularly strong in low-dimensional systems. Recently it has been studied in quasi-two-dimensional Heisenberg antiferromagnets.[5] As mentioned above, a similar problem has been studied in Ref. 4 and, recently in the context of application to high-T_c metal oxide superconductors, in the model of itinerant electron antiferromagnetism (the SDW model) in Refs. 8 and 9. In contrast to Ref. 4, the authors of Ref. 9 abandoned the idea of a self-consistent approach to spin fluctuations, giving the correlation function of the latter in a model form and restricting the calculation to the usual random phase approximation.

Meanwhile, a rigorous self-consistent procedure in the SDW model must allow for several basic points. Specifically, renormalization of the bare electron-electron interaction by spin fluctuations causes it to become retarded, so that the gap in the elementary excitation spectrum is energy-dependent, like the superconducting gap in the model of phonon superconductivity. To calculate the self-energy parts (normal and anomalous) of the Green's functions, it is necessary to use a system of Eliashberg equations with a renormalized

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electron-electron interaction vertex. Furthermore, at all stages we must check the system invariance with respect to spin rotations, which, in particular, causes the spectrum of transverse spin fluctuations to be gapless (the Goldstone collective mode is present). In the present study we will try to carry out this program.

2. BASIC EQUATIONS

Consider a system unstable against triplet electron-hole pairing, i.e., against transition to a state with a spin density wave.[10] We write the Hamiltonian in the form

$$H = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) a^+_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{U}{2N} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} a^+_{\mathbf{k},\sigma} a^+_{\mathbf{k}',-\sigma} a_{\mathbf{k}'-\mathbf{q},-\sigma} a_{\mathbf{k}+\mathbf{q},\sigma}, \tag{1}$$

where $\varepsilon(\mathbf{k}) = \xi(\mathbf{k}) - \mu$ is the electron dispersion law, μ is the chemical potential, U is the potential of electron-electron interaction, N is the number of sites, and σ is the electron spin.

We assume that for a certain set of quasimomenta $\mathbf{k}$ the spectrum $\varepsilon(\mathbf{k})$ satisfies the "nesting" condition $\varepsilon(\mathbf{k}) = -\varepsilon(\mathbf{k}+\mathbf{Q})$, where $\mathbf{Q}$ is equal to half the reciprocal lattice vector. Consider the case of pure doubling of the antiferromagnet structure. It is convenient to introduce band indices "1" and "2" to denote the nested portions of the Fermi surface and the creation and annihilation operators for electrons with momentum $\mathbf{k}$ and spin σ on the corresponding portions, $a^+_{i\mathbf{k}\sigma}$ and $a_{i\mathbf{k}\sigma}$, where $i = 1$ and 2. The momentum-conservation law allows only those scattering processes which are shown in Fig. 1. In what follows we will restrict the discussion to the model in which the Fermi surface consists of spherical sections with identical radii, i.e., to the case of equal electron and hole concentration ($\mu = 0$).

We introduce, in a usual manner, the temperature Green's functions:

$$G^{\alpha\beta}_{ij}(\mathbf{k},\tau) = -\langle T_\tau a_{i\mathbf{k}\alpha}(\tau) a^+_{j\mathbf{k}\beta}(0)\rangle. \tag{2}$$

The anomalous (in the band indices) Green's functions G_{ij} [and their self-energy parts Σ_{ij} ($i \neq j$), see below] in (2) give rise to antiferromagnetic ordering. The normal Green's functions G_{ii} (and their self-energy parts Σ_{ii}) have spin structure of the form $G^{\alpha\beta}_{ii} = G_{ii}\delta_{\alpha\beta}$ and the anomalous ones (G_{ij} and Σ_{ij} with $i \neq j$) have triplet structure. We assume that the SDW is linearly polarized. Then we have $\Sigma^{\alpha\beta}_{12} = \Sigma_{12}\delta^{\alpha\beta}_z$, where δ_z is the third Pauli matrix, and the direction of the quantization axis coincides with the direction of SDW polarization. In what follows we will denote the components of the matrices G_{ij} and Σ_{ij} in spin space by G^σ_{ij} and Σ^σ_{ij} to allow explicitly for the sign of the spin projection on the z axis. It is evident that

$$\Sigma^\sigma_{ij} = (-1)^{i+j}\Sigma^{-\sigma}_{ij}.$$

The Green's functions obey the same relation, so in what follows we will write the index σ only on the anomalous Green's functions and their self-energy parts, bearing in mind $\Sigma^\sigma_{ij} \equiv \sigma\Sigma_{ij}$ ($i \neq j, \sigma = \pm 1$).

The Green's functions (2) obey the following equations of motion:

$$\begin{pmatrix} i\omega - \varepsilon_1(\mathbf{k}) - \Sigma_{11}(\mathbf{k}, i\omega) & -\Sigma^\sigma_{12}(\mathbf{k}, i\omega) \\ -\Sigma^\sigma_{21}(\mathbf{k}, i\omega) & i\omega - \varepsilon_2(\mathbf{k}) - \Sigma_{22}(\mathbf{k}, i\omega) \end{pmatrix} \times \begin{pmatrix} G_{11}(\mathbf{k}, i\omega) & G^\sigma_{12}(\mathbf{k}, i\omega) \\ G^\sigma_{21}(\mathbf{k}, i\omega) & G_{22}(\mathbf{k}, i\omega) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3}$$

where $i\omega = i(2n+1)T$ is the fermion Matsubara frequency and T is the temperature.

