PHYSICAL REVIEW B VOLUME 41, NUMBER 13 1 MAY 1990

Low-temperature properties of the quasi-two-dimensional antiferromagnetic Heisenberg model

Bang-Gui Liu*
Center of Theoretical Physics, Chinese Center of Advanced Science and Technology (World Laboratory), Beijing 100080, People's Republic of China

(Received 5 July 1989; revised manuscript received 29 December 1989)

By means of a two-sublattice approach to antiferromagnets, we found that the ground state of a quasi-two-dimensional cubic-lattice antiferromagnet ($J_z/J_{xy} \ll 1$) is a Néel antiferromagnetic state with a mean magnetic moment of $0.6\mu_B$ (μ_B is the Bohr magneton) and that low-temperature moment decreases with the square of the temperature. The coefficient of the temperature-squared term approaches infinity when $J_z/J_{xy}=0$. The z-direction coupling ($J_z>0$) is essential to keep three-dimensional Néel ordering at nonzero temperature and to obtain a nonzero Néel temperature. The low-temperature specific heat capacity is proportional to the temperature squared.

It is observed that $La_{2-x}(Ba,Sr)_xCuO_4$ ($x<0.03$) and $RBa_2Cu_3O_{6+y}$ ($y<0.4$; R=rare-earth element) exhibit three-dimensional (3D) Néel antiferromagnetic (AFM) ordering with a magnetic moment of about $0.6\mu_B$ (where μ_B is the Bohr magneton).[1] Further experiments affirm that their excitations are 2D spin waves. The 2D Heisenberg coupling constants J of La_2CuO_4 and $RBa_2Cu_3O_6$ are 950 and 1300 K, respectively.[2] Coupling between CuO_2 planes is much weaker than in-plane coupling. The copper oxide materials can be described by a quasi-2D Hubbard model on a simple cubic lattice with large on-site Coulomb repulsion.[3] There are no dopants in the idealistic CuO_2 planes which correspond to La_2CuO_4 and $RBa_2Cu_3O_6$. The corresponding Hubbard model is half filled. Because of the large on-site Coulomb repulsion, the Hubbard model is equivalent to the following spin-$\frac{1}{2}$ Heisenberg AFM model:

$$H=\sum_{\langle ij\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\,. \tag{1}$$

$J_{ij}=J$ only for the nearest-neighboring i and j sites within one CuO_2 plane and $J_{ij}=gJ$ ($g\le 1$) when i and j are nearest-neighboring sites in the z direction.

If $g=0$ the Hamiltonian (1) reduces to the 2D Heisenberg AFM model

$$H=J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{2}$$

where i and j take on values within the CuO_2 planes.

Reference 4 used the (2+1)-dimension nonlinear sigma model to approach (2) and found that the correlation length had renormalized classical behavior $\kappa^{-1}=\exp(-A/T)$, where A/T is not equivalent to zero when T approaches zero. Reference 5 used a mean-field method to investigate (2). Their models provided a Bose-liquid description of the excitations but they were unable to given a unique magnetic moment in Néel AFM states. Reference 6, by means of a Monte Carlo method, obtained the Néel AFM ground state of the 2D AFM Heisenberg model on 32×32 sites of a square lattice, whose staggered moment is equivalent to 0.334 ± 0.001. These results are limited to the 2D model (2).

In this paper we use a two-sublattice method to investigate the Hamiltonian (1). We obtain the Néel AFM ground states for all g. The average staggered moments of the ground states increase with parameter g. They are 0.606 and $0.844\mu_B$ when $g=0$ and 1, respectively. Low-temperature staggered moments are shown to decrease with the square of the temperature, but the coefficient of the temperature-squared term approaches infinity when g is equal to zero. This implies that the 2D AFM Heisenberg model has no AFM ordering at any finite temperature. The z-direction coupling is essential to keep the 3D AFM ordering at nonzero temperature and to obtain a nonzero Néel temperature. Further, we calculate its low-temperature specific-heat capacity. There is no linear term in the specific-heat capacity when g is very small. This is in agreement with experimental data.[7]

First, as in Ref. 8, we divide the simple cubic lattice into two sublattices, indicated by a and b, so that all nearest-neighboring sites of every a (b) sublattice site belong to sublattice b (a). Sublattice a (b) is a face-centered cubic lattice. $\mathbf{S}_a$ and $\mathbf{S}_b$ indicate spin operators on sublattices a and b, respectively. a_i and b_j indicate operators introduced by the Holstein-Primakoff transformation corresponding to $\mathbf{S}_a$ and $\mathbf{S}_b$, respectively. After the Holstein-Primakoff transformation, a_i and b_j are transferred into momentum space (k_x,k_y,k_z). As a result, the Hamiltonian (1) can be expressed in terms of a_k and b_k.

