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Current carriers in a quantum two-dimensional antiferromagnet

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Abstract. The interaction of current carriers with localized moments in a two-dimensional Heisenberg antiferromagnet is considered in the s - d exchange model (both using perturbation theory and in the limit of infinitely large s - d parameter) and in the t - J model. It is demonstrated that at low $T \ll J$ the electron spectrum has the same structure as in the ground state despite the absence of long-range magnetic order. The influence of spin dynamics on the manifestations of the Kondo effect is investigated, and the corresponding T -linear term in resistivity is obtained. The problem of the formation of a narrow quasi-particle peak near the band bottom due to spin dynamics is discussed. Using the Schwinger boson or Dyson–Maleev representation yields, unlike the linear magnon theory, an appreciable bare bandwidth of a hole in the t - J model, which is proportional to the sublattice magnetization quantum contraction.

1. Introduction

The idea about the decisive role of strong inter-electron correlations and, in particular, of local magnetic moments in the problem of high- T_c superconductivity, put forward by Anderson [1], has stimulated great interest in the problem of electron-spin interactions in two-dimensional (2D) systems (see [2–4]). In these papers, the t - J model (the $U = \infty$ Hubbard model with inclusion of the direct Heisenberg interaction J) at temperature $T = 0$ was employed. The standard description of a 2D Heisenberg antiferromagnet at finite T is quite different from that at $T = 0$ because of destruction of the long-range magnetic order. One might suppose that the structure of the electron spectrum at $T \ll J$ is weakly disturbed by thermal fluctuations since the correlation length ξ is exponentially large [5, 6] and the short-range order is very strong. However, formal treatment of the finite- T case is not trivial. Recent works on 2D Heisenberg magnets using the Schwinger-boson technique [7–9] or the Dyson–Maleev representation [10] give the possibility to resolve this problem. This is one of the issues of the present paper. Besides the s - d exchange model with the s - d parameter $I \rightarrow \pm \infty$ (which includes the t - J model as a particular case) we consider the broad-band s - d model using perturbation theory in I . (In this connection, it should be noted that both the narrow-band and the broad-band limit may be realized for different electron groups in copper oxide layers.)

The structure of the paper is as follows. In section 2 we describe the Schwinger-boson formalism and discuss the second-order correction to the electron self-energy (in

particular, the antiferromagnetic gap). In section 3 we consider the corresponding many-electron corrections to the density of states. Besides that, we calculate the third-order Kondo contributions, which turn out to be more important. In section 4 we treat the problem of the formation of a quasi-particle band near the band bottom due to spin dynamics in the broad band s - d model. In section 5 we consider the same problem in the narrow-band s - d model and t - J model. In appendix 1 we carry out a comparison with approaches using the Dyson–Maleev and Holstein–Primakoff representations, and in appendix 2 we analyse the structure of the perturbation series in the s - d model.

2. The Schwinger-boson representation and the second-order correction to the electron self-energy

We proceed with the Hamiltonian of the s - d exchange model

$$H = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} - I \sum_{i\sigma\sigma'} S_i c_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma'} + H_d \quad (1)$$

where $c_{k\sigma}^\dagger$ are the conduction electron annihilation operators, S_i are the localized spin operators, $\boldsymbol{\sigma}$ are the Pauli matrices, I is the s - d exchange parameter,

$$H_d = J \sum_{\langle ij \rangle} S_i S_j = \frac{1}{2} \sum_q J_q S_{-q} S_q \quad (2)$$

is the Heisenberg Hamiltonian. When describing the antiferromagnetic state within approaches [7–10], no anomalous averages $\langle S_Q \rangle$ (sublattice magnetization) occur, and the long-range magnetic order is manifested by the delta-like singularity of the pair correlation function $\langle S_q S_{-q} \rangle$ at $q = Q$ ($Q = (\pi, \pi)$ for a square lattice). Such a picture of the ground state of an antiferromagnet was discussed earlier in detail in [11]. For 2D systems this description turns out to be suitable since it yields a ‘smooth’ transition to the case of finite temperatures.

Consider the Schwinger representation of spin operators

$$S_i = \frac{1}{2} \sum_{\sigma\sigma'} b_{i\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} b_{i\sigma'} \quad (3)$$

$$\sum_{\sigma} b_{i\sigma}^\dagger b_{i\sigma} = 2S \quad (4)$$

where $b_{i\sigma}$ are Bose operators, and S is the value of the localized spins. In the mean-field approximation the constraint (4) is taken into account by introducing the Lagrange multiplier λ , which is independent of site index i , and the anomalous averages describing the singlet pairing are constructed from $\langle b_{i\uparrow} b_{j\downarrow} \rangle$. The onset of long-range ordering corresponds to the Bose–Einstein condensation for quasi-momenta $k = \pm Q/2$. To treat this formally one may include the interaction with an external magnetic field h [8]. Using the Bogoliubov transformation

$$\begin{aligned} b_{Q/2+k\uparrow} &= \cosh \theta_k \alpha_k - \sinh \theta_k \beta_{-k}^\dagger \\ b_{Q/2-k\downarrow} &= \cosh \theta_k \beta_{-k} - \sinh \theta_k \alpha_k^\dagger \end{aligned} \quad (5)$$

we diagonalize the Hamiltonian (2) to obtain

$$H_d = \sum_k (E_{k\alpha} \alpha_k^\dagger \alpha_k + E_{k\beta} \beta_k^\dagger \beta_k) + \text{const} \quad (6)$$

where, for the square lattice,

$$E_{k\alpha,\beta} = E_k \mp (\frac{1}{2}\hbar - 2J\langle S^z \rangle) \quad E_k = (\lambda^2 - \gamma_k^2)^{1/2} \quad (7)$$

$$\sinh 2\theta_k = \gamma_k/E_k \quad \cosh 2\theta_k = \lambda/E_k \quad (8)$$

$$\gamma_k = \frac{1}{2}\gamma(\sin k_x + \sin k_y). \quad (9)$$

Equations for γ and λ , which are obtained from (4), (5) and (8), read

$$2S + 1 = \frac{1}{N} \sum_k \frac{\lambda}{E_k} (1 + N_{k\alpha} + N_{k\beta}) \quad (10)$$

$$1 = \frac{1}{2N} \sum_k \frac{J}{E_k} (\sin k_x + \sin k_y)^2 (1 + N_{k\alpha} + N_{k\beta}) \quad (11)$$

where $N_{k\alpha,\beta} = N(E_{k\alpha,\beta})$ are the Bose distribution functions and N is the number of lattice sites.