We represent the self-energy parts of the normal Green's functions as a sum of odd and even (in frequency) terms

$$\Sigma_{ii}(\mathbf{k}, i\omega) = i\omega[1 - Z_i(\mathbf{k}, i\omega)] + S_i(\mathbf{k}, i\omega), \tag{4}$$

where the functions $Z_i(\mathbf{k}, i\omega)$ and $S_i(\mathbf{k}, i\omega)$ are even in $i\omega$.

The Dyson equation for the self-energy parts is

$$\Sigma^\sigma_{ij}(k) = \frac{T}{N}\sum_{i\nu}\sum_{\mathbf{p}}\sum_{m,n=1}^{2} UG^{-\sigma}_{mn}(p) - \frac{T^2}{N^2}\sum_{i\nu,i\eta}\sum_{\mathbf{p},\mathbf{q}}\sum_{\substack{l,m,n,\\ r,s,t=1}} UG^\sigma_{rs}(q) \times G^{-\sigma}_{tl}(q+p-k)G^{-\sigma}_{mn}(p)V_{stnj}(q, p+q-k, p, k), \tag{5}$$

where $p = (\mathbf{p}, i\nu)$, $k = (k, i\omega)$, $q = (\mathbf{q}, i\eta)$; $i\nu$, $i\eta$ and $i\omega$ are the fermion Matsubara frequencies, and $V_{stnj}(p_1,p_2,p_3,p_4)$ is the vertex part of the two-particle Green's function constructed using the operators of the bands s, t, n, and j. In (5) and in what follows, without mentioning it, we will take into account, in the sums over band indices, only allowed combinations (Fig. 1) of indices of the Green's functions and self-energy parts.

In the block V we single out two groups of diagrams which correspond to scattering processes with and without spin flip. This step is absolutely natural due to the character of the bare interaction U corresponding to scattering of particles with opposite spins. The simplest diagrams in these groups are ladder and polarization diagrams. When the two sets of diagrams are summed they yield effective potentials in the longitudinal and transverse spin channels, which can be represented graphically (Fig. 2) or in the analytic form

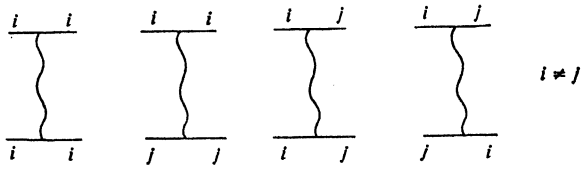

FIG. 1

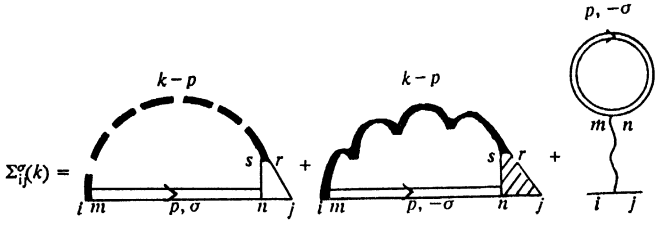

FIG. 2

$$\Sigma_{ij}^{\sigma}(k)=\frac{T}{N}\sum_{i\nu}\sum_{\mathbf{p}}\sum_{m,n,r,s=1}^{2}\{\Lambda_{ms}^{ir}(k-p)\Gamma_{nj}^{sr}(k-p,p,k)G_{mn}^{\sigma}(p)$$

$$+[U+\theta_{ms}^{ir}(k-p)\tilde{\Gamma}_{nj}^{sr}(k-p,p,k)]G_{mn}^{-\sigma}(p)\},\quad(6)$$

where $\Lambda_{ms}^{ir}(k-p)$ and $\theta_{ms}^{ir}(k-p)$ are the propagators of longitudinal and transverse spin fluctuations, respectively, and Γ_{nj}^{sr} and $\tilde{\Gamma}_{nj}^{sr}$ are the vertices in corresponding channels.

In the effective potentials in (6) we will distinguish the contributions of low-frequency spin fluctuations with characteristic energies $\omega\lesssim 2\Delta$ (Δ is on the order of half the gap width in the electron spectrum). The contributions of high frequency fluctuations are taken into account in the initial dispersion law through renormalization of quasiparticle mass and chemical potential (as in the usual theory of Fermi liquid). In the low-frequency part of the effective potentials we take the vertices Γ and $\tilde{\Gamma}$ in static approximation. In this case their role reduces to renormalization of the bare irreducible block (in fact, to renormalization of the constant U).