$$H=-NJZ/4+\sum_k JZ[a_k^\dagger a_k+b_k^\dagger b_k+r(k)\times(a_k b_k+a_k^\dagger b_k^\dagger)]\,, \tag{3}$$

where N is the total site number of the lattice, $Z=4+2g$ is the effective nearest-neighbor number, and

$$r(k)=(2\cos k_x+2\cos k_y+2g\cos k_z)/Z\,. \tag{4}$$

By means of a Bogoliubov transformation the Hamiltonian (3) is diagonalized to be (for details see Callaway[8])

$$H=E_0+\sum_k e(k)[A^\dagger(k)A(k)+B^\dagger(k)B(k)]\,, \tag{5}$$

where

$$A(k)=u(k)a_k-v(k)b_k^{\dagger}, \tag{6}$$

$$B(k)=u(k)b_k-v(k)a_k^{\dagger}, \tag{7}$$

$$E_0=-NJZ\left[1+\left(1-4/N\sum_k[1-r^2(k)]^{1/2}\right)\right], \tag{8}$$

$$e(k)=JZ[1-r^2(k)]^{1/2}. \tag{9}$$

$u(k)$ and $v(k)$ in the above equations satisfy $u^2-v^2=1$ and $u^2+v^2=1/[1-r^2(k)]^{1/2}$. The mean a-spin operator $S^z=2/N\sum_i S_{ai}^z=2/N\sum_i(\frac{1}{2}-a_i^{+}a_i)$ can be expressed in terms of $A(k)$ and $B(k)$ as

$$S^z=\tfrac{1}{2}-2/N\sum_k\{u^2(k)A^{\dagger}(k)A(k)+v^2(k)B(k)B^{\dagger}(k)+u(k)v(k)[A(k)B(k)+A^{\dagger}(k)B^{\dagger}(k)]\}. \tag{10}$$

Because the ground state $|\rangle$ is defined by $A|\rangle=B|\rangle=0$, the mean value of the spin z component in the ground state is given by

$$S_0^z=\tfrac{1}{2}-2/N\sum_k v^2(k)=1-1/N\sum_k 1/[1-r^2(k)]^{1/2}. \tag{11}$$

The above k summation can be transformed into k integration. For small g, we obtain

$$S_0^z=1-1/16\pi^3\int d^3k/[1-r^2(k)]^{1/2}. \tag{12}$$

S_0^z varies with the parameter g. $S_0^z=0.303$ and 0.422 when $g=0$ and 1, respectively. These results are in agreement with Anderson's result[9] and Monte Carlo results.[6] S_0^z increases with g when $0<g<1$. Since $S_0^z<\frac{1}{2}$, the ground state is not a precise Néel AFM state, but a renormalized Néel AFM state with average staggered magnetic moment $2S_0^z\mu_B$. When $g=0$ and 1, the average moments are 0.606 and $0.844\mu_B$, respectively. These are quantitatively in agreement with experimental data.[1]

On the other hand, we can make use of the thermodynamical Green's-function method to investigate the Hamiltonian (1). This method was proposed originally by Bogoliubov to investigate ferromagnetic models.[10] Afterwards it was used in Ref. 11 to investigate AFM models. This method allows us to obtain finite temperature properties of Hamiltonian (1). To use this method, first, one has to define some necessary thermodynamical Green's functions; second, one constructs equations of motion of these Green's functions; third, one makes some proper cutoff approximations to obtain appropriate results. From Hamiltonian (1) we derive the following average z component $\langle S^z\rangle$ of a spin at temperature T (detailed calculation shall be included in another paper):

$$\langle S^z\rangle=\tfrac{1}{2}(1+W)=\tfrac{1}{2}-W/2, \tag{13}$$

where W is defined by

$$W=1/N\sum_k\{JZ\coth[\langle S^z\rangle e(k)/2T]/e(k)-1\}. \tag{14}$$

Equations (13) and (14) are enough to determine the average staggered magnetic moment $\langle S^z\rangle$ at any nonzero finite temperature T.

$\langle S^z\rangle$ can be worked out at low temperature.

$$\langle S^z\rangle=S_0^z-f(g)(T/JZS)^2+O(T/JZS)^4. \tag{15}$$

In the above equation $S=\frac{1}{2}$ for the case we discuss and $f(g)=(2+g)^{3/2}/6g^{1/2}$. $f(1)=\sqrt{3}/2$ is in agreement with the spin-wave theory given by Oguchi and Kubo.[12]