Consider the case where $T = 0$. Then $\lambda = \gamma$ and, for $\hbar > 0$, $N_{k\alpha}$ (but not $N_{k\beta}$) contains a condensate term at $E_{k\alpha} = 0$, i.e.

$$k = \pm Q/2 \quad E_k = \frac{1}{2}\hbar - 2J\langle S^z \rangle \propto \hbar. \quad (12)$$

Then we have

$$N_{\pm Q/2} = N\langle S^z \rangle = NE_{Q/2} n_B / \lambda \quad (13)$$

with $2n_B$ being the density of condensed bosons. Equation (10) yields

$$n_B = S + \frac{1}{2} - \frac{1}{2N} \sum_k [1 - \frac{1}{4}(\sin k_x + \sin k_y)^2]^{-1/2} = S - 0.197 \quad (14)$$

so that n_B equals the sublattice magnetization of the Néel antiferromagnet with account of the zero-point spin-wave correction.

At finite T , the spectrum contains a gap and the condensate is absent. Then we may put $\hbar = 0$, $N_{k\alpha,\beta} = N_k$ from the beginning.

We calculate the one-electron retarded anticommutator Green function

$$G_k^\sigma(E) = \langle\langle c_{k\sigma} | c_{k\sigma}^\dagger \rangle\rangle_E = [E - \varepsilon_k - \Sigma_k(E)]^{-1}. \quad (15)$$

To second order in I we obtain for the self-energy (cf [12])

$$\Sigma_k(E) = \frac{I^2}{N} \sum_q \int_{-\infty}^{\infty} d\omega K_{q\omega} \left(\frac{1 - f_{k+q}}{E - \varepsilon_{k+q} + \omega} + \frac{f_{k+q}}{E - \varepsilon_{k+q} - \omega} \right) \quad (16)$$

where $f_k = f(\varepsilon_k)$ is the Fermi function, $K_{q\omega}$ is the spectral density for the Hamiltonian H_d ,

$$\begin{aligned} K_{q\omega} &= -\frac{1}{\pi} N(\omega) \text{Im}(\langle\langle S_q^+ | S_{-q}^- \rangle\rangle_\omega + \langle\langle S_q^z | S_{-q}^z \rangle\rangle_\omega) \\ &= \sum_{mn} w_m |(S_q)_{mn}|^2 \delta(\omega + E_n - E_m) \end{aligned}$$

$$H_d|m\rangle = E_m|m\rangle \quad w_m = \exp(-E_m/T)/\text{Tr} \exp(-H_d/T). \quad (17)$$

Using the spectral representation (17) we obtain $K_{q\omega}$ from the spin Green functions, which are expressed in terms of polarization operators of non-interacting bosons α and β . The result reads

$$K_{q\omega} = \frac{1}{4N} \sum_k \sum_{\mu, \nu = \alpha, \beta} \{ \cosh^2(\theta_k - \theta_{k+q}) N_{k\mu} (1 + N_{k+q, \nu}) \delta(\omega + E_{k+q, \nu} - E_{k\mu}) \\ + \frac{1}{2} (1 + \delta_{\mu\nu}) \sinh^2(\theta_k - \theta_{k+q}) [N_{k\mu} N_{k+q, \nu} \delta(\omega - E_{k+q, \nu} - E_{k\mu}) \\ + (1 + N_{k\mu})(1 + N_{k+q, \nu}) \delta(\omega + E_{k+q, \nu} + E_{k\mu})] \}. \quad (18)$$

As follows from (13), at $T = 0$, $h \rightarrow 0$, the spectral density contains the delta-like contribution

$$\delta K_{q\omega} = \frac{3}{2} n_B^2 N \delta_{qQ} \delta(\omega). \quad (19)$$

The factor of $3/2$ in (19) is an artifact of the Schwinger-boson approach (which yields $\langle S_i^2 \rangle = \frac{3}{2} S(S+1)$, thereby violating the sum rule because of an approximate treatment of the constraint (4) in the mean-field approximation); it is absent when using, e.g., the Dyson–Maleev representation (see appendix 1). Hereafter we omit this factor when considering electron properties. Then we get from (16) and (19)

$$\delta \Sigma_k(E) = I^2 n_B^2 / (E - \varepsilon_{k+Q}). \quad (20)$$

After substituting this contribution into (15) we obtain the standard antiferromagnetic gap in the electron spectrum.

Now we treat the case of finite T . At $k \rightarrow \pm Q/2$ we have [8]

$$E_k^2 = \frac{\lambda^2}{2} [(k \mp Q/2) + \xi^{-2}] \quad (21)$$

where

$$\xi \propto \exp[(\pi\lambda/2T)n_B] \quad (22)$$

is the correlation length. At $q = Q$ the integral in (18) is almost divergent at the points $k = \pm Q/2$ (with the cut-off $|k \mp Q/2| \sim \xi^{-1}$). Expanding $N_k \approx T/E_k$ we write down the corresponding singular contribution in the form

$$\delta K_{q\omega} = \frac{3}{2} [(2T/\pi\lambda) \ln \xi]^2 \Delta_q \Delta_\omega = \frac{3}{2} n_B^2 \Delta_q \Delta_\omega \quad (23)$$

where Δ_q and Δ_ω are $\delta(q - Q)$ and $\delta(\omega)$ like functions smeared on the scales ξ^{-1} and $\omega_\xi \sim \lambda/\xi \sim J/\xi$, respectively. The quantity ω_ξ coincides with the characteristic scaling frequency in [6].

