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Disordered ground-state properties of a double-layer Heisenberg antiferromagnet

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Abstract. The disordered ground-state properties of a double-layer quantum antiferromagnet are investigated in the bond operator representation. The intralayer and interlayer couplings are J and $J_\perp$, respectively. In a mean-field approximation, we obtain a spin gap which decreases with increasing ratio $\lambda = J/J_\perp$ and disappears at the value $\lambda_c = 0.292$. In the region $0 \leqslant \lambda \leqslant \lambda_c$, we calculate the disordered ground-state energy, the intralayer and interlayer nearest-neighbour singlet strengths, and the correlation length.

1. Introduction

There is an intimate connection between antiferromagnetism and superconductivity in layered copper oxide compounds; the $S = \frac{1}{2}$ square-lattice antiferromagnetic copper–oxygen planes might be a vital component of the mechanism of high-temperature superconductivity [1,2]. In most high-T_c materials the appearance of superconductivity is almost accompanied by the disappearance of the antiferromagnetic long-range order [3,4]. It was recently suggested [5–7] that the unusual normal-state magnetic properties of the high-T_c superconducting cuprates are characteristic of two-dimensional quantum antiferromagnets close to the critical point of a zero-temperature order–disorder transition. In the disordered phase there is an energy gap towards spin excitations. In order to obtain the critical point, Sachdev and Bhatt [8] introduced a new representation of $S = \frac{1}{2}$ quantum spins in terms of the bond operator to study the two-dimensional antiferromagnetic system and found that the magnetically disordered columnar dimerization phase was stable for the ratio λ_c of intradimer to interdimer coupling strength less than 0.46. Katoh and Imada [9] also investigated the phase diagram of the $S = \frac{1}{2}$ antiferromagnetic Heisenberg model on a dimerized square lattice using the quantum Monte Carlo simulations and found that the spin gap appeared above $\lambda_c = 0.538$.

In La_2CuO_4 the basic structural unit is a single CuO_2 plane, weakly coupling to the other CuO_2 planes. Unlike La_2CuO_4, in $YBa_2Cu_3O_{6+x}$ the basic structural unit is a pair of CuO_2 planes, separated from the next pair of CuO_2 planes by the relatively inert CuO chains [10]. Investigation of the two-layer quantum Heisenberg antiferromagnet relates closely to the superconducting mechanism of the $YBa_2Cu_3O_{6+x}$ series. When the interplane coupling $J_\perp = 0$, each of the two independent planes has long-range order at $T = 0$ and the spectrum

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is gapless. However, for a small ratio $\lambda = J/J_\perp$ of the intralayer and interlayer coupling, there is a tendency for the neighbouring spins in adjacent planes to form singlets, and there is a gap for spin-1 excitations and no long-range order. The critical coupling λ_c at which the spin gap disappears was calculated by various methods. Hida obtained the critical coupling $\lambda_c = 0.236$ by the modified spin-wave method [11], and $\lambda_c = 0.391$ by the series expansion method [12]. Millis and Monien [13] gave $\lambda_c = 0.223$ by the Schwinger boson mean-field calculation. Sandvik and Scalapino [14] found that $\lambda_c = 0.398$ by the modification of the Handscomb quantum Monte Carlo algorithm. In these references there are no systematic investigations of the properties of disordered ground state in the double-layer quantum antiferromagnet.

The purpose of this paper is to investigate the disordered ground-state properties of a double-layer dimerized Heisenberg antiferromagnet in the bond operator representation. In section 2 we shall give the model Hamiltonian in the bond operator representation, derive the equation of motion for the retarded Green function and give the analytical expressions for the spin gap, the ground-state energy and the related physical quantities. The results of numerical calculation and discussion are given in section 3. The last section 4 is devoted to a summary.

2. Hamiltonian and analytical results

Let us consider the double-layer square lattice Heisenberg model; the intralayer and the interlayer nearest-neighbour antiferromagnetic couplings are J and $J_\perp$, respectively. The Hamiltonian is as follows:

$$H = J_\perp \sum_i S_{1i} S_{2i} + J \sum_m \sum_{\langle i,j \rangle} S_{mi} S_{mj} \tag{2.1}$$

where $\langle i, j \rangle$ is a pair of nearest-neighbours in each layer, and S_{mi} is a spin-$\frac{1}{2}$ operator at site i in layer m ($m = 1$ or 2 indicates the two layers). The lattice constant is taken to be equal to unity. With the interlayer coupling $J_\perp = 0$, each of the two independent layers has long-range order at $T = 0$. For a small $J/J_\perp$ ratio, the nearest-neighbour spins on different layers form a singlet pair; thus in the two-layer structure, dimerization may occur in a perpendicular direction to planes, and the antiferromagnetic long-range order should be suppressed.

