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Spin excitations in the $S = \frac{1}{2}$ Heisenberg antiferromagnetic model on a square lattice

A F Barabanov†, L A Maksimov‡, O A Starykh† and G V Uimin§

† Vereschagin Institute for High Pressure Physics, 142092 Troitsk, Moscow Region, USSR

‡ Kurchatov Institute for Atomic Energy, 123182 Moscow, USSR

§ Landau Institute for Theoretical Physics, 142432 Moscow, USSR

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Abstract. We investigate the properties of the two-dimensional quantum $S = \frac{1}{2}$ Heisenberg antiferromagnetic model on a square lattice by means of a block approach. The lattice is divided into four spin square blocks and the Hamiltonian is expressed in terms of low-energy block states. In the framework of the mean-field theory based on the 'auxiliary-boson' formalism, we show that the spin excitation spectrum contains one singlet mode with the temperature-dependent gap and three degenerate triplet modes. The asymptotic low-temperature spin–spin correlations are proportional to $R^{-3/2}\exp[-R(1/\xi_1 + 1/\xi_2)]$, where $\xi_1 = \exp(\tilde{A}/T)$, $\xi_2 =$ constant and $\tilde{A} \simeq 0.5J$. The uniform susceptibility tends to zero in agreement with numerical results; the energy per site is close to $-0.57J$. Beyond the mean-field theory we find gapless collective excitations analogous to the gapless mode in the neutral Fermi gas with attraction.

1. Introduction

Recent neutron experiments [1, 2] indicate that the spin subsystem of the high-T_c superconductor CuO_2 planes may be described in a first approximation by the $S = \frac{1}{2}$ Heisenberg antiferromagnetic Hamiltonian on a square lattice. The theoretical background for such a description is based on the the generalized two-band Hubbard model [3, 4] which takes into account strong intrasite Coulomb repulsion between two holes on Cu ions. It is known that, for non-zero temperatures, spin-correlation functions $\langle S_0 S_r\rangle \to 0$ at $r \to \infty$, i.e. long-range order (LRO) is absent [5].

For the ground state at $T = 0$ the numerical method indicates the existence of LRO [6–8], although there is no rigorous analytical proof of this fact. These methods give reliable values for the ground-state energy $\varepsilon_0 = E_0/N = -0.665J$ and the first correlation functions $K_g = -0.115$ and $K_{2g} = 0.071$, where $\boldsymbol{g}$ is the nearest-neighbour vector. It is interesting that different variational ground-state functions—the Néel-like and non-magnetic (the resonance valence bonds)—have similar energies [8].

A recent analytical analysis of the model is carried out in the mean-field (MF) approximation by representing spin site operators S_r^i as the Fermi (spinons) [9, 10] or the Bose [11] operators $a_{r\sigma}$. The MF approximation is based on the order parameters $\langle a_{r\sigma} a_{r+g-\sigma}\rangle$. In both cases (Fermi and Bose) the $\hat{a}$-operator representation for the spin site operators is rigorous only if the local constraint $\Sigma_\sigma a_{r\sigma}^+ a_{r\sigma} = 1$ is fulfilled on each site.

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The main drawback of the above-mentioned considerations is the substitution of the local constraint by the analogous one averaged over sites, i.e. 'constraint in average'. As already known, such an approximation is valid at $S \gg 1$. In the case of a small spin ($S = \frac{1}{2}$), it leads to essential breakdown of the sum rule; the self-consistent value $\langle S_r^2 \rangle$ calculated with operators $a_{r\sigma}$ happens to be $\frac{3}{2}$ times greater than $S^2 = \frac{3}{4}$ [11, 12]. Because of the 'constraint in average' the ground-state energy $\varepsilon_0/J = -0.845$ (-0.416) and nearest spin-correlation functions $K_g = -0.168$ (-0.114) found in the Bose (Fermi) approach do not fit the numerical results.

Our consideration will be close to the Bose approach in [11]. Let us summarize the main results of this work. The elementary excitation spectrum $\omega(k)$ describes two degenerate branches with spin $\frac{1}{2}$. There is a temperature-dependent gap proportional to the inverse correlation length $\xi = \exp(A/T)$, $A = 1.16J$. At $T \to 0$ the uniform susceptibility χ remains finite, the specific heat C is proportional to T^2, the spin-correlation function K_r at large r is proportional to $r^{-1}\exp(-\kappa r)$, $\kappa = \xi^{-1}$. Expressions for the structure factor $S(\boldsymbol{q}, \omega) = \langle S^z(\boldsymbol{q}, 0) S^z(-\boldsymbol{q}, t) \rangle_\omega$ and $S(\boldsymbol{q}) = \int d\omega\, S(\boldsymbol{q}, \omega)$ show a peak for the antiferromagtic wavevector $\boldsymbol{q} = (\pi/g, \pi/g)$.