At $T \ll J$ one has $\omega_\xi \ll T$ and we may neglect the smearing, so that the description of the antiferromagnetic gap by (20) holds despite the absence of long-range order. The temperature dependence of the gap may be obtained if one retains the terms of the next order in $\ln \xi$. Using for ξ the result of [8] yields corrections to n_B that are proportional to $T \ln T$. However, the more accurate consideration [6] shows that the pre-exponential factor in (22) does not depend on T . Then we have in (20) $n_B \rightarrow S_{\text{ef}}(T)$ with

$$S_{\text{ef}}(T) = n_B (1 - \text{const} \cdot T/J). \quad (24)$$

To obtain an analogue of the term describing the interaction of an electron with

antiferromagnetic spin waves we have to consider the expression (18) at $|\mathbf{q} - \mathbf{Q}| \gg \xi^{-1}$. Picking out the contributions 'linear' in n_B , i.e. putting $E_k \rightarrow 0, N_k = T/E_k$, but retaining N_{k+q} and vice versa, we derive

$$\begin{aligned} \delta_1 K_{q\omega} = & \frac{T}{E_{q+Q/2}} \frac{1}{N} \sum_k \frac{\lambda^2 - \gamma_k \gamma_{k+q}}{E_k^2} [(1 + N_{q+Q/2})\delta(\omega + E_{q+Q/2}) \\ & + N_{q+Q/2} \delta(\omega - E_{q+Q/2})] \approx \frac{1}{2} n_B \left(\frac{1 - \varphi_q}{1 + \varphi_q} \right)^{1/2} \\ & \times \{ [1 + N(\omega_q)] \delta(\omega + \omega_q) + N(\omega_q) \delta(\omega - \omega_q) \} \end{aligned} \quad (25)$$

where, for $q, |\mathbf{q} - \mathbf{Q}| \gg \xi^{-1}$,

$$\omega_q = \lambda(1 - \varphi_q^2)^{1/2} \approx E_{q+Q/2} \quad \varphi_q \equiv \frac{1}{2}(\cos q_x + \cos q_y) \quad (26)$$

so that ω_q coincides with the magnon frequency of the square-lattice antiferromagnet with λ being the renormalized spin-wave bandwidth.

Substituting (20) and (25) into (16) gives

$$\begin{aligned} \Sigma_k(E) = & \frac{I^2 S_{\text{eff}}^2(T)}{E - \varepsilon_{k+Q}} + \frac{I^2}{N} n_B \sum_{q, |\mathbf{q}-\mathbf{Q}| > \xi^{-1}} \left(\frac{1 - \varphi_q}{1 + \varphi_q} \right)^{1/2} \\ & \times \left(\frac{1 - f_{k+q} + N(\omega_q)}{E - \varepsilon_{k+q} - \omega_q} + \frac{f_{k+q} + N(\omega_q)}{E - \varepsilon_{k+q} + \omega_q} \right). \end{aligned} \quad (27)$$

This expression has the same structure as that for the usual conducting antiferromagnet (cf [13, 14]). Both the dependence $S_{\text{eff}}(T)$ and the contributions due to the Bose distribution functions result in corrections to the electron spectrum of order $I^2(T/J)$.

3. Many-electron contributions to the electron self-energy and the Kondo anomalies

The Fermi distribution functions in (27) lead to a sharp energy dependence of the electron density of states

$$g(E) = -\frac{1}{\pi} \sum_k \text{Im } G_k(E) \quad (28)$$

in the region $|E| \ll JS$ near the Fermi level ($E = 0$). The corresponding 'non-quasi-particle' contribution [15, 16] has the form

$$\begin{aligned} \delta g(E) = & -\frac{1}{\pi} \sum_k \frac{\text{Im } \Sigma_k(E)}{(E - \varepsilon_k)^2} = \frac{1}{N} \sum_{qk} \frac{I^2 n_B}{(E - \varepsilon_k)^2} \left(\frac{1 - \varphi_q}{1 + \varphi_q} \right)^{1/2} \\ & \times \{ [1 - f_{k+q} + N(\omega_q)] \delta(E - \varepsilon_{k+q} - \omega_q) \\ & + [f_{k+q} + N(\omega_q)] \delta(E - \varepsilon_{k+q} + \omega_q) \}. \end{aligned} \quad (29)$$

At $T = 0, |E| \ll \lambda$ we obtain

$$\delta g(E) \propto I^2 n_B \sum_q |\mathbf{q}| [f(E - \lambda q/\sqrt{2}) + f(-E - \lambda q/\sqrt{2})] \propto I^2 n_B (E/\lambda)^2. \quad (30)$$

Such a dependence may be observed in transport properties and tunnelling experiments.

It should be noted that an analogous contribution to $g(E)$ occurs in second order in the interaction with acoustic phonons.

Consider now the terms of third order in I which describe the Kondo effect and lead to a stronger dependence of $\Sigma(E)$. They were discussed in [12] for a 3D antiferromagnet. To treat the 2D case we may use the general expression for the Kondo contribution to the self-energy in the periodic s-d model, valid for arbitrary spin dynamics (see equation (14) in [12]). This may be rewritten in the suitable form.

$$\begin{aligned} \delta\Sigma_k^{(3)}(E) &= i\varepsilon_{\alpha\beta\gamma} \frac{I^3}{N^2} \sum_{pq} f_{k+q} \int_0^\infty dt \int_0^\infty dt' \{ \exp[i(E - \varepsilon_{k+q})t] \\ &\quad - \exp[i(\varepsilon_{k+p-q} - \varepsilon_{k+q})t] \} \exp[i(E - \varepsilon_{k+p})t'] \\ &\quad \times \langle [S_{-q}^\alpha(t), S_{q-p}^\beta] S_p^\gamma(t') \rangle_d \end{aligned} \quad (31)$$

where $\varepsilon_{\alpha\beta\gamma}$ is the unit antisymmetric tensor, $S^\alpha(t)$ and $\langle \dots \rangle_d$ stand for the Heisenberg representation and the average with the Hamiltonian H_d . The dependence $S_p^\gamma(t')$ may be neglected since it is not important for cutting off the logarithmic divergence. Using the rotational symmetry, the Schwinger-boson representation (3) and (5)–(7), we derive