The spin-wave analysis cannot be used to study the dimerization phase; instead we use the bond operator representation for quantum $S = \frac{1}{2}$ spins [8]. In this representation, two spins S_1 and S_2 are placed on a pair of nearest-neighbour sites in the two layers. The four states in the Hilbert space can be combined to form a singlet state $|s\rangle$ and three triplet states $|t_x\rangle$, $|t_y\rangle$ and $|t_z\rangle$. The single and triplet creation operators are defined as follows:

$$\begin{aligned}
s^+|0\rangle &= |s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\
t_x^+|0\rangle &= |t_x\rangle = -\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \\
t_y^+|0\rangle &= |t_y\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \\
t_z^+|0\rangle &= |t_z\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle).
\end{aligned} \tag{2.2}$$

A representation of the spins S_{1i} and S_{2i} in terms of these singlet and triplet operators is given by

$$\begin{aligned} S_{1\alpha} &= \tfrac{1}{2}(s^+ t_\alpha + t_\alpha^+ s - \mathrm{i}\epsilon_{\alpha\beta\gamma} t_\beta^+ t_\gamma) \\ S_{2\alpha} &= \tfrac{1}{2}(-s^+ t_\alpha - t_\alpha^+ s - \mathrm{i}\epsilon_{\alpha\beta\gamma} t_\beta^+ t_\gamma) \end{aligned} \tag{2.3}$$

where α, β and γ represent the components along the x, y and z axes, respectively, repeated indices are summed over and ϵ is the totally antisymmetric tensor. The restriction that the physical states are either singlet or triplet leads to the constraint

$$s^+ s + t_\alpha^+ t_\alpha = 1. \tag{2.4}$$

Taking the singlet and triplet operators at each site to satisfy the bosonic commutation relations and, using equations (2.3) and (2.4), one can reproduce the spin-$\frac{1}{2}$ $SU(2)$ algebra of the spins S_{1i} and S_{2i}.

Substituting equations (2.3) and (2.4) into equation (2.1), we can rewrite the Hamiltonian as follows:

$$\begin{aligned} \frac{H}{J_\perp} = \sum_i [(-\tfrac{3}{4} - \tilde{\mu}) s_i^+ s_i + (\tfrac{1}{4} - \tilde{\mu}) t_{i\alpha}^+ t_{i\alpha} + \tilde{\mu}] + \frac{\lambda}{2} \sum_{\langle i,j \rangle} (s_i^+ s_j t_{j\alpha}^+ t_{i\alpha} + s_i^+ s_j^+ t_{i\alpha} t_{j\alpha} + \mathrm{HC}) \\ + \frac{\lambda}{2} \sum_{\langle i,j \rangle} (1 - \delta_{\beta\gamma})(t_{i\beta}^+ t_{j\beta}^+ t_{i\gamma} t_{j\gamma} - t_{j\beta}^+ t_{i\gamma}^+ t_{i\beta} t_{j\gamma} + \mathrm{HC}) \end{aligned} \tag{2.5}$$

where $\lambda = J/J_\perp$ and $\tilde{\mu} = \mu/J_\perp$. The chemical potential μ is introduced to impose the constraint of equation (2.4). According to [8, 15], we take $\langle s_j \rangle = \bar{s}$, which means that the s bosons are condensed, omit the third term on the right-hand side of equation (2.5) because it does not change the results significantly even for $\lambda = 1$ [15] and perform the Fourier transformation of the operators $t_{i\alpha}^+ = (1/\sqrt{N}) \sum_k t_{k\alpha}^+ \exp(\mathrm{i}kr_i)$, where N is the total number of sites in each layer. Thus we finally obtain the mean-field Hamiltonian as follows:

$$\frac{H}{J_\perp} = N(-\tfrac{3}{4}\bar{s}^2 - \tilde{\mu}\bar{s}^2 + \tilde{\mu}) + \sum_k [A(k) t_{k\alpha}^+ t_{k\alpha} + B(k)(t_{k\alpha}^+ t_{-k\alpha}^+ + t_{k\alpha} t_{-k\alpha})] \tag{2.6}$$

where

$$\begin{aligned} A(k) &= \tfrac{1}{4} - \tilde{\mu} + \lambda \bar{s}^2 \eta_k \\ B(k) &= \lambda \bar{s}^2 \eta_k \end{aligned} \tag{2.7}$$

with $\eta_k = \cos k_x + \cos k_y$.