For the frequency-dependent effective potentials Λ and θ, as well as for the Green's functions we introduce the Lehman spectral representation

$$\Lambda_{mn}^{ij}(\mathbf{k}-\mathbf{p},i\zeta)=\int_0^{\infty}d\Omega\left(\frac{1}{i\zeta-\Omega}-\frac{1}{i\zeta+\Omega}\right)L_{mn}^{ij}(\mathbf{k}-\mathbf{p},\Omega),$$

$$\theta_{mn}^{ij}(\mathbf{k}-\mathbf{p},i\zeta)=\int_0^{\infty}d\Omega\left(\frac{1}{i\zeta-\Omega}-\frac{1}{i\zeta+\Omega}\right)T_{mn}^{ij}(\mathbf{k}-\mathbf{p},\Omega),\quad(7)$$

$$G_{mn}^{\sigma}(\mathbf{p},i\nu)=-\int_{-\infty}^{\infty}\frac{d\varepsilon}{\pi}\frac{\operatorname{Im}G_{mn}^{\sigma Ret}(\mathbf{p},\varepsilon)}{i\nu-\varepsilon},$$

where $i\zeta$ and $i\nu$ are the even and odd Matsubara frequencies. The label *Ret* denotes the retarded Green's function.

Substituting (7) into (6), we can sum over the Matsubara frequencies in the Dyson equations (6). As mentioned above, the vertices Γ and $\tilde{\Gamma}$ are regarded as constants included in Λ and θ. After summation we have

$$\Sigma_{ij}^{\sigma}(\mathbf{k},i\omega)=-\frac{1}{N}\sum_{\mathbf{p}}\sum_{m,n=1}^{\infty}\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\{\int_0^{\infty}[L_{mn}^{ij}(\mathbf{k}-\mathbf{p},\Omega)$$

$$\times\operatorname{Im}[G_{mn}^{\sigma Ret}(\mathbf{p},\varepsilon)]$$

$$+T_{mn}^{ij}(\mathbf{k}-\mathbf{p},\Omega)\operatorname{Im}[G_{mn}^{-\sigma Ret}(\mathbf{p},\varepsilon)]]K(\Omega,\varepsilon,i\omega)d\Omega$$

$$-U\operatorname{Im}[G_{mn}^{-\sigma Ret}(\mathbf{p},\varepsilon)]n_F(\varepsilon)\},\quad(8)$$

where

$$K(\Omega,\varepsilon,i\omega)=\frac{n_B(\Omega)+n_F(-\varepsilon)}{\Omega+\varepsilon-i\omega}-\frac{n_B(\Omega)+n_F(\varepsilon)}{\Omega-\varepsilon+i\omega},$$

and $n_{F,B}(\varepsilon)$ are the Fermi–Dirac and Bose–Einstein distribution functions, respectively.

When the bands are filled, with $\mu=0$, and the "nesting" is ideal, the Green's functions, as seen from (3) and (4), have the form

$$G_{11,22}(\mathbf{k},i\omega)=[i\omega Z(\mathbf{k},i\omega)\pm\xi(\mathbf{k})]D^{-1}(\mathbf{k},i\omega),$$

$$G_{12,21}^{\sigma}(\mathbf{k},i\omega)=\Sigma_{12,21}^{\sigma}(\mathbf{k},i\omega)D^{-1}(\mathbf{k},i\omega),\quad(9)$$

where

$$D(\mathbf{k},i\omega)=[i\omega Z(\mathbf{k},i\omega)]^2-\xi^2(\mathbf{k})-\Sigma_{12}^{\sigma}(\mathbf{k},i\omega)\Sigma_{21}^{\sigma}(\mathbf{k},i\omega).$$

Indeed, in the mean field approximation we have the following relation between the Green's functions $G_{11}(\mathbf{k},i\omega)$ and $G_{22}(\mathbf{k},i\omega)$:

$$G_{22}(\mathbf{k},i\omega)=-G_{11}(\mathbf{k},-i\omega),$$

which is the consequence of the electron-hole symmetry (of the bands 1 and 2). Suppose that this relation also holds for the exact Green's functions. This requirement leads to

$$Z(\mathbf{k},i\omega)\equiv Z_1(\mathbf{k},i\omega)=Z_2(\mathbf{k},i\omega)$$

and

$$S(\mathbf{k},i\omega)\equiv S_1(\mathbf{k},i\omega)=-S_2(\mathbf{k},i\omega).$$

Here S is a correction to the chemical potential. Since it is determined mainly by the high-frequency contribution, we assume that it is already allowed for and in what follows we omit the quantities $S_{1,2}$, which leads to the relations (9).

Note that the system (8) is formally similar to the system of Eliashberg equations.[11] In the piecewise-spherical model of the Fermi surface (and only this model is considered) we change over from summation over $\mathbf{p}$ in (8) to integration over ξ and $q=|\mathbf{k}-\mathbf{p}|$ and the angle φ. As a result, the self-energy parts are frequency—rather than momentum-dependent. By means of analytic continuation in (8) to the real frequency axis, $i\omega\to\omega+i\delta$, we find for the retarded self-energy parts the following equations (for brevity we omit the labels *Ret*):

$$\Sigma_{ij}^{\sigma}(\omega)=\sum_{m,n=1}^{2}\int_{-\infty}^{\infty}d\varepsilon\left\{n_F(\varepsilon)UN(0)\operatorname{Re}\left[\frac{A_{mn}^{-\sigma}(\varepsilon)}{D(\varepsilon)}\right]\right.$$

$$\left.+\int_0^{\infty}d\Omega\left\{f_{mn}^{ij}(\Omega)\operatorname{Re}\left[\frac{A_{mn}^{\sigma}(\varepsilon)}{D(\varepsilon)}\right]+g_{mn}^{ij}(\Omega)\operatorname{Re}\left[\frac{A_{mn}^{-\sigma}(\varepsilon)}{D(\varepsilon)}\right]\right\}\right.$$