$$\begin{aligned} \langle [S_{-q}^\alpha(t), S_{q-p}^\beta] S_p^\gamma \rangle_d &= - (i/2) \varepsilon_{\alpha\beta\gamma} \langle [S_{-q}^+(t), S_{q-p}^-] S_p^z \rangle_d \\ &= - (i/4) \varepsilon_{\alpha\beta\gamma} \frac{1}{N} \sum_k \left[\left(\frac{\lambda^2}{E_k E_{k+q}} + 1 \right) \exp[i(E_{k+q} - E_k)t] \right. \\ &\quad \left. - \frac{1}{2} \left(\frac{\lambda}{E_k} + 1 \right) \left(\frac{\lambda}{E_{k+q}} - 1 \right) \exp[-i(E_{k+q} + E_k)t] - \frac{1}{2} \left(\frac{\lambda}{E_k} - 1 \right) \left(\frac{\lambda}{E_{k+q}} + 1 \right) \right. \\ &\quad \left. \times \exp[i(E_{k+q} + E_k)t] \right] \langle (b_{k+q, \uparrow}^\dagger b_{k+q-p, \uparrow} - b_{k+p, \downarrow}^\dagger b_{k, \downarrow}) S_p^z \rangle_d. \end{aligned} \quad (32)$$

Neglecting contributions of the order of the magnon frequency, the expression in the large square brackets may be replaced by

$$\exp[i(E_{k+q} - E_k)t] + \cos[(E_{k+q} + E_k)t].$$

Picking out in (32) the ‘singular’ term proportional to n_B^2 , we get

$$\delta\Sigma_k^{(3)}(E) = 2n_B^2 \frac{I^3}{N} \sum_{k'} \frac{f_{k'}(E - \varepsilon_{k'})}{(E - \varepsilon_{k'})^2 - \omega_{k-k'}^2} [(\varepsilon_{k'} - \varepsilon_{k'+Q})^{-1} - (E - \varepsilon_{k+Q})^{-1}]. \quad (33)$$

This expression coincides with equation (29) in [12], obtained for the usual Néel state. Averaging over the angle between the vectors k and k' and calculating the imaginary part of the average, we derive for the self-energy on the Fermi surface ($\varepsilon_k = 0$) at $|E| < \bar{\omega}$ ($\bar{\omega} \sim Jk_F$ is a characteristic magnon frequency)

$$\begin{aligned} \text{Im} \Sigma_k^{(3)}(E) &= -2\pi S_{\text{eff}}^2(T) \frac{I^3}{N} \sum_{k'} \frac{f_{k'} \text{sgn}(E - \varepsilon_{k'})}{[\bar{\omega}^2 - (E - \varepsilon_{k'})^2]^{1/2}} \\ &\quad \times [(\varepsilon_{k'} - \varepsilon_{k'+Q})^{-1} - (E - \varepsilon_{k+Q})^{-1}] \approx -2\pi I^3 S_{\text{eff}}^2(T) \\ &\quad \times (\pi/2 - \sin^{-1} |E|/\bar{\omega}) (\varepsilon_{k+Q}^{-1} - \langle \varepsilon_{k'+Q}^{-1} \rangle_F) \end{aligned} \quad (34)$$

where $\langle \dots \rangle_F$ stands for the average in k' over the Fermi surface. Thus, owing to spin dynamics ($\omega_q \propto q$ at $q > \xi^{-1}$), we have in 2D the linear energy dependence for the

damping of electron states with $|E| \ll \bar{\omega}$, in contrast with the usual Kondo behaviour $\text{Im } \delta\Sigma(E) \propto \ln|E|$ (which takes place at $|E| \gg \omega$). As follows from the analytical properties of $\Sigma(E)$, the dependence $|E| = E \text{sgn } E$ in $\text{Im } \Sigma(E)$ corresponds to the contribution $E \ln|E|$ in $\text{Re } \Sigma(E)$. (In three dimensions, we have $\text{Im } \delta\Sigma(E) \propto |E|E$, $\text{Re } \delta\Sigma(E) \propto E^2 \ln|E|$ [12].) The contribution of order $E \ln|E/J|$ in $\text{Re } \Sigma_F(E)$ leads to the $T \ln T$ dependence of the Fermi surface cross sections. This may be observed in investigations of the de Haas–van Alphen effect.

The contribution to the conductivity $\sigma(T)$ due to the ‘Kondo’ scattering may be estimated as ($v_k = \partial \varepsilon_k / \partial k$)

$$\begin{aligned} \delta\sigma(T) &\propto \frac{1}{N} \sum_k \left(-\frac{\partial f_k}{\partial \varepsilon_k} \right) v_k^2 [-\text{Im } \Sigma_k^{(3)}(E)] \\ &\propto I^3 n_B^2 (1 - \text{const} \cdot T) (\langle v_k^2 / \varepsilon_{k+Q} \rangle_F - \langle v_k^2 \rangle_F \langle \varepsilon_{k+Q}^{-1} \rangle_F). \end{aligned} \tag{35}$$

This term is linear in T at $T \ll J$ owing to both the dependence $S_{\text{eff}}(T)$ and the energy dependence of the damping. The sign of $\delta\sigma(T)$ depends on the sign of I and on the shape of the Fermi surface.

Similar to the case of one Kondo impurity [17], the ‘Kondo’ terms may be summed up in the ‘parquet’ approximation, which is reliable for $I > 0$ (see also appendix 2). This does not change the dependence of non-analytic corrections to $\Sigma(E)$, which clearly contradicts the Fermi liquid theory (where the leading non-analytic contribution $\delta\Sigma(E) \propto E^3 \ln E$ in any dimensions [18]). For $I < 0$, one might assume that the local moments are compensated and the Fermi-liquid picture is restored below some temperature T_K^* , which is an analogue of the Kondo temperature (cf the situation in heavy-fermion systems). On the other hand, it is possible that the Fermi-liquid theory is violated up to $T = 0$, similar to the situation in a conducting ferromagnet [15, 16].

4. Formation of the quasi-particle band in the broad-band s–d model

Now we investigate more accurately the structure of the electron spectrum near the band bottom for a single current carrier taking into account spin dynamics. This problem was considered for the t – J model in [2–4]. Investigation of the broad-band s–d model, where a well defined perturbation expansion exists, before the narrow-band case seems to be instructive.