Our approach is based on the block method, which allows us to account for spin correlations [13] already in the zero approximation without breakdown of the square symmetry of the problem. Let us divide the plane into four site square blocks and find all block eigenstates $\nu_{\boldsymbol{R}}$, where $\boldsymbol{R}$ is the block vector index. As will be seen below, the main difference between our and the above-mentioned studies based on the single site states $a_{r\sigma}$ are as follows: the block solution of the problem in the MF approximation and 'constraint in average' violate the sum rule only slightly, i.e. the use of block states effectively corresponds to a spin increase. In particular it gives a proper description of the correlation functions at small distance, a decrease in the correlation length ξ with respect to [11] and qualitative changes in the character of the elementary excitations. We shall also show the presence of collective gapless excitations in the system.

2. Block formulation for the Hamiltonian

The complete set of the four site square block states $\nu_{\boldsymbol{R}}$ is formed by 16 states: one singlet with energy $\varepsilon_\varphi = -2J$; one triplet $\psi_{\boldsymbol{R},m}$ $(m = \pm 1, 0)$ with energy $\varepsilon_\psi = -J$; two triplets and one singlet with energy 0; five $S = 2$ states with energy $2J$, where J is an exchange integral. We shall treat the problem in the subspace of four energy low-lying block states $\varphi_{\boldsymbol{R}}$ and $\psi_{\boldsymbol{R},m}$. In conclusion we shall discuss the influence of the next energy states on the results.

The explicit form of the block wavefunctions $\varphi_{\boldsymbol{R}}$ and $\psi_{\boldsymbol{R},m}$ is

$$\varphi_{\boldsymbol{R}} = Z_{\boldsymbol{R}}^{\varphi,0}|0\rangle \qquad Z_{\boldsymbol{R}}^{\varphi,0} = \frac{1}{2\sqrt{3}}(1 + \hat{C} + \hat{C}^2 + \hat{C}^3)\left(\begin{vmatrix} + & + \\ - & - \end{vmatrix} - \begin{vmatrix} + & - \\ - & + \end{vmatrix}\right)$$

$$\psi_{\boldsymbol{R},0} = Z_{\boldsymbol{R}}^{\psi_0,0}|0\rangle \qquad Z_{\boldsymbol{R}}^{\psi_0,0} = \frac{1}{\sqrt{2}}(1 - \hat{C})\begin{vmatrix} + & - \\ - & + \end{vmatrix} = \frac{1}{\sqrt{2}} = \left(\begin{vmatrix} + & - \\ - & + \end{vmatrix} - \begin{vmatrix} - & + \\ + & - \end{vmatrix}\right). \tag{1}$$

Here $|0\rangle$ is the block vacuum, $\hat{C}$ is the block rotation operator by $\pi/2$ and $\begin{vmatrix} \sigma_2 & \sigma_1 \\ \sigma_3 & \sigma_4 \end{vmatrix}$ is a product of the four Fermi creation operators for one-electron states with a spin

projection $\sigma_i/2$; $i = 1, 2, 3, 4$ is the site index of the block $\boldsymbol{R}$. The states $\psi_{\boldsymbol{R},m}$, $m = \pm 1$, can be easily constructed by acting on $\psi_{\boldsymbol{R},0}$ by $S^{\pm}_{\boldsymbol{R}}$ block spin operators.

In our reduced subspace the Heisenberg Hamiltonian takes the form ($|m\rangle \equiv |\psi_m\rangle$):

$$H = h + T_1 + T_2 \qquad h = h_0 + V \qquad h_0 = \sum_{\boldsymbol{R}} \left(\varepsilon_\varphi Z^{\varphi\varphi}_{\boldsymbol{R}} + \sum_m \varepsilon_\psi Z^{mm}_{\boldsymbol{R}} \right)$$

$$V = \rho \sum_{\boldsymbol{R},\boldsymbol{g},m} (-1)^m (Z^{m,\varphi}_{\boldsymbol{R}} Z^{-m,\varphi}_{\boldsymbol{R}+2\boldsymbol{g}} + \text{HC}) \qquad \rho = -\frac{J}{6} \tag{2}$$

$$T_1 = 2\rho \sum_{\boldsymbol{R},\boldsymbol{g},m} Z^{m,\varphi}_{\boldsymbol{R}} Z^{\varphi,m}_{\boldsymbol{R}+2\boldsymbol{g}} \qquad T_2 = \frac{J}{16} \sum_{\boldsymbol{R},\boldsymbol{g}} S_{\boldsymbol{R}} S_{\boldsymbol{R}+2\boldsymbol{g}}$$

$$S_{\boldsymbol{R}} = \sum_{m_1,m_2} S_{m_1,m_2} Z^{m_1,m_2}_{\boldsymbol{R}}.$$