In order to calculate the energy of the ground state and related physical quantities, we define the following retarded function:

$$G(k,\omega) = \begin{bmatrix} \langle\langle t_{k\alpha} | t_{k\alpha}^+ \rangle\rangle_\omega & \langle\langle t_{-k\alpha} | t_{k\alpha} \rangle\rangle_\omega \\ \langle\langle t_{-k\alpha}^+ | t_{k\alpha}^+ \rangle\rangle_\omega & \langle\langle t_{k\alpha}^+ | t_{k\alpha} \rangle\rangle_\omega \end{bmatrix}. \tag{2.8}$$

Using the technique of the equation of motion for the Green function, we obtain the solution of the Green function:

$$G(k,\omega) = \frac{1}{\omega^2 - \omega_k^2} \begin{bmatrix} \omega + A(k) & -B(k) \\ -B(k) & -\omega + A(k) \end{bmatrix} \tag{2.9}$$

where

$$\omega_k = J_\perp \sqrt{A(k)^2 - B(k)^2}. \tag{2.10}$$

Using the spectral theorem and equation (2.9), we obtain the correlation functions

$$\langle t_{k\alpha}^{+} t_{k\alpha}\rangle = \frac{J_\perp A(k) - \omega_k}{2\omega_k}$$
$$\langle t_{k\alpha}^{+} t_{-k\alpha}^{+}\rangle = \langle t_{k\alpha} t_{-k\alpha}\rangle = \frac{-J_\perp B(k)}{2\omega_k} \tag{2.11}$$

and the ground-state energy per site

$$\frac{E_g}{J_\perp} = -\tfrac{1}{16} - \tfrac{1}{2}(\tfrac{3}{4} + \tilde{\mu})\bar{s}^2 + \tfrac{3}{4}\tilde{\mu} + \frac{1}{4NJ_\perp}\sum_k \omega_k. \tag{2.12}$$

The mean-field parameter $\bar{s}$ and the chemical potential $\tilde{\mu}$ are determined by using the minimization condition of the ground-state energy: $\partial E_g/\partial \bar{s} = 0$, and $\partial E_g/\partial \tilde{\mu} = 0$. Thus we obtain the self-consistent equations on $\bar{s}$ and $\tilde{\mu}$ as follows:

$$\tfrac{3}{2} + 2\tilde{\mu} = \frac{\lambda}{(2\pi)^2}\int_{-\pi}^{\pi}\int \frac{\eta_k}{\sqrt{1 + D\eta_k}}\,dk_x\,dk_y \tag{2.13}$$

$$3 - 2\bar{s}^2 = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int \frac{1 + 0.5D\eta_k}{\sqrt{1 + D\eta_k}}\,dk_x\,dk_y \tag{2.14}$$

where

$$D = \frac{2\lambda\bar{s}^2}{0.25 - \tilde{\mu}}. \tag{2.15}$$

For each λ, the self-consistent solutions of $\tilde{\mu}$ and $\bar{s}$ are given by equations (2.13) and (2.14) and are used to determine the excitation spectrum of the spin-triplet state obtained from equation (2.10) as

$$\omega_k = J_\perp(0.25 - \tilde{\mu})\sqrt{1 + D\eta_k}. \tag{2.16}$$

The dispersion relation of equation (2.16) can be parametrized to obtain the spin-wave velocity V_s and the spin stiffness D_s

$$V_s = J_\perp(0.25 - \tilde{\mu})\sqrt{0.5D} \tag{2.17}$$

$$D_s = J_\perp(0.25 - \tilde{\mu})\frac{D}{4\sqrt{1 + 2D}}. \tag{2.18}$$

The excitation spectrum (2.16) has a minimum at $k_x = k_y = \pi$ and the spin gap is given by

$$\Delta = J_\perp(0.25 - \tilde{\mu})\sqrt{1 - 2D}. \tag{2.19}$$

Using the spin-wave velocity V_s and the spin gap Δ, we can calculate the intralayer spin–spin correlation length as [15]

$$\xi = \frac{V_s}{\Delta} = \sqrt{\frac{D}{2(1 - 2D)}}. \tag{2.20}$$

Using equations (2.3) and (2.11), we can also obtain the intralayer nearest-neighbour spin–spin correlation function

$$\langle S_{1i} S_{1j}\rangle = \frac{\bar{s}^2}{4} I_1 + \tfrac{1}{12} I_1 I_2 \tag{2.21}$$