$$\left.\times K(\Omega,\varepsilon,\omega+i\delta)\right\},\quad(10)$$

where $N(0)$ is the density of states at the Fermi level in the paramagnetic phase;

$$D(\varepsilon)=\{[\varepsilon Z(\varepsilon)]^2-\Sigma_{12}^{\sigma}(\varepsilon)\Sigma_{21}^{\sigma}(\varepsilon)\}^{1/2},$$

$$A_{11,22}^{\sigma}(\varepsilon)=\pm|\varepsilon|Z(\varepsilon),$$

$$A_{12,21}^{\sigma}(\varepsilon)=\sigma\Sigma_{12,21}(\varepsilon)\operatorname{sign}\varepsilon,\quad\sigma=\pm1,\quad(11)$$

$$f_{mn}^{ij}(\Omega)=\frac{1}{4\pi^2v_F}\int_0^{q_m}L_{mn}^{ij}(q,\Omega)qdq,$$

$$g_{mn}^{ij}(\Omega)=\frac{1}{4\pi^2v_F}\int_0^{q_m}T_{mn}^{ij}(q,\Omega)qdq,$$

v_F is the velocity on the Fermi surface, and q_m is found from the condition $cq_m \sim 2\Delta$, where c is the spin wave velocity.

The system (10) is not yet closed, since the effective potentials entering into it through the quantities f and g are themselves defined through $\Sigma_{ij}(\omega)$.

3. EFFECTIVE POTENTIALS

To find the form of effective potentials we will use something like the random-phase approximation, but with the exception that we will use, as an irreducible element, the effective point interaction U^*, which allows in the static approximation for vertex corrections in the irreducible polarization loop rather than the bare interaction U. The irreducible polarization loop, in contrast to that calculated in the random phase approximation, must be constructed not with the help of mean-field Green's functions of electrons and holes, but using the Green's functions of electrons and holes moving in the field of spin fluctuations whose propagators are constructed in turn with the help of the same Green's functions rather than the Green's functions of the approximation of lowest order in the fluctuations, as in the perturbation theory approach. In this sense we can speak of carrier motion in the self-consistent field of the spin fluctuations.

To find the interaction U^* correctly we need to retain the gapless transverse mode in the spectrum of spin fluctuations, i.e., satisfy the Goldstone theorem. In practice, this requirement means that the denominator of the pair correlation function of transverse spin fluctuations vanishes in the static long-wavelength limit.

Since the bare interaction only leads to scattering of particles with opposite spins, the transverse and longitudinal spin scattering channels do not get mixed up. We have the following expressions for Λ^{ij}_{mn} and θ^{ij}_{mn}:

$$\Lambda_1(q) \equiv \Lambda^{ii}_{ii}(q) = \Lambda^{ij}_{ij}(q) = -U[U^* l_1(q)]^3[1 - U^* l_1(q)]^{-1},$$

$$\Lambda_2(q) \equiv \Lambda^{ii}_{jj}(q) = \Lambda^{ij}_{ji}(q) = -U[U^* l_2(q)]^3[1 - U^* l_2(q)]^{-1},$$

$$\theta_1(q) \equiv \theta^{ii}_{ii}(q) = \theta^{ij}_{ij}(q) = -UU^*\{\pi_1(q)[1 - U^*\pi_2(q)] + U^*\pi_3^2(q)\}R^{-1}(q),$$

$$\theta_2(q) \equiv \theta^{ij}_{ji}(q) = \theta^{ii}_{jj}(q) = -UU^*\{\pi_2(q)[1 - U^*\pi_1(q)] + U^*\pi_3^2(q)\}R^{-1}(q),$$

$$\theta^{ii}_{ij}(q) = \theta^{ij}_{ii}(q) = \theta^{ii}_{ii}(q) = \theta^{ii}_{ji}(q) = -UU^*\pi_3(q)R^{-1}(q), \qquad (12)$$

where $i, j = 1, 2$, $i \neq j$, $q = (\mathbf{q}, \omega)$, and

$$R(q) = [1 - U^*\pi_1(q)][1 - U^*\pi_2(q)] - [U^*\pi_3(q)]^2.$$

We have introduced [in Eq. (12)] the notation $l_{1,2}(q)$ and $\pi_i(q)$, $i = 1, 2, 3$, for the irreducible polarization operators in the longitudinal and transverse channels. (The longitudinal channel corresponds to fluctuations of the SDW amplitude, and the transverse one to fluctuations of the SDW polarization vector direction.) They result from summation of elementary loops constructed using the Green's functions with self-energy parts obeying (10), i.e., the Green's functions of electrons and holes moving in the self-consistent field of the spin fluctuations. We have

$$l_1(q) = \sum_{i,j=1}^{2} P^{ij}_{ij}(q, \sigma, \sigma),$$

$$l_2(q) = \sum_{i,j=1}^{2} [P^{ii}_{jj}(q, \sigma, \sigma) + P^{ij}_{ji}(q, \sigma, \sigma)](1 - \delta_{ij}),$$

$$P^{ij}_{mn}(q, \alpha, \beta) = -\frac{T}{N}\sum_{i\nu}\sum_{\mathbf{p}} G^{\alpha}_{ij}(p + q)G^{\beta}_{nm}(p),$$