Here $Z^{\nu_1,\nu_2}_{\boldsymbol{R}}$ is the Hubbard projection operator which transforms the block $\boldsymbol{R}$ from the state ν_1 to ν_2; V describes the transformation of the neighbouring blocks from φ to ψ_m and vice versa; T_1 is the singlet–triplet exchange interaction; T_2 is the exchange interaction between triplets; $2\boldsymbol{g}$ is the nearest-neighbour block vector.

In the following we shall consider only the Hamiltonian h. Justification for omitting the terms T_1 and T_2 will be given later in section 3.

Let us introduce the boson fields $a_{\boldsymbol{R}}$, $b_{\boldsymbol{R},m}$ for the operators $Z^{\nu_1,\nu_2}_{\boldsymbol{R}}$. The 'constraint in average' is enforced by a 'chemical potential' λ:

$$Z^{\varphi\varphi}_{\boldsymbol{R}} = a^+_{\boldsymbol{R}} a_{\boldsymbol{R}} \qquad Z^{m_1,m_2}_{\boldsymbol{R}} = b^+_{\boldsymbol{R},m_1} b_{\boldsymbol{R},m_2} \qquad Z^{m,\varphi}_{\boldsymbol{R}} = b^+_{\boldsymbol{R},m} a_{\boldsymbol{R}}$$
$$n_a + 3n_b = 1 \qquad n_a = \langle a^+_{\boldsymbol{R}} a_{\boldsymbol{R}} \rangle \qquad n_b = \langle b^+_{\boldsymbol{R},m} b_{\boldsymbol{R},m} \rangle. \tag{3}$$

In this approximation, h describes the four-component Bose gas with an interaction which transforms triplet boson $b_{\boldsymbol{R},m}$ to singlet $a_{\boldsymbol{R}}$ and vice versa. We shall discuss the non-magnetic state of the system so that the thermal average $\langle a^+ b \rangle = 0$ but the following abnormal averages are non-zero:

$$\Delta_a = \Delta^*_a = \langle a_{\boldsymbol{R}} a_{\boldsymbol{R}+2\boldsymbol{g}} \rangle \qquad \Delta_b = \Delta^*_b = (-1)^m \langle b_{\boldsymbol{R},m} b_{\boldsymbol{R}+2\boldsymbol{g},-m} \rangle. \tag{4}$$

In the MF approximation the Hamiltonian h takes the form

$$h^{\text{MF}} = h^a + h^b + E_0 \tag{5}$$

where

$$h^a = \lambda \sum_{\boldsymbol{R}} a^+_{\boldsymbol{R}} a_{\boldsymbol{R}} + 3\Delta_b \rho \sum_{\boldsymbol{R},\boldsymbol{g}} (a^+_{\boldsymbol{R}} a^+_{\boldsymbol{R}+2\boldsymbol{g}} + \text{HC})$$

$$h^b = (\varepsilon + \lambda) \sum_{\boldsymbol{R},m} b^+_{\boldsymbol{R},m} b_{\boldsymbol{R},m} + \Delta_a \rho \sum_{\boldsymbol{R},\boldsymbol{g},m} (-1)^m (b^+_{\boldsymbol{R},m} b^+_{\boldsymbol{R}+2\boldsymbol{g},-m} + \text{HC})$$

and

$$E_0 = N_0 \varepsilon_\varphi - N_0 \rho 24 \Delta_a \Delta_b - N_0 \lambda \qquad \varepsilon = \varepsilon_\psi - \varepsilon_\varphi = J.$$

$N_0 = N/4$, the number of blocks, and h^{MF} invariance with respect to rotation in the spin space is provided by the Δ_b phase $(-1)^m$ in equation (4).