Performing summation of higher-order terms in the ‘non-crossing’ approximation (see appendix 2) we obtain for the self-energy

$$\begin{aligned} \Sigma_k(E) &= \Phi_k(E) - I^2 n_B^2 / \Phi_{k+Q}(E) \\ \Phi_k(E) &= \frac{I^2}{N} \sum_{|q-Q| > \xi^{-1}} \int_{-\infty}^{\infty} d\omega K_{q\omega} G_{k+q}(E + \omega). \end{aligned} \tag{36}$$

For $T = 0$ we have

$$\Phi_k(E) = \frac{I^2}{N} n_B \sum_q \left(\frac{1 - \varphi_q}{1 + \varphi_q} \right)^{1/2} G_{k+q}(E - \omega_q). \quad (37)$$

By analogy with the consideration in [2] we use the 'dominant pole' approximation

$$G_k(E) = a_k / (E - \varepsilon_k^*) + G_{\text{inc}}(k, E) \quad (38)$$

$$a_k = \left(1 - \frac{\partial}{\partial E} \text{Re} \Sigma_k(E) \Big|_{E=\varepsilon_k^*} \right)^{-1} \quad (39)$$

where a_k is the residue at the pole,

$$\varepsilon_k^* \approx \varepsilon_{\text{min}} + a_k(\varepsilon_k - \varepsilon_{\text{min}}) \approx \varepsilon_{\text{min}} + a|t|k^2$$

is the spectrum of new quasi-particles, G_{inc} is an incoherent contribution to the Green function and t is the transfer integral. Near the band bottom ($k = 0$, $E = \varepsilon_{\text{min}}$), $\Phi_{k+Q}(E)$ does not lead to divergences and the second term in (36) may be neglected (it is principal near the band top $k = Q$, $E = \varepsilon_{\text{max}}$). Substituting (38) into (36) we obtain in 2D the estimation

$$a^{-1} - 1 = \frac{I^2}{N} \sum_q \frac{n_B a q / \sqrt{8}}{(\lambda q / \sqrt{2} + a|t|q^2)^2} \propto \frac{I^2}{J|t|}. \quad (40)$$

Then at $I^2 \gg J|t|$ we have the 'heavy-fermion' situation with

$$m^*/m = a^{-1} \sim I^2/J|t| \gg 1. \quad (41)$$

In the three-dimensional case we have

$$a^{-1} - 1 \propto (I^2 S / t^2) \ln |t| / JS \quad (42)$$

(similar divergences were treated in [19]).

The terms with the Bose functions in (25) yield corrections to a^{-1} , which are proportional to $T/(J\xi)$, i.e. exponentially small. Therefore the consideration of the quasi-particle band formation in the present and next sections holds at finite $T \ll J$.

Thus the picture of the electron spectrum in a 2D antiferromagnet near the band bottom is as follows. At small $|I| \ll |Jt|^{1/2}$ the spectral density $(-1/\pi) \text{Im} G_k(E)$ is concentrated in the delta-like pole contribution, whereas the incoherent part is small (of order $I^2/(Jt^2)$). As $|I|$ increases, the spectral weight passes into the incoherent contribution, the effective mass of the undamped quasi-particles becoming large. As we shall see in the following section, the results (40)–(42) are qualitatively valid even at $|I| \rightarrow \infty$ if we replace $|I| \rightarrow |t|/S$.

It is interesting to note that similar results may be obtained in the case of interaction of conduction electrons with acoustic phonons. Indeed, the corresponding self-energy may be obtained from the second term in (25) if we replace

$$I^2 n_B [(1 - \varphi_q)/(1 + \varphi_q)]^{1/2} \rightarrow \Lambda^2 q \quad q \rightarrow 0$$

where $\Lambda \propto \kappa$ is a constant of the electron–phonon interaction, $\kappa = (m/M)^{1/4}$ being the adiabatic parameter. Since the phonon frequency $\omega_q \propto \kappa^2$, the estimate for the residue reads

$$a^{-1} - 1 \sim \Lambda^2 / (\bar{\omega}|t|) \sim 1.$$

Let us carry out a comparison with the case of the usual paramagnet without strong

antiferromagnetic correlations. In the latter case, the matrix element of the electron-spin interaction is a constant (instead of $q^{1/2}$ at $q \rightarrow 0$), and the spin frequency is proportional to q^2 and imaginary,

$$K_{q\omega} = \frac{S(S+1)}{\pi} \frac{D_s q^2}{\omega^2 + (D_s q^2)^2} \tag{43}$$

where $D_s \sim JS^2$ is the spin diffusion constant. Then the *ansatz* (38) gives

$$a^{-1} = 1 + \frac{S(S+1)I^2}{\pi N} \sum_q \frac{a(aq^2|t| - D_s q^2)}{[(aq^2t)^2 + (D_s q^2)^2]^2}$$

which results in $a = 0$ for both the 2D and the 3D cases because of the divergence of the integral at small q . This demonstrates the significance of well defined ‘magnons’ for the existence of undamped electron states. We can search for damped quasi-particles if we replace in (39) $\epsilon_k^* \rightarrow \epsilon_k^* - i\Gamma_k$. The damping Γ_k in the dominant pole approximation may be estimated as

$$\Gamma_k = -\text{Im} \int_{-\infty}^{\infty} d\omega \frac{I^2}{N} \sum_q K_{q\omega} \frac{a_{k+q}}{\epsilon_k^* - \epsilon_{k+q}^* + \omega} \tag{44}$$

Then we obtain at $k \rightarrow 0$

$$\Gamma_k \propto \frac{I^2 JS^3}{at^2} \times \begin{cases} |\ln k| & \text{2D} \\ 1 & \text{3D.} \end{cases} \tag{45}$$

Solving the equation for a gives

$$a^{-1} \propto \begin{cases} (|t|/JS)^{1/2} & \text{2D} \\ 1 + \text{const}(I^2 S/|t|J)^{1/2} & \text{3D.} \end{cases} \tag{46}$$

(In 2D we neglect logarithmic corrections.) Thus the residue of the damped quasi-particles may also be small. However, it is difficult to separate them from the background of the incoherent contribution.