$$\pi_1(q) = \sum_{i,j=1}^{2} P^{ij}_{ij}(q, \sigma, -\sigma),$$

$$\pi_2(q) = \sum_{i,j=1}^{2} [P^{ij}_{ji}(q, \sigma, -\sigma) + P^{ii}_{jj}(q, \sigma, -\sigma)](1 - \delta_{ij}),$$

$$\pi_3(q) = \sum_{i,j=1}^{2} [P^{ii}_{ij}(q, \sigma, -\sigma) + P^{ij}_{ii}(q, \sigma, -\sigma)](1 - \delta_{ij})$$

$$= \sum_{i,j=1}^{2} [P^{ji}_{ii}(q, \sigma, -\sigma) + P^{ii}_{ji}(q, \sigma, -\sigma)](1 - \delta_{ij}). \qquad (13)$$

The existence of the gapless transverse mode means that we have the relation $R(0,0) = 0$ which, because the polarization operator $\pi_3(\mathbf{q},\omega)$ is odd in frequency, can be written in the form

$$1 - U^*\pi_2(0, 0) = 0. \qquad (14)$$

In the non-self-consistent random phase approximation in which polarization operators are constructed with the help of mean-field Green's functions the condition (14) coincides with the self-consistency equation for the mean-field order parameter and is automatically fulfilled for $U^* = U$. In our case Eq. (14) gives the effective interaction U^*.

Thus, the expressions (10)–(14) form a closed system of equations which self-consistently describe low-frequency spin fluctuations of the SDW in the model with electron and hole Fermi surfaces composed of nested spherical parts. Note that Eqs. (12)–(14) are independent of the specific form of the electron spectrum and, together with (8), comprise a system of equations valid, in principle, for the solution of the problem when portions of the Fermi surface are nested anisotropically. However this case is beyond the scope of the present study.

4. SOLUTION IN THE WEAK COUPLING LIMIT AT $T = 0$

Let us rewrite the system of equations for zero temperature:

$$\omega[1 - Z(\omega)] = \int_{-\infty}^{\infty} d\varepsilon \int_{0}^{\infty} d\Omega [f_1(\Omega) - f_2(\Omega) + g_1(\Omega) - g_2(\Omega)] \times \mathrm{Re}\left[\frac{A_{11}(\varepsilon)}{2D(\varepsilon)}\right]\left(\frac{1 + \mathrm{sign}\,\varepsilon}{\Omega + \varepsilon - \omega - i\delta} - \frac{1 - \mathrm{sign}\,\varepsilon}{\Omega - \varepsilon + \omega + i\delta}\right),$$

$$\Sigma^{\sigma}_{12}(\omega) = \int_{-\infty}^{\infty} d\varepsilon \left\{UN(0)\mathrm{Re}\left[\frac{A^{-\sigma}_{12}(\varepsilon) + A^{-\sigma}_{21}(\varepsilon)}{2D(\varepsilon)}\right](1 - \mathrm{sign}\,\varepsilon)\right.$$

$$+\frac{1}{2}\int_0^\infty d\Omega\Big\{g_1(\Omega)\mathrm{Re}\left[\frac{A_{12}^{-\sigma}(\varepsilon)}{D(\varepsilon)}\right]$$

$$+g_2(\Omega)\mathrm{Re}\left[\frac{A_{21}^{-\sigma}(\varepsilon)}{D(\varepsilon)}\right]+f_1(\Omega)\mathrm{Re}\left[\frac{A_{12}^{\sigma}(\varepsilon)}{D(\varepsilon)}\right]$$

$$+f_2(\Omega)\mathrm{Re}\left[\frac{A_{21}^{\sigma}(\varepsilon)}{D(\varepsilon)}\right]\Big\}\left(\frac{1+\mathrm{sign}\,\varepsilon}{\Omega+\varepsilon-\omega-i\delta}-\frac{1-\mathrm{sign}\,\varepsilon}{\Omega-\varepsilon+\omega+i\delta}\right)\Big\}, \tag{15}$$

where the quantities $f_{1,2}(\Omega)$ and $g_{1,2}(\Omega)$ are defined in terms of $\Lambda_{1,2}(q)$ and $\theta_{1,2}(q)$ taken from (12), just as the quantities $f_{mn}^{ij}(\Omega)$ are defined in terms of $L_{mn}^{ij}(q)$, etc., in (11).

We represent $\Sigma_{12}^{\sigma}(\omega)$ and $\Sigma_{21}^{\sigma}(\omega)$ in the following form:

$$\Sigma_{12,21}^{\sigma}(\omega)=\sigma[\Sigma^{s}(\omega)\pm\Sigma^{a}(\omega)+\omega[\Sigma^{os}(\omega)\pm\Sigma^{oa}(\omega)]], \tag{16}$$

where

$$\sigma[\Sigma^{s,a}(\omega)+\omega\Sigma^{os,a}(\omega)]=\frac{1}{2}[\Sigma_{12}^{\sigma}(\omega)\pm\Sigma_{21}^{\sigma}(\omega)],\quad \sigma=\pm 1.$$