Using the momentum representation for h^a (h^b) and the u–v transformation a_k, b_k, α_k, β_k (see Appendix) we diagonalized the Hamiltonian (5):

$$h^a = \sum_k [\omega_{k,\alpha}\alpha_k^+\alpha_k + \tfrac{1}{2}(\omega_{k,\alpha} - \lambda)] \qquad \omega_{k,\alpha} = (\lambda^2 - 4\rho_{k,a}^2)^{1/2}$$

$$h^b = \sum_{k,m} \{\omega_{k,\beta}\beta_{k,m}^+\beta_{k,m} + \tfrac{1}{2}[\omega_{k,\beta} - (\varepsilon + \lambda)]\}$$

$$\omega_{k,\beta} = [(\varepsilon + \lambda)^2 - 4\rho_{k,b}^2]^{1/2} = c_b[2\eta^2 + 2(1 - \gamma_k^2)]^{1/2} \qquad c_b = 4\rho\Delta_a \tag{6}$$

$$\rho_{k,a} = 12\Delta_b\rho\gamma_k \qquad \rho_{k,b} = 4\Delta_a\rho\gamma_k \qquad \gamma_k = \tfrac{1}{2}[\cos(k_x 2g) + \cos(k_y 2g)].$$

3. The one-particle spectrum and the correlation functions

Self-consistent equations for abnormal average and constraint yield the system of three equations for finding Δ_a, Δ_b and λ:

$$\Delta_a = -12\rho\Delta_b N_0^{-1} \sum_k \frac{\gamma_k^2(1 + 2n_{k,\alpha})}{\omega_{k,\alpha}}$$

$$\Delta_b = -4\rho\Delta_a N_0^{-1} \sum_k \frac{\gamma_k^2(1 + 2n_{k,\beta})}{\omega_{k,\beta}} \tag{7}$$

$$n_a + 3n_b = 1.$$

Here

$$n_a = N_0^{-1} \sum_k \langle a_k^+ a_k \rangle = N_0^{-1} \sum_k [(n_{k,\alpha} + \tfrac{1}{2})\lambda\omega_{k,\alpha}^{-1} - \tfrac{1}{2}]$$

$$n_b = N_0^{-1} \sum_k \langle b_{k,m}^+ b_{k,m} \rangle = N_0^{-1} \sum_k [(n_{k,\beta} + \tfrac{1}{2})(\varepsilon + \lambda)\omega_{k,\beta}^{-1} - \tfrac{1}{2}]$$

where $n_{k,\alpha(\beta)} = n(\omega_{k,\alpha(\beta)})$ is the Bose occupation function.

System (7) has a solution with Δ_a, $\Delta_b \neq 0$ at $T < T_0 = 0.3J$. In this temperature range the Hamiltonian (6) describes one mode of singlet excitations and three degenerate modes of triplet excitations. The spectrum analysis is simple for the low-temperature limit. According to [11] it is convenient to express $\omega_{k,\alpha}$ as $\omega_{k,\alpha} = c_a[\kappa^2 + 2(1 - \gamma_k^2)]^{1/2}$ where κ serves as a cut-off in momentum integrations in (7); κ determines the inverse correlation length. At low temperatures the numerical solution of (7) yields

$$c_a = 12 \times \sqrt{2}\rho\Delta_b \qquad \Delta_b = 0.128 \qquad \Delta_a = 0.905 \qquad \lambda = 0.512J$$

$$\kappa = \exp(-\tilde{A}/T) \qquad \tilde{A} = 0.506J. \tag{8}$$

The value $\tilde{A}$ (equation (8)) is half the corresponding value A from [11]; this means a relative decrease in the correlation length ξ.

The triplet excitation spectra $\omega_{k,\beta}$ (equation (6)) have a finite gap $\eta \simeq 0.75J$ in contrast with $\omega_{k,\alpha}$ which have an exponentially small gap at $T \to 0$.

Note that the average number of triplet states is non-zero and $3n_b = 0.17$. The specific heat is proportional to T^2. The mean energy value ε_0 per site, equal to $-0.573J$, lies between the bosonic and fermionic one-site approach values.

To take into account the omitted term T_1, we tried to introduce the 'kinetic' averages $\tilde{\Delta}_a = \langle a_R^+ a_{R+2g} \rangle$, $\tilde{\Delta}_b = \langle b_{R,m}^+ b_{R+2g,m} \rangle$ together with the averages (4). This leads to the

addition of two corresponding equations in system (7). We found that solution of this new system gives zero values for $\tilde{\Delta}_a$, $\tilde{\Delta}_b$; so, in the Hartree–Fock MF approximation, T_1 vanishes. As to the term T_2, it can be seen that it contains four triplet operators and so is proportional to $n_b^2 \ll 1$. Our solution is unusual because of the finite gap in the triplet excitation spectrum in contrast with the usual massless spin-wave excitations. Nevertheless, as we shall show in section 4, in addition to the massless singlet excitations there exists a gapless branch of collective excitations.