5. The electron spectrum in the narrow-band *s-d* and *t-J* models

Now we pass to the limit of the strong interaction of conduction electrons with local moments. For $|I| \rightarrow \infty$ we have to use in the Hamiltonian the many-electron *X*-operator representation [20], which yields

$$H = \sum_{k\sigma} \epsilon_k g_{k\sigma\alpha}^\dagger g_{k\sigma\alpha} + H_d \quad \alpha = \text{sgn } I \tag{47}$$

$$g_{i\sigma+}^\dagger = \sum_{M=-S}^S \left(\frac{S + \sigma M + 1}{2S + 1} \right)^{1/2} |iM + \sigma/2, +\rangle \langle iM| \tag{48}$$

$$g_{i\sigma-}^\dagger = \sum_{M=-S}^S \left(\frac{S - \sigma M}{2S + 1} \right)^{1/2} |iM + \sigma/2, -\rangle \langle iM|$$

where $|iM\rangle$ is the empty state on site i with the localized spin projection M , and $|i\mu, \alpha\rangle$

is the state with a conduction electron, the total spin on the site $S + \alpha/2$ and its projection μ . The t - J model, widely used in the theory of high- T_c superconductivity,

$$H = \sum_k t_k X_k^{0\alpha} X_k^{\sigma 0} + H_d \tag{49}$$

($|i0\rangle$ is the hole state) is a particular case of the narrow-band model with $I \rightarrow -\infty$. Indeed, one can see that the Hamiltonian (49) coincides with (47) for $\alpha = -$, $S = 1/2$ if we replace $\epsilon_k \rightarrow 2t_k$.

The equation of motion for the one-particle Green function

$$G_{k\alpha}^\sigma(E) = \langle\langle g_{k\alpha\sigma} | g_{k\alpha\sigma}^+ \rangle\rangle_E \tag{50}$$

has the form (cf (21))

$$(E - P_\alpha \epsilon_k) G_{k\alpha}^\sigma(E) = P_\alpha + \frac{\alpha}{2S+1} \frac{1}{N} \sum_q \epsilon_{k+q} B_{kq\alpha}^\sigma(T) \tag{51}$$

$$B_{kq\alpha}^\sigma(E) = \langle\langle \sigma S_{-q}^z g_{k+q,\sigma\alpha} + S_{-q}^{-\sigma} g_{k+q,-\sigma\alpha} | g_{k\alpha}^+ \rangle\rangle_E \tag{52}$$

$$P_+ = \frac{S+1}{2S+1}, \dots, P_- = \frac{S}{2S+1}. \tag{53}$$

Expanding spin operators in the eigenstates of the Hamiltonian H_d (cf [12]) and carrying out the decoupling in the equation for B (which is possible to first order in the inverse nearest-neighbour number $1/z$) we get

$$B_{kq\alpha}(E) = \int_{-\infty}^{\infty} d\omega \frac{K_{q\omega}/(2S+1)}{E - P_\alpha \epsilon_{k+q} + \omega} [1 + \epsilon_k G_{k\alpha}(E)]. \tag{54}$$

Substituting (54) into (51), picking out the singular contribution and replacing the energy denominators by the exact Green functions (the latter may be justified, similar to the case of the broad-band s - d model, within perturbation theory in $1/z$, see [21]), we obtain

$$G_{k\alpha}(E) = \left(Z_{k\alpha}(E) + \frac{n_B^2 \epsilon_{k+Q}/(2S+1)^2}{E - Z_{k+Q,\alpha}(E) \epsilon_{k+Q}} \right) \times \left(E - Z_{k\alpha}(E) \epsilon_k - \frac{n_B^2 \epsilon_k \epsilon_{k+Q}/(2S+1)^2}{E - Z_{k+Q,\alpha}(E) \epsilon_{k+Q}} \right)^{-1} \tag{55}$$

$$Z_{k\alpha}(E) = P_\alpha + \frac{1}{N} \sum_{|q-Q|>\xi-1} \frac{\epsilon_{k+q}}{(2S+1)^2} \times \int_{-\infty}^{\infty} d\omega K_{q\omega} Z_{k+q,\alpha}^{-1}(E+\omega) G_{k+q,\alpha}(E+\omega). \tag{56}$$

Consider first the ‘mean-field’ approximation where $Z_\alpha = P_\alpha$. Then the spectrum contains two quasi-particle bands (cf [13])

$$E_{1,2}(k) = \frac{P_\alpha}{2} (\epsilon_k + \epsilon_{k+Q}) \pm \left(\frac{P_\alpha^2}{4} (\epsilon_k - \epsilon_{k+Q})^2 + \frac{S_{\text{cf}}^2(T)}{(2S+1)^2} \epsilon_k \epsilon_{k+Q} \right)^{1/2}. \tag{57}$$

In the nearest-neighbour approximation where $\epsilon_k = 4t\varphi_k$, $\epsilon_{k+Q} = -\epsilon_k$ we have

$$E_{1,2}(k) = \pm \frac{\epsilon_k}{2S+1} \times \begin{cases} [S^2 - S_{\text{cf}}^2(T)]^{1/2} & \alpha = - \\ [(S+1)^2 - S_{\text{cf}}^2(T)]^{1/2} & \alpha = +. \end{cases} \tag{58}$$

At $T = 0$, $I < 0$ (and in the t - J model) the bandwidth in the mean-field approximation

does not vanish due to zero-point contraction of n_B only. This bandwidth is absent when using the Holstein–Primakoff representation (see [2, 3] and appendix 2). Note that in the t - J model the band is reduced by the factor of 0.4, which is not numerically small. At $I > 0$ the bandwidth does not vanish even when neglecting zero-point oscillations (i.e. in the large- z limit), although it is formally small in $1/2S$.

It should be mentioned that decomposing of Fermi-type X -operators into ‘holon’ and ‘spinon’ (i.e. Schwinger-boson) operators and calculating the holon Green function instead of the total Green function (50) do not give the narrowing of the bare band, which is unreasonable.