From (15) and (16) we get

$$\Sigma^{s}(\omega)=2UN(0)\int_0^W d\varepsilon\,\mathrm{Re}\left[\frac{\Sigma^{s}(\varepsilon)-\varepsilon\Sigma^{os}(\varepsilon)}{D(\varepsilon)}\right]+\int_0^\infty d\varepsilon\int_0^\infty d\Omega[f_1(\Omega)$$

$$+f_2(\Omega)-g_1(\Omega)-g_2(\Omega)]\mathrm{Re}\left[\frac{\Sigma^{s}(\varepsilon)}{D(\varepsilon)}\right]K_{+}(\Omega,\varepsilon,\omega+i\delta), \tag{17}$$

$$\Sigma^{a}(\omega)=\int_0^\infty d\varepsilon\int_0^\infty d\Omega[f_1(\Omega)-f_2(\Omega)-g_1(\Omega)+g_2(\Omega)]\mathrm{Re}\left[\frac{\Sigma^{a}(\varepsilon)}{D(\varepsilon)}\right]$$

$$\times K_{+}(\Omega,\varepsilon,\omega+i\delta), \tag{18}$$

$$\omega\Sigma^{os}(\omega)=\int_0^\infty d\varepsilon\int_0^\infty d\Omega[f_1(\Omega)+f_2(\Omega)-g_1(\Omega)-g_2(\Omega)]$$

$$\times\mathrm{Re}\left[\frac{\varepsilon\Sigma^{os}(\varepsilon)}{D(\varepsilon)}\right]K_{-}(\Omega,\varepsilon,\omega+i\delta), \tag{19}$$

$$\omega\Sigma^{oa}(\omega)=\int_0^\infty d\varepsilon\int_0^\infty d\Omega[f_1(\Omega)-f_2(\Omega)-g_1(\Omega)+g_2(\Omega)]$$

$$\times\mathrm{Re}\left[\frac{\varepsilon\Sigma^{oa}(\varepsilon)}{D(\varepsilon)}\right]K_{-}(\Omega,\varepsilon,\omega+i\delta), \tag{20}$$

$$\omega[1-Z(\omega)]=\int_0^\infty d\varepsilon\int_0^\infty d\Omega[f_1(\Omega)-f_2(\Omega)+g_1(\Omega)-g_2(\Omega)]$$

$$\times\mathrm{Re}\left[\frac{\varepsilon Z(\varepsilon)}{D(\varepsilon)}\right]K_{-}(\Omega,\varepsilon,\omega+i\delta). \tag{21}$$

Here

$$K_{\pm}(\Omega,\varepsilon,\omega)=(\Omega+\varepsilon-\omega)^{-1}\pm(\Omega+\varepsilon+\omega)^{-1}.$$

In the first term in (17) we have cut off the integral at the upper limit: W is an energy on the order of half the band width ($2W\sim t$). It is evident from Eqs. (17)–(20) that $\Sigma^{a}(\omega)$ and $\Sigma^{oa,s}(\omega)$ are low-energy quantities. We will consider them approximately constant, i.e., $\Sigma^{a}(\omega)=\Sigma^{a}(0)$, etc. It follows from the requirement of system compatibility that $\Sigma^{a}(0)=\Sigma^{os,a}(0)=0$, and Eqs. (18)–(20) become identities.

To solve Eqs. (17)–(21) we introduce an ansatz of the McMillan type:[12]

$$\Delta(\varepsilon)\equiv\frac{\Sigma^{s}(\varepsilon)}{Z(\varepsilon)}=\begin{cases}\Delta_0, & \varepsilon<\Omega_0\\ \Delta_\infty, & \varepsilon>\Omega_0\end{cases}, \tag{22}$$

where Ω_0 is the characteristic energy scale of spin fluctuations ($\Omega_0\sim 2\Delta_0$) and

$$Z(\varepsilon)=\begin{cases}Z_0, & \varepsilon<\Omega_0\\ Z_\infty, & \varepsilon>\Omega_0\end{cases}. \tag{23}$$

As follows from (21), $Z(\omega)$ is a low-energy quantity, i.e., we have $Z_\infty=1$ in (23). With the help of Eqs. (22) and (23) the equations for Δ_0, Δ_∞, Z_0, and U^* take the form

$$1-Z_0=2\int_0^\infty d\Omega F_z(\Omega)\left[\int_{\Delta_0}^{\Omega_0}\frac{\varepsilon d\varepsilon}{(\varepsilon+\Omega)^2\sqrt{\varepsilon^2-\Delta_0^2}}\right.$$

$$\left.+\int_{\Omega_0}^\infty\frac{\varepsilon d\varepsilon}{(\varepsilon+\Omega)^2\sqrt{\varepsilon^2-\Delta_\infty^2}}\right], \tag{24}$$

$$\Delta_0 Z_0=\Delta_\infty+2\int_0^\infty d\Omega F_s(\Omega)\left[\int_{\Delta_0}^{\Omega_0}\frac{\Delta_0 d\varepsilon}{(\varepsilon+\Omega)\sqrt{\varepsilon^2-\Delta_0^2}}\right.$$

$$\left.+\int_{\Omega_0}^\infty\frac{\Delta_\infty d\varepsilon}{(\varepsilon+\Omega)\sqrt{\varepsilon^2-\Delta_\infty^2}}\right], \tag{25}$$

$$\Delta_\infty=2UN(0)\left[\int_{\Delta_0}^{\Omega_0}\frac{\Delta_0 d\varepsilon}{\sqrt{\varepsilon^2-\Delta_0^2}}+\int_{\Omega_0}^\infty\frac{\Delta_\infty d\varepsilon}{\sqrt{\varepsilon^2-\Delta_\infty^2}}\right], \tag{26}$$

$$1=2U^*N(0)\left[\int_{\Delta_0}^{\Omega_0}\frac{d\varepsilon}{Z_0\sqrt{\varepsilon^2-\Delta_0^2}}+\int_{\Omega_0}^\infty\frac{d\varepsilon}{\sqrt{\varepsilon^2-\Delta_\infty^2}}\right]. \tag{27}$$