Let us discuss the sum rule and the uniform magnetic susceptibility at low temperatures. The block and site spin operators S_R^j and $S_{R,i}^j$ ($j = x, y, z$) are expressed by the operators $Z_R^{\nu_2,\nu_1}$ and, hence, a_R and $b_{R,m}$. The expressions for z-components are given by

$$\begin{aligned} S_R^j &= Z_R^{1,1} - Z_R^{-1,-1} = b_{R,1}^+ b_{R,1} - b_{R,-1}^+ b_{R,-1} \\ S_{R,i}^j &= (-1)^{i+1} 6^{-1/2} (Z_R^{\varphi,\psi_0} + Z_R^{\psi_0,\varphi}) + \tfrac{1}{4} \sum_m m Z_R^{m,m} \\ &= (-1)^{i+1} 6^{-1/2} (a_R^+ b_{R,0} + b_{R,0}^+ a_R) + \tfrac{1}{4} (b_{R,1}^+ b_{R,1} - b_{R,-1}^+ b_{R,-1}). \end{aligned} \tag{9}$$

It is not difficult to find the x- and y-components.

Violation of the sum rule could be checked by comparing the values for $\langle (S^z)^2 \rangle$ which have been obtained by boson operator substitution at different steps of the calculation. On the one hand, we have

$$\langle (S_R^z)^2 \rangle = \langle (Z_R^{1,1} - Z_R^{-1,-1})^2 \rangle = \langle Z_R^{1,1} + Z_R^{-1,-1} \rangle = \langle b_{R,1}^+ b_{R,1} + b_{R,-1}^+ b_{R,-1} \rangle = 2n_b \tag{10a}$$

and, on the other hand,

$$\begin{aligned} \langle S_R^z S_R^z \rangle &= \langle (Z_R^{1,1} - Z_R^{-1,-1})(Z_R^{1,1} - Z_R^{-1,-1}) \rangle \\ &= \langle (b_{R,1}^+ b_{R,1} - b_{R,-1}^+ b_{R,-1})(b_{R,1}^+ b_{R,1} - b_{R,-1}^+ b_{R,-1}) \rangle \\ &= 2 \left(N_0^{-1} \sum_k \langle b_{k,1}^+ b_{k,1} \rangle \right) \left(N_0^{-1} \sum_k \langle b_{k,1} b_{k,1}^+ \rangle \right) = 2n_b(1 + n_b). \end{aligned} \tag{10b}$$

Here we use $\Sigma_k \langle b_{k,1}^+ b_{k,-1}^+ \rangle = 0$ which follows from the u–v transformation.

A comparison of (10a) and (10b) shows that the sum rule violation is proportional to n_b^2 ($n_b \simeq 0.06$) in our case, i.e. small.

The temperature dependence of the uniform susceptibility is given by

$$\begin{aligned} \chi(T) &= g^2 \mu_b^2 T^{-1} \sum_{r_2} \langle S_{r_1}^z S_{r_2}^z \rangle = g^2 \mu_b^2 T^{-1} N^{-1} \sum_{r_1, r_2} \langle S_{r_1}^z S_{r_2}^z \rangle \\ &= g^2 \mu_b^2 T^{-1} N^{-1} \sum_{R_1, R_2} \langle S_{R_1}^z S_{R_2}^z \rangle \\ &= g^2 \mu_b^2 T^{-1} N^{-1} \sum_k 2n_{k,\beta}(1 + n_{k,\beta}) \sim T^{-1} \exp\left(\frac{-C_b \eta}{T} \right). \end{aligned} \tag{11}$$

Thus $\chi(T \to 0) \to 0$ as in the fermionic approach [10]. The exponential decay is determined by the gap in the triplet excitation spectrum.

To investigate the correlation function

$$K^{jj}(r_1, r_2) = K^{jj}(\boldsymbol{R}_1, i_1; \boldsymbol{R}_2, i_2) = \langle S^j_{\boldsymbol{R}_1, i_1} S^j_{\boldsymbol{R}_2, i_2} \rangle$$

we must consider the special case $\boldsymbol{R}_1 = \boldsymbol{R}_2$. In this case when both site spins belong to one block we must use the block states (1) to find K^{jj}. Straightforward calculations yield the fact that K^{jj} is independent of j and is given by