where

$$I_1 = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int \frac{\cos k_x}{\sqrt{1+D\eta_k}}\,\mathrm{d}k_x\,\mathrm{d}k_y \tag{2.22}$$

$$I_2 = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int \sqrt{1+D\eta_k}\cos k_x\,\mathrm{d}k_x\,\mathrm{d}k_y \tag{2.23}$$

and the interlayer nearest-neighbour spin–spin correlation function

$$\langle S_{1i}S_{2i}\rangle = 0.25 - \bar{s}^2. \tag{2.24}$$

3. Computation results and discussion

In figure 1, we present the result of the spin gap as a function of λ obtained from equation (2.19). From figure 1, we can see that the spin gap decreases with increasing value of λ and becomes zero at $\lambda_c = 0.292$. The value of λ_c is larger than that given by both the modified spin-wave method [11] and the Schwinger boson mean-field method [13] but is smaller than that given by both the series expansion method [12] and the quantum Monte Carlo method [14]. In the range $0 < \lambda < \lambda_c$, the system is in a magnetically disordered phase and has a spin gap. At $\lambda = 0$, the spin gap has the maximum value of $J_\perp$, which is just equal to the energy difference between the triplet state and the singlet state of the two-spin-$\frac{1}{2}$ system.

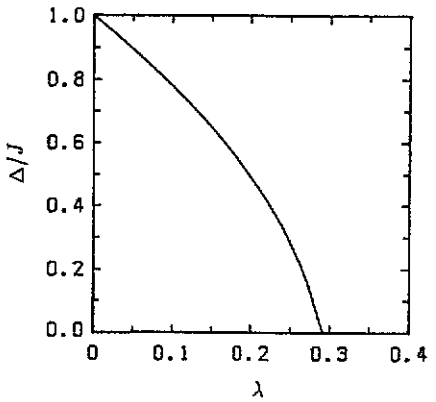

Figure 1. The spin gap Δ as a function of λ $(= J/J_\perp)$.

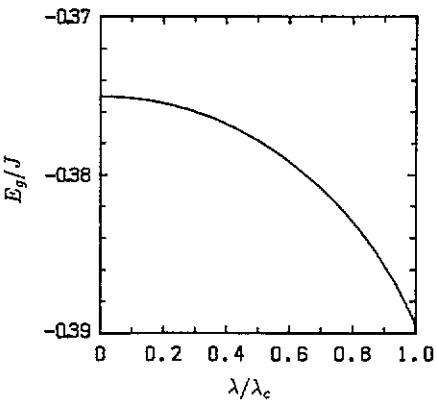

Figure 2. The disordered ground-state energy E_g as a function of λ/λ_c.

In figures 2–7, the unit of the horizontal axis is normalized by λ_c. The curve of the disordered ground-state energy E_g versus λ/λ_c is shown in figure 2. At the critical coupling λ_c, the energy is $-0.389J_\perp$, which is smaller than that given by the modified spin-wave method in which it is $-0.371J_\perp$ [11]. The ground-state energy decreases with increasing value of λ.

Computation results of the spin velocity V_s and the spin stiffness D_s versus λ/λ_c are shown in figure 3 and figure 4, respectively. We see that the spin-wave velocity and spin stiffness decrease with decreasing λ. At $\lambda = 0$, $V_s = D_s = 0$, it is easy to understand that there is no spin wave in the independent two-spin-$\frac{1}{2}$ system. At the critical coupling λ_c, the spin-wave velocity is $1.88J_\perp$; it is smaller than that obtained by the spin-wave theory for the two-layer system [14].

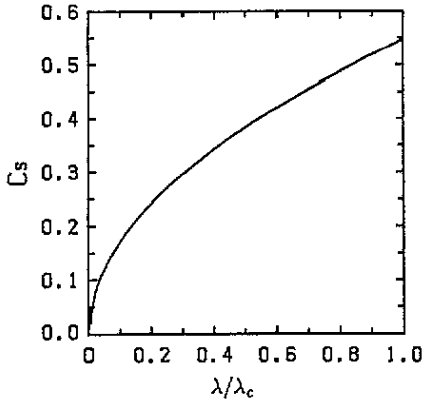

Figure 3. The spin-wave velocity C_s as a function of λ/λ_c.

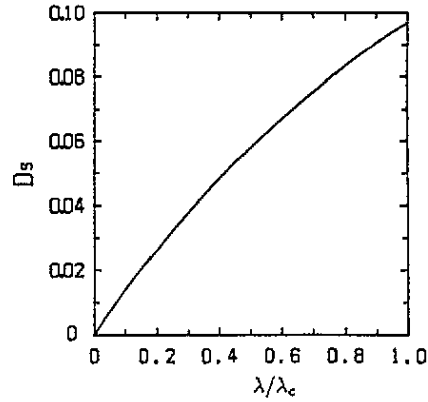

Figure 4. The spin-wave stiffness D_s as a function of λ/λ_c.