As well as in the broad-band case, the second term in (56) leads to qualitative changes in the structure of the spectrum near the band bottom due to spin dynamics. Using (25) we obtain at $T \rightarrow 0$

$$Z_{k\alpha}(E) = P_\alpha + \frac{n_B}{(2S + 1)^2} \frac{1}{N} \sum_q \left(\frac{1 - \varphi_q}{1 + \varphi_q} \right)^{1/2} \varepsilon_{k+q} \times Z_{k+q,\alpha}^{-1}(E - \omega_q) G_{k+q,\alpha}(E - \omega_q). \tag{59}$$

Then we may employ the dominant pole approximation

$$G_{k\alpha}(E) = Z_{k\alpha}(E) [a_k / (E - \varepsilon_k^*) + \tilde{G}_{inc}(k, E)] \tag{60}$$

and repeat the calculations of the previous section with the obvious replacement $I^2 \rightarrow (t/2S)^2$, corrections to Z_α in (60) not being important. We derive

$$a^{-1} - 1 \propto \begin{cases} |t|/(JS^2) & 2D \\ (1/S) \ln(|t|/JS) & 3D \end{cases} \tag{61}$$

which is in agreement with [2]. The presence of the finite bandwidth in the mean-field approximation does not influence the result (61), concerning the formation of a new quasi-particle band. However, it must be rather important for the incoherent part of the spectrum.

6. Conclusions

In the present paper we have demonstrated that introducing an RVB-type order parameter gives the possibility to describe the electron spectrum in systems with destroyed long-range order and to confirm the physically reasonable statement that the form of the spectrum is determined mainly by the short-range order. We have investigated electron states in a 2D quantum antiferromagnet with both weak and strong electron-spin interaction. It would be interesting to analyse in a similar way effects of short-range order in 3D magnets above the ordering temperature. The problem of destroyed (or almost destroyed) charge ordering in systems such as Sm_3Se_4 , Fe_3O_4 , etc [22], may also be mentioned in this connection.

We have calculated many-electron corrections to the electron spectrum. Most interesting are the results concerning the manifestations of the Kondo effect, which turn out to depend on the space dimensionality due to spin dynamics.

An important issue is the formation of the energy scale of order J in the electron spectrum. It may arise both due to many-electron Kondo-like divergences near E_F (see also [12]) and for a single current carrier near the band bottom. Simultaneous consideration of these effects, which may lead to a richer and more interesting picture of electron spectrum in 2D magnetic quantum systems, is an exciting problem.

Appendix 1. Comparison with Dyson–Maleev and Holstein–Primakoff representations

Consider an antiferromagnet divided into A and B sublattices. Following [10] we may introduce the Dyson–Maleev representation

$$\begin{aligned} S_l^- &= (2S)^{1/2} a_l^\dagger & S_l^+ &= (2S)^{1/2} [1 - (1/2S) a_l^\dagger a_l] a_l \\ S_l^z &= S - a_l^\dagger a_l & l &\in A \\ S_m^- &= (2S)^{1/2} b_m & S_m^+ &= (2S)^{1/2} b_m^\dagger [1 - (1/2S) b_m^\dagger b_m] \\ S_m^z &= -S + b_m^\dagger b_m & m &\in B \end{aligned} \quad (\text{A1.1})$$

with a_l, b_m the ideal-boson operators, and put on each site $\langle S^z \rangle = 0$, i.e.

$$\langle a_l^\dagger a_l \rangle = \langle b_m^\dagger b_m \rangle = S. \quad (\text{A1.2})$$

Using the Bogoliubov transformation

$$\begin{aligned} \alpha_k &= \cosh \theta_k \alpha_k - \sinh \theta_k \beta_k^\dagger \\ b_k^\dagger &= \cosh \theta_k \beta_k^\dagger - \sinh \theta_k \alpha_k \end{aligned} \quad (\text{A1.3})$$

we can diagonalize the Heisenberg Hamiltonian to obtain

$$\begin{aligned} H_d &= \sum_k' \omega_k (\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + \text{const} \\ \langle \alpha_k^\dagger \alpha_k \rangle &= \langle \beta_k^\dagger \beta_k \rangle = N(\omega_k) \equiv N_k \end{aligned} \quad (\text{A1.4})$$

and

$$\omega_k = (\lambda^2 - \gamma^2 \varphi_k^2)^{1/2} \quad \tanh 2\theta_k = \gamma \varphi_k / \lambda \quad (\text{A1.5})$$

where \sum_k' stands for the sum over the reduced Brillouin zone. The equations for λ and γ , which are similar to (10) and (11), are derived in [10]. At $T = 0$, $\lambda = \gamma + O(1/N)$, and the $1/N$ correction may describe, as well as inclusion of the external magnetic field (cf [7, 9]), the Bose condensate formation,

$$(1 - \gamma^2 / \lambda^2)^{-1/2} = N n_B. \quad (\text{A1.6})$$

As follows from (A1.1) and (A1.2), the transverse spin correlation function $\langle S_{-q}^- S_q^+ \rangle$ is identically zero, and the longitudinal correlation function has the delta-like singularity at $q = Q$. Calculating the corresponding spectral density gives

$$\begin{aligned} K_{q\omega} &= K_{q\omega}^{zz} = \frac{1}{N} \sum_k' \{ \cosh^2(\theta_k - \theta_{k+q}) N_k (1 + N_{k+q}) \delta(\omega + \omega_{k+q} - \omega_k) \\ &\quad + \frac{1}{2} \sinh^2(\theta_k - \theta_{k+q}) [N_k N_{k+q} \delta(\omega - \omega_{k+q} - \omega_k) \\ &\quad + (1 + N_k)(1 + N_{k+q}) \delta(\omega + \omega_{k+q} + \omega_k)] \} \end{aligned} \quad (\text{A1.7})$$

$$\delta K_{q\omega} = N n_B^2 \delta_{qQ} \delta(\omega). \quad (\text{A1.8})$$

Similar to (18), expression (A1.7) may be used to calculate the electron spectrum. Unlike (19), (A1.8) does not contain the factor $3/2$ since the Dyson–Maleev representation maintains the sum rule $\langle S_i^z \rangle = S(S + 1)$. On the other hand, it violates the rotational symmetry, in contrast with the ‘isotropic’ Schwinger-boson representation.

Now we consider the linear Holstein-Primakoff representation, where, instead of corresponding formulae in (A1.1),

$$S_l^+ = (2S)^{1/2} a_l \quad S_m^+ = (2S)^{1/2} b_m^+ \tag{A1.9}$$

Of course, it is applicable for $T = 0$ only.