$$\begin{aligned} K^{jj}(\boldsymbol{R}_1, i_1; \boldsymbol{R}_2, i_2) = (-1)^{i_1+i_2} 3^{-1} N_0^{-1} \Big[\Big(\sum_k \exp(\mathrm{i}k\boldsymbol{R}) \langle a_k^+ a_k \rangle \Big) \Big(\sum_k \exp(\mathrm{i}k\boldsymbol{R}) \langle b^+_{k,0} b_{k,0} \rangle \Big) \\ + \Big(\sum_k \exp(\mathrm{i}k\boldsymbol{R}) \langle a_k^+ a^+_{-k} \rangle \Big) \Big(\sum_k \exp(\mathrm{i}k\boldsymbol{R}) \langle b_{k,0} b_{-k,0} \rangle \Big) \Big] \\ + 8^{-1} N_0^{-1} \Big[\Big(\sum_k \exp(\mathrm{i}k\boldsymbol{R}) \langle b^+_{k,1} b_{k,1} \rangle \Big)^2 - \Big(\sum_k \exp(\mathrm{i}k\boldsymbol{R}) \langle b^+_{k,1} b^+_{-k,-1} \rangle \Big)^2 \Big] \end{aligned} \tag{12}$$

$\boldsymbol{R} = \boldsymbol{R}_2 - \boldsymbol{R}_1 \neq \boldsymbol{0}$

$$K^{jj}(\boldsymbol{R}_1, i_1; \boldsymbol{R}_1, i_2) = \begin{cases} -(\frac{1}{6} n_a + \frac{1}{4} n_b) & |i_1 - i_2| \neq 2 \\ \frac{1}{12}(n_a + 3n_b) = \frac{1}{12} & |i_1 - i_2| = 2. \end{cases}$$

Here as before $i = 1, 2, 3, 4$ is the site index in a block.

As can be seen from (12) the leading part of K^{jj} connected with the average $\langle a_k^+ a_k \rangle$ has different signs at odd and even sublattices; so correlations exhibit antiferromagnetic character.

Using the explicit form of $\omega_{k,\alpha}$ ($\omega_{k,\beta}$) it is easy to find the asymptotic spin–spin correlations at a large distance $\boldsymbol{R}$:

$$\begin{aligned} &K^{jj}(\boldsymbol{R} = \boldsymbol{R}_1 - \boldsymbol{R}_2) \sim T\sqrt{\xi_1} R^{-3/2} \exp(-R/\xi) \qquad \xi^{-1} = \xi_1^{-1} + \xi_2^{-1} \\ &\xi_1 = \kappa^{-1} = \exp(\tilde{A}/T) \qquad \xi_2 = (2^{1/2}\eta)^{-1}. \end{aligned} \tag{13}$$

As is clear from (13) the low-temperature asymptotic behaviour of K^{jj} is determined by the triplet gap η. The correlation length is much smaller in comparison with the one-site bosonic approach [11]. At $T = 0$, $\xi = \xi_2$ and hence there is no LRO in the ground state.

To find the correlation function $K^{jj}(r_1, r_1 + r)$ at small distance $r \sim \boldsymbol{g}$, it is natural to define the function $K^{jj}(r)$ which is constructed by averaging of $K^{jj}(r_1, r_1 + r)$ on r_1 inside the block. Such an averaging reconstructs the translational symmetry with initial periods g_x, g_y. In principle, despite the plane division into blocks this symmetry must be conserved by taking into account the complete set of 16 block states. The values of the first spin-correlation functions obtained from (12) at $T = 0$ are

$$K_1 = K^{jj}(\boldsymbol{g}) = -0.097 \qquad K_2 = K^{jj}(2\boldsymbol{g}) = 0.037.$$

These values are in qualitative agreement with the results of numerical methods: $K_1 = -0.117$, $K_2 = 0.07$ [6]. For comparison it is possible to obtain $K_1 = -0.168$ from the one-site bosonic method [11].

4. Gapless excitations

Let us consider the existence of gapless excitations in our treatment of the model. A gapless mode for collective sound-like excitations with a small momentum is known to

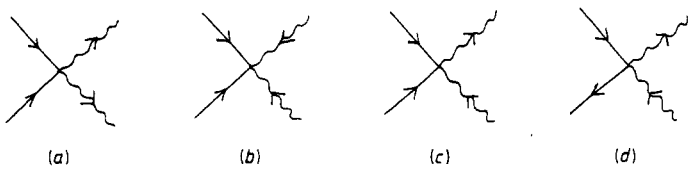

Figure 1. Typical vertices which determine collective excitations.