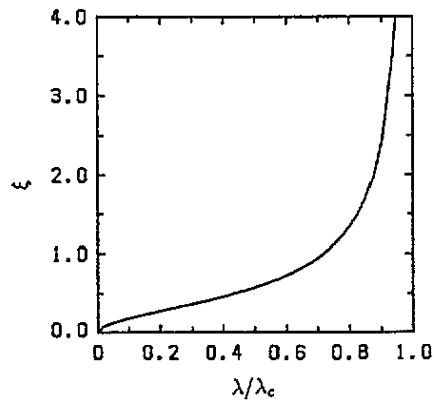

Figure 5. The correlation length ξ as a function of λ/λ_c.

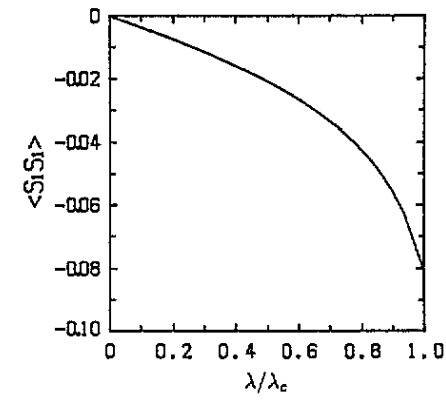

Figure 6. The intralayer nearest-neighbour spin–spin correlation $\langle S_{1i} S_{1j} \rangle = \langle S_{2i} S_{2j} \rangle$ as a function of λ/λ_c.

The computation result of the correlation length ξ versus λ/λ_c is shown in figure 5. We see that the correlation length increases with increasing λ. At the critical coupling λ_c the correlation length is infinite; it is a feature of the antiferromagnetic order–disorder transition occurring at $T = 0$. In the range $0 \leqslant \lambda \leqslant \lambda_c$, the correlation length is finite; this is very different from that given by the modified spin-wave method. In the modified spin-wave method, the correlation length vanishes in this parameter region. Because the correlation length is finite in our calculation, the disordered phase is the spin-liquid phase rather than the singlet gas phase [11]. This conclusion is consistent with that obtained by the series expansion method [12].

The calculated intralayer and interlayer nearest-neighbour spin–spin correlation are shown in figure 6 and figure 7, respectively. At $\lambda = 0$, we obtain correctly the values of 0 and -0.75 for the intralayer and interlayer spin–spin correlations. At critical coupling, the value of the interlayer spin–spin correlation is -0.685; it is slightly smaller than the value of -0.645 given by the modified spin-wave method [11]. The value of the intralayer

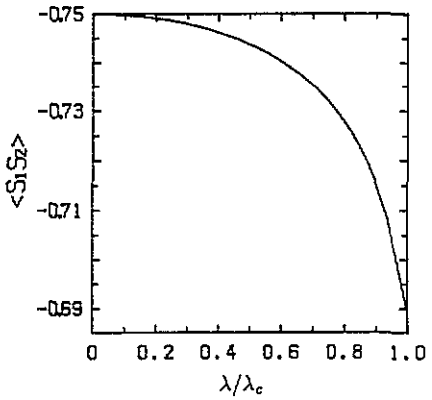

Figure 7. The interlayer nearest-neighbour spin–spin correlation $\langle S_{1l} S_{2l} \rangle$ as a function of λ/λ_c.

spin–spin correlation is finite in the disordered phase, which is different from that obtained by the modified spin-wave method in which the value is zero.

4. Summary

In this paper, we have investigated the properties of the disordered ground state of the double-layer Heisenberg antiferromagnet with spin-$\frac{1}{2}$ in the bond operator representation. In the mean-field approximation, the spin gap which decreases with increasing ratio of the intralayer coupling J and the interlayer coupling $J_\perp$ is obtained, and it becomes zero at $\lambda(= J/J_\perp) = 0.292$. The other physical quantities, such as the ground-state energy, the spin-wave velocity and stiffness, the correlation length, and the intralayer and interlayer nearest-neighbour spin–spin correlation functions, are calculated in the region $0 < \lambda < \lambda_c$. The results have shown that both the correlation length and the interlayer spin–spin correlation are finite, which is different from that given by the modified spin-wave method; the disordered phase is the spin-liquid phase rather than the singlet gas phase.

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