For simplicity, we restrict ourselves to the treatment of the t - J model

$$H = t \sum_{\langle lm \rangle} (X_l^{0\sigma} Y_m^{0\sigma} + Y_m^{0\sigma} X_l^{0\sigma}) + H_d \tag{A1.10}$$

$$X_l^{0\sigma} = |l0\rangle\langle l\sigma| \quad Y_m^{0\sigma} = |m0\rangle\langle m\sigma|.$$

The equation of motion for the Green function

$$G_{k\sigma}^A(E) = \langle\langle X_k^{0\sigma} | X_{-k}^{0\sigma} \rangle\rangle_E \tag{A1.11}$$

at $\sigma = \uparrow$ reads

$$EG_{k\uparrow}^A(E) = \frac{1}{2} + \langle S_A^z \rangle + \frac{1}{N} \sum_q' \langle\langle (t_{k-q} a_q + t_k b_{-q}^+) Y_{k-q}^{-0} | X_{-k}^{0+} \rangle\rangle_E \tag{A1.12}$$

where we have used the relations

$$X_l^{+\dagger} = 1 - a_l^+ a_l \approx 1 \quad Y_m^{+0} = Y_m^{+-} Y_m^{-0} = b_m^+ Y_m^{-0}. \tag{A1.13}$$

Carrying out a decoupling in the equation of motion for the Green function on the right-hand side of (A1.12) we obtain

$$\left(E - \frac{1}{N} \sum_q' \langle\langle (t_{k-q} a_q + t_k b_{-q}^+) (t_{k-q} a_q^+ + t_k b_{-q}^-) \rangle\rangle / E \right) G_{k\uparrow}^A(E) = \frac{1}{2} + \langle S_A^z \rangle. \tag{A1.14}$$

Replacing the factor $1/E$ by the exact Green function, using the Bogoliubov transformation (which has the same form (A1.3)) and restoring spin dynamics we derive the integral equation

$$G_{k\uparrow}^A(E) = \left(\frac{1}{2} + \langle S_A^z \rangle \right) \left(E - \frac{1}{N} \sum_q' (t_{k-q} \cosh \theta_q - t_k \sinh \theta_q)^2 G_{k-q,\uparrow}^A(E - \omega_q) \right)^{-1} \tag{A1.15}$$

which agrees with the corresponding result of [2]. Note that the Green function $G_{k\downarrow}^A$ is proportional to the small factor $1/2 - \langle S_A^z \rangle$. This is in contrast with the consideration of section 5, where the result does not depend on σ . The difference of both pictures of the electron spectrum in the antiferromagnetic (AFM) state is rather instructive (compare with the treatment of NMR experiments in the state without magnetic sublattices, but with long-range AFM order [11]).

Appendix 2. Perturbation theory in the broad-band s-d model

Writing down the sequence of equations of motion in the s-d model with $\langle S_Q \rangle = 0$ we obtain the expansion of the Green function for a single current carrier in the form

$$G_k(E) = (E - \varepsilon_k)^{-1} + (E - \varepsilon_k)^{-2} \left(\frac{I^2}{N} \sum_q \frac{K_q}{E - \varepsilon_{k+q}} - \frac{I^3}{N^2} \sum_{qp} \langle\langle (S_{q-p} \sigma)(S_p \sigma)(S_{-q} \sigma) \rangle\rangle (E - \varepsilon_{k+q})^{-1} (E - \varepsilon_{k+q-p})^{-1} \right)$$

$$\begin{aligned}
& + \frac{I^4}{N^3} \sum_{qpr} \langle (S_{q-p+r} \sigma)(S_{-r} \sigma)(S_p \sigma)(S_{-q} \sigma) \rangle (E - \varepsilon_{k+q})^{-1} \\
& \times (E - \varepsilon_{k+q-p})^{-1} (E - \varepsilon_{k+q-p+r})^{-1} + \dots
\end{aligned} \tag{A2.1}$$

where spin dynamics is omitted for brevity, $K_q = \langle S_{-q} S_q \rangle$.

We employ the decoupling

$$\langle (S_{q-p+r} \sigma)(S_{-r} \sigma)(S_p \sigma)(S_{-q} \sigma) \rangle = \delta_{pq} K_q K_r + \delta_{pr} K_q K_p + \delta_{q,-r} K_p K_q \tag{A2.2}$$

which may be justified in the quasi-classical case. The first term on the right-hand side of (A2.2) yields the expansion of the Dyson equation (15), the second term corresponds to the expansion of the denominator in (16) and the third 'connected' term is a vertex correction. It is common practice to neglect contributions of the latter type (the 'non-crossing' approximation). Then we have

$$\Sigma_k(E) = \frac{I^2}{N} \sum_q K_q \left(E - \varepsilon_{k+q} - \frac{I^2}{N} \sum_{p \neq q} \frac{K_p}{E - \varepsilon_{k+q-p} - \dots} \right)^{-1}. \tag{A2.3}$$

This procedure may be repeated in higher orders of perturbation theory. Picking out the singular contributions to spin correlation functions and restoring spin dynamics we derive expression (36).

Now we analyse the third-order correction to the self-energy. We use the identity

$$\langle (S_{q-p} \sigma)(S_p \sigma)(S_{-q} \sigma) \rangle = K_p - K_{p-q} - K_q. \tag{A2.4}$$

The first term in (A2.4) yields a connected contribution, and other terms give multiple-scattering corrections, which may be summed up in all orders of perturbation theory to obtain

$$I \rightarrow I_{\text{ef}}(E) = \frac{I}{1 - IR(E)} \quad R(E) = \frac{1}{N} \sum_k \frac{1}{E - \varepsilon_k} \tag{A2.5}$$

in the second-order contribution to $\Sigma_k(E)$, $I_{\text{ef}}(E)$ (T matrix) being of the order of the bandwidth for large $|I|$.

It should be noted that in the case of a finite band filling the approximation (A2.5) corresponds to the 'parquet' approximation in the Kondo problem [17], where

$$R(E) \rightarrow \frac{1}{N} \sum_q \frac{1 - 2f_q}{E - \varepsilon_q}. \tag{A2.6}$$

This approximation enables one to remove logarithmic (in the absence of spin dynamics) divergences at $I > 0$ only.

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