exist in a system with a gap in a one-particle excitation spectrum [14, 15]. Such a situation takes place for neutral attracting Fermi particles. For charged particles (e.g. in superconductors) this mode transforms to plasma waves. In our case one-particle Bose excitations are neutral and have a gap in the spectrum. Collective excitations with momentum $\boldsymbol{q}$ must be described by the following operators:

$$\begin{aligned} A_{qk} &= \alpha_{q-k}\alpha_k & A^+_{qk} &= \alpha^+_{-k}\alpha^+_{k-q} \\ B^m_{qk} &= \beta_{q-k,m}\beta_{k,-m} & B^{m+}_{qk} &= \beta^+_{-k,-m}\beta^+_{k-q,m} \end{aligned} \tag{14}$$

To find the spectrum of these excitations in the framework of the Hamiltonian (2) we must go beyond the MF approximation (5) and take into account the off-diagonal terms V':

$$V' = N_0^{-1} \sum_{m,k_1,k_2,q\neq 0} (-1)^m \rho_{k_1,k_2}(a^+_{k_1}a^+_{q-k_1}b_{q-k_2,m}b_{k_2,-m} + \text{HC}) \tag{15}$$

$$\rho_{k_1,k_2} = 2\rho\{\cos[2g(k_{1x} - k_{2x})] + \cos[2g(k_{1y} - k_{2y})]\}.$$

After the u–v transformation the interaction V' yields the vertices shown in figure 1 where the full line corresponds to the singlet excitations α_k (α^+_k), and the wavy line to the triplet excitations β_k (β^+_k). These vertices contain the product of the $u_{k,\alpha(\beta)}$- and $v_{k,\alpha(\beta)}$-quadratic combinations (see Appendix).

The interaction constant ρ is numerically only small ($\frac{1}{6}$) relative to the energy level difference $\varepsilon_\psi - \varepsilon_\varphi$. Nevertheless we shall treat the problem in the framework of the perturbation theory on ρ. Then in the ladder approximation the vertices in figures 1(a) and 1(b) lead to the closed system of equations for eight Green functions connected with excitations (14). By omission of non-uniform terms as in [14] it is possible to obtain the system which determines the collective excitation spectrum $\omega(q)$. The explicit form of the system is given in the Appendix. The gapless spectrum $\omega(q = 0) = 0$ exists if the solution (A2) exists for $\omega, q \to 0$. In this limit it is possible to construct two equations for the Green functions $\langle A_k|\rangle$, $\langle B_k|\rangle$:

$$\langle A_k|\rangle = \langle (A^+_{qk} - A_{qk})|\rangle_{q\to 0} \qquad \langle B_k|\rangle = \sum_m (-1)^m \langle (B^{m+}_{qk} - B^m_{qk})|\rangle_{q\to 0}$$

$$\begin{aligned} \langle A_k|\rangle &= -(1 + 2n_{k,\alpha})(2\omega_{k,\alpha})^{-1} N_0^{-1} \sum_{k_1} 2\rho_{k,k_1}\langle B_{k_1}|\rangle \\ \langle B_k|\rangle &= -(1 + 2n_{k,\beta})(2\omega_{k,\beta})^{-1} N_0^{-1} \sum_{k_1} 6\rho_{k,k_1}\langle A_{k_1}|\rangle. \end{aligned} \tag{16}$$

It is not difficult to show that the existence condition for the solution (16) strictly coincides with that giving the self-consistent solution of (7) for Δ_a, Δ_b. This ensures that the collective excitations (14) have a gapless spectrum at $T < T_0$. It may be shown that

the vertices in figures 1(c) and 1(d) do not alter equations (16). To obtain the explicit expression for $\omega(q)$ and to investigate the stability of the spectrum, it is necessary to solve the rather complex system (A2). The analysis yields that the spectrum is linear in q and vertices of the type in figures 1(c) and 1(d) must be taken into account to find the velocity of sound.

5. Conclusion

The most strange result that we found is the triplet excitation gap. We think that it is an artifact of the auxiliary boson approach in the described block method simultaneously with the 'constraint in average'. The analogous situation occurs in the one-dimensional $S = \frac{1}{2}$ Heisenberg antiferromagnet. The Schwinger boson approach [11] gives a non-zero gap in the spin-wave spectrum in contrast with the exact solution [16]. Nevertheless it is possible to construct gapless collective Schwinger boson excitations as in Section 4. Thus these modes are Goldstone modes; however, it is difficult for us to investigate their thermodynamic properties.

In conclusion we shall discuss the possible influence of high-energy block states on our results. The low-lying part of the one-particle spectrum is determined by the singlet states φ_R; the triplet excitations have a finite gap. This result will remain the same if we take into account the states ν_R with an energy greater than $-J$. These states will decrease the triplet gap η and the number n_a of singlet states and increase the temperature T_0; however the temperature dependence of $C(T)$ and $\chi(T)$ will not change. The corrections due to high-lying states may increase $|K_1|$ and decrease the correlation length. Finally we would like to emphasize that the inclusion of the high-lying energy states will not influence the existence of collective gapless excitations.