Here

$$F_{z,s}(\Omega)=f_1(\Omega)\mp f_2(\Omega)-[g_2(\Omega)\mp g_1(\Omega)]. \tag{28}$$

Now the most difficult problem is the self-consistent calculation of spin-fluctuation propagators, which reduces, in fact, to the calculation of the irreducible polarization operators (13). Such calculations are carried out, in general,

only numerically. It is possible to find the lowest corrections to the mean-field solution analytically. For this purpose we expand the polarization operators $\pi_i(q)$ $(i = 1,2,3)$ in (13) in small q and ω (in the sense that $v_F q, \omega \ll \Delta_0$):

$$\pi_i(\mathbf{q}, \omega) \approx \pi_i(0, 0) + b_i \mathbf{q}^2 + c_i \omega^2.$$

In $\pi_i(0,0)$ we use the ansatz (22) and (23) to find U^* from Eq. (14) for the spin-fluctuation spectrum. When we calculate the coefficients b_i and c_i, it is sufficient to set $\Delta(\varepsilon) = \Delta_0 = \text{const}$ and not to distinguish between Δ_0 and Δ_∞ in the terms of Eqs. (24) and (25) containing the spectral characteristics of the fluctuations $F_{z,s}(\Omega)$. The calculation of the latter reduces to the well-known calculation of the resonant parts of spin-fluctuation propagators in the random phase approximation, but with the difference that we have Δ_0 instead of the mean-field SDW amplitude and the irreducible loop must be multiplied by Z_0^{-1}. In this approximation $\Omega_0 = 2\Delta_0$ holds in (22) and (23). The quantities $l_{1,2}(q,\omega)$ are calculated in the same way. Thus, we find that the amplitude mode spectrum has the Einstein form with frequency Ω_0. In the weak coupling limit $[UN(0) \ll 1]$, with the qualifications made above, the quantities $F_{z,s}(\Omega)$ in (28) are written in the following way:

$$F_{z,s}(\Omega) = \frac{U}{U^*}[A_{z,s}\theta(\Omega_0 - \Omega) + B_{z,s}\delta(\Omega - \Omega_0), \tag{29}$$

where

$$A_{z,s} = -\frac{6Z_0\Delta_0^2}{(2\pi)^2 v_F^3 N(0)}, \quad B_{z,s} = \pm\frac{6Z_0\Delta_0^3}{(2\pi)^2 v_F^3 N(0)},$$

$\theta(\Omega) = \frac{1}{2}(1 + \text{sign}\,\Omega)$, and $\delta(\Omega)$ is the Dirac delta-function.

Substituting (29) into (24) and (25) we find the following equations to second order in Δ_0/W:

$$1 - Z_0 = 2\int_{\Delta_0}^{\infty}\left(A_z\Omega_0 + \frac{B_z\varepsilon}{\varepsilon + \Omega_0}\right)\frac{d\varepsilon}{(\varepsilon + \Omega_0)\sqrt{\varepsilon^2 - \Delta_0^2}}$$

$$\equiv -\zeta\left(\frac{\Delta_0}{2W}\right)^2, \tag{30}$$

$$\Delta_0 Z_0 = \Delta_\infty + 2\Delta_0\int_{\Delta_0}^{\infty}\left[A_s\ln\left(1 + \frac{\Omega_0}{\varepsilon}\right) + \frac{B_s}{\varepsilon + \Omega_0}\right]\frac{d\varepsilon}{\sqrt{\varepsilon^2 - \Delta_0^2}}$$

$$\equiv \Delta_\infty - \beta\Delta_0\left(\frac{\Delta_0}{2W}\right)^2. \tag{31}$$

The signs of ζ and β are chosen, as can easily be seen, so that $\zeta > 0$ and $\beta > 0$ hold (see Appendix).

Dividing (31) by Δ_0 and then adding (31) to (30), we find for the quantity

$$\delta \equiv \Delta_\infty/\Delta_0 - 1$$

the following expression:

$$\delta = (\zeta + \beta)(\Delta_0/2W)^2. \tag{32}$$

Here we have used

$$\frac{U}{U^*} = \frac{\Delta_\infty}{Z_0\Delta_0}\frac{I_0 + Z_0 I_\infty}{I_0 + (1+\delta)I_\infty} \approx 1 + \beta\left(\frac{\Delta_0}{2W}\right)^2\frac{I_0}{I_0 + I_\infty}, \tag{33}$$

which follows from Eqs. (26) and (27), where

$$I_0 \equiv \int_{\Delta_0}^{\Omega_0}\frac{d\varepsilon}{\sqrt{\varepsilon^2 - \Delta_0^2}},$$

$$I_\infty \equiv \int_{\Omega_0}^{W}\frac{d\varepsilon}{\sqrt{\varepsilon^2 - \Delta_\infty^2}} \approx \ln\frac{2W}{\Delta_0} - \left(\frac{\Delta_0}{2W}\right)^2$$

$$- I_0 + \frac{\delta\Delta_0^2}{\sqrt{\Omega_0^2 - \Delta_0^2}(\Omega_0 + \sqrt{\Omega_0^2 - \Delta_0^2})}.$$

Thus, according to Eq. (32), the $\Delta(\varepsilon)$ high-frequency limit differs from the low-frequency one by the factor of (Δ_0/W).[2] To find Δ_0 as a function of the bare interaction U and band width, we use Eq. (26), which yields

$$2UN(0) = -\left[\ln\frac{\Delta_0}{2W} + \left(\frac{\Delta_0}{2W}\right)^2 C\right]^{-1}, \tag{34}$$

where

$$C = 1 + (\zeta + \beta)\left[I_0 + \frac{1}{2UN(0)} - \frac{\Delta_0^2}{\sqrt{\Omega_0^2 - \Delta_0^2}(\Omega_0 + \sqrt{\Omega_0^2 - \Delta_0^2})}\right]. \tag{35}$$

To find the mean-field solution, we must omit the term in $(\Delta_0/W)^2$ in the right-hand side of Eq. (34). Since we have $C > 0$ [Eq. (35)], the solution of (34) is smaller in magnitude than the mean-field one, which reflects partial suppression of SDW ordering by quantum spin fluctuations. In the weak-coupling limit the term $(\zeta + \beta)/2UN(0)$ dominates in (35), and (34) reduces to

$$1 + \delta = 2UN(0)\ln(2W/\Delta_0).$$

As can easily be seen, the role of spin fluctuations reflected by the quantity δ [see (32)] reduces, in fact, to attenuation of the bare coupling constant in a certain frequency range.

5. CONCLUSION

The scheme of allowing self-consistently for quantum spin fluctuations in antiferromagnets with a spin density wave, suggested above, in principle allows different macroscopic characteristics (for example, the sublattice magnetization or SDW amplitude) to be calculated using numerical methods for the solution of Eqs. (10)–(14).

The SDW amplitude S calculated as

$$S = \text{Sp}\int\frac{d^3p}{(2\pi)^3}\int\frac{d\varepsilon}{2\pi i}G_{12}^{\sigma}(\mathbf{p}, \varepsilon)\sigma_z$$

with $\Delta(\varepsilon)$ and $Z(\varepsilon)$ from (22) and (23) is mainly determined by the high-frequency limit of $\Delta(\varepsilon)$, i.e., by the quan-

tity Δ_∞. At the same time low-frequency spectral characteristics, e.g., the gap in the density of states together with the absorption edge, are given by Δ_0.

The density of states calculated in the usual manner as

$$\rho(\varepsilon) = N(0)\mathrm{Re}\left(\frac{|\varepsilon|}{\sqrt{\varepsilon^2 - \Delta^2(\varepsilon)}}\right)$$

with the ansatz (22) has a gap, which is a consequence of the presence of long-range order. The discontinuity in $\rho(\varepsilon)$ at the frequency Ω_0 is related to the choice of the ansatz (22) and has no physical meaning.

In comparison with the schemes suggested in Refs. 4, 6, 8, and 9 to allow for spin fluctuations, the requirement formulated in (14) that the Goldstone theorem be satisfied and allowance for retardation of effective potentials, as follows from (29), lead to enhancement of spin-fluctuation effects by the factor $U/U^* > 1$. Therefore Δ_0 in this scheme is smaller than the relevant parameters in the theories which are not self-consistent in terms of spin fluctuations, which allows larger coupling constants U to be treated using the smallness of the parameter Δ_0/W.

Note that for the systems in which the Fermi surface has anisotropic parts (in particular, for the system considered in Ref. 6) the method of solution of Eqs. (8) and (12)–(14) used in the present study is inapplicable due to impossibility of straightforward changing from integration over momentum to integration over frequency.

APPENDIX

It follows from (30) and (31) that

$$\zeta = \frac{3}{\pi^2}\int_1^\infty \frac{(x+4)dx}{(x+2)^2\sqrt{x^2-1}}, \qquad \text{(A1)}$$

and

$$\beta = \frac{3}{\pi^2}\left[\int_1^\infty \frac{\ln(1+2/x)dx}{\sqrt{x^2-1}} + \int_1^\infty \frac{dx}{(x+2)\sqrt{x^2-1}}\right]. \qquad \text{(A2)}$$

We have used here the following estimates:

$$v_F \sim 2Wa, \quad N(0) \sim 1/2Wa^3,$$

where a is the lattice constant.

The integral (A1) and the second term in (A2) are easily reduced to tabulated integrals. To estimate the first term in (A2), which is not expressible in terms of elementary functions, we split the integration interval into two regions: $1 < x < 2$ and $x > 2$. In the first region the main contribution comes from $x \sim 1$. In the second region we expand the logarithm in a power series. As a result, we have $\zeta = 0.37$, $\beta = 0.99$.

[1)] Here and in what follows we mean invariance with respect to SDW polarization vector rotations.

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