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Appendix

Let us represent the explicit form for the u–v transformation a, b, α, β and equations for two-particle Green functions which determine the spectrum $\omega(q)$ for the collective excitations (14) as follows:

$$a_k = u_{k\alpha}\alpha_k - v_{k\alpha}\alpha^+_{-k} \qquad b_{k,m} = u_{k,\beta}\beta_{k,m} - (-1)^m v_{k,\beta}\beta^+_{-k,-m} \qquad m = 0, \pm 1$$

$$u_{k,\alpha} = [\tfrac{1}{2}(\lambda + \omega_{k,\alpha})\omega^{-1}_{k,\alpha}]^{1/2}$$

$$u_{k,\beta} = [\tfrac{1}{2}(\varepsilon + \lambda + \omega_{k,\beta})\omega^{-1}_{k,\beta}]^{1/2} \tag{A1}$$

$$v_{k,\alpha(\beta)} = (u^2_{k,\alpha(\beta)} - 1)^{1/2}.$$

The Green function equations for operators A_{qk} and a singlet combination B_{qk} of operators B^m_{qk} (14) have the form

$$B_{qk} = \sum_m (-1)^m \beta_{q-k,m}\beta_{k,-m} \qquad B^+_{qk} = \sum_m (-1)^m \beta^+_{-k,-m}\beta^+_{k-q,m}$$

$$(z - \omega_{k_1,\alpha} - \omega_{q_1,\alpha})\langle A_{qk_1}|\rangle = N_0^{-1} \sum_{k_2} R_\alpha(k_1, k_2, q)(\gamma^{-+}_{\alpha\beta}\langle B^+_{qk_2}|\rangle + \gamma^{--}_{\alpha\beta}\langle B_{qk_2}|\rangle)$$

$$(z + \omega_{k_1,\alpha} + \omega_{q_1,\alpha})\langle A^+_{qk_1}|\rangle = -N_0^{-1} \sum_{k_2} R_\alpha(k_1, k_2, q)(\gamma^{--}_{\alpha\beta}\langle B^+_{qk_2}|\rangle + \gamma^{-+}_{\alpha\beta}\langle B_{qk_2}|\rangle)$$

$$(z - \omega_{k_1,\beta} - \omega_{q_1,\beta})\langle B_{qk_1}|\rangle = 3N_0^{-1} \sum_{k_2} R_\beta(k_1, k_2, q) \quad (\gamma^{-+}_{\beta\alpha}\langle A^+_{qk_2}|\rangle + \gamma^{--}_{\beta\alpha}\langle A_{qk_2}|\rangle)$$

$$(z + \omega_{k_1,\beta} + \omega_{q_1,\beta})\langle B^+_{qk_1}|\rangle = 3N_0^{-1} \sum_{k_2} R_\beta(k_1, k_2, q)(\gamma^{--}_{\beta\alpha}\langle A^+_{qk_2}|\rangle + \gamma^{-+}_{\beta\alpha}\langle A_{qk_2}|\rangle) \qquad \text{(A2)}$$

$$\gamma^{-+}_{\alpha\beta}(k_1, k_2, q) = u_{k_1\alpha}u_{q_1\alpha}v_{q_2\beta}v_{k_2\beta} + v_{k_1\alpha}v_{q_1\alpha}u_{q_2\beta}u_{k_2\beta}$$

$$\gamma^{--}_{\alpha\beta}(k_1, k_2, q) = u_{k_1\alpha}u_{q_1\alpha}u_{q_2\beta}u_{k_2\beta} + v_{k_1\alpha}v_{q_1\alpha}v_{q_2\beta}v_{k_2\beta}$$

$$R_\alpha(k_1, k_2, q) = 2[\rho_{k_1,k_2}(1 + n_{q_1,\alpha}) + \rho_{q_1,k_2}n_{k_1,\alpha}]$$

$$z = \omega + \mathrm{i}0 \qquad q_1 = q - k_1 \qquad q_2 = q - k_2.$$

Expressions for $\gamma_{\beta\alpha}$, R_β can be found by the formal index exchange $\alpha \rightarrow \beta$ in the expressions for $\gamma_{\alpha\beta}$, R_α. We have already mentioned that the non-uniform terms in the RHS of equation (A2) were omitted. At $\omega, q \rightarrow 0$ the system (A2) gives equations (16).

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