$f(g)$ approaches infinity when g tends to zero. This means the coefficient of the second term approaches infinity when $g=0$. As a result, in two dimensions there is no AFM ordering above zero temperature. In order to get 3D Néel AFM ordering, g must be nonzero. As long as $g>0$, there is 3D Néel AFM ordering at finite Néel temperature $T_N>0$. To make this clearer we expand Eq. (14) in terms of $\langle S^z\rangle$. Noticing that $\langle S^z\rangle$ approaches zero when temperature T tends to T_N, we obtain

$$\langle S^z\rangle=\tfrac{1}{2}[3/G(1-T/T_N)T/T_N]^{1/2}, \tag{16}$$

where

$$T_N=JZ/4G, \tag{17}$$

$$G=2/N\sum_k 1/[1-r^2(k)]. \tag{18}$$

If $g>0$, G is finite so that T_N is larger than zero. If $g=0$, G tends to infinity and $T_N=0$. Again we come to the conclusion that there is no AFM ordering at any nonzero temperature in 2D Heisenberg antiferromagnets. When $g>0$, there are AFM phase transitions at Néel temperature T_N.

Concerning the copper oxide materials, we see that the coupling in the z direction, although very small with respect to the in-plane coupling, is essential to keep the 3D Néel AFM ordering. If the z-direction coupling is equivalent to zero, the 2D Heisenberg is obtained. But there is no magnetic ordering at finite temperature.

For small g and k, spin-wave energy is given by

$$E(k)=2J(k_x^2+k_y^2)^{1/2}. \tag{19}$$

Internal energy at low temperature is given by

$$E=\text{ground-state energy}+0.047NT^3/J^2. \tag{20}$$

Specific heat capacity is given by

$$c=0.14(T/J)^2. \tag{21}$$

The specific-heat capacity is proportional to temperature squared. This means that the copper oxide materials without doping, such as La_2CuO_4 and $RBa_2Cu_3O_6$, have no linear temperature term in specific-heat capacity at low temperature. This is in complete agreement with experimental data.[7]

Summarily, we make use of the two-sublattice approach to investigate the quasi-two-dimensional Heisenberg AFM model. It is found that the ground state of the quasi-2D ($g\ll 1$) Heisenberg AFM model is an AFM Néel state with a renormalized mean magnetic moment of $0.6\mu_B$, similar to the 2D Heisenberg AFM model. At low finite temperature, the magnetic moment is decreased with the square of the temperature, which is similar to

that in three dimensions. But the coefficient of the temperature-squared term approaches infinity when $g=0$ ($J_z/J_{xy}=0$). This is in agreement with the fact that there is no magnetic ordering at finite temperature in two dimensions. This means that the z direction coupling is essential to keep 3D AFM ordering at finite temperature in the copper oxide materials. There are AFM phase transitions when $g>0$, or $J_z/J_{xy}>0$, at the Néel temperature $T_N>0$. The low-temperature specific-heat capacity is proportional to the temperature squared. Therefore there is no linear temperature term in the specific-heat capacity in La_2CuO_4 and $RBa_2Cu_3O_6$ materials.

*Mailing address: Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, People's Republic of China.

[1]A. Aharony, R. J. Birgeneau, A. Coniglio, M. A. Kastner, and H. E. Stanley, Phys. Rev. Lett. **60**, 1330 (1988); K. B. Lyons, F. A. Fleury, L. F. Schneemeyer, and J. V. Waszczak, *ibid.* **60**, 732 (1988); J. W. Lynn, W-H. Li, H. A. Mook, B. C. Sales, and Z. Fisk, Phys. Rev. B **37**, 9844 (1988); Phys. Rev. Lett. **60**, 2781 (1988); J. M. Tranquada *et al.*, *ibid.* **60**, 156 (1988); J. H. Brewer *et al.*, *ibid.* **60**, 1073 (1988).

[2]M. Sato, S. Shamato, J. M. Tranquada, G. Shirane, and B. Keimer, Phys. Rev. Lett. **61**, 1317 (1988); R. J. Birgeneau, D. R. Gabbe, H. P. Jenssen, M. A. Kastner, P. J. Picone, T. R. Thueston, G. Shirane, Y. Endoh, M. Sato, K. Yamada, Y. Hitaka, M. Oda, Y. Enomoto, M. Suzuki, and T. Murakami; Phys. Rev. B **38**, 6614 (1988); G. Shirane, Y. Endoh, R. J. Birgeneau, A. Kastner, Y. Hidaka, M. Oda, M. Suzuki, and T. Murakami, Phys. Rev. Lett. **59**, 1613 (1987); G. Aeppli, S. M. Hayden, H. A. Mook, Z. Fisk, S-W. Cheong, D. Rytz, J. P. Remeika, G. P. Espinosa, and A. S. Cooper, *ibid.* **62**, 2052 (1989).

[3]P. W. Anderson, Science **235**, 1196 (1987), and references therein.

[4]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).

[5]A. Auerbach and D. P. Arovas, Phys. Rev. Lett. **61**, 617 (1988).

[6]J. Carlson, Phys. Rev. B **40**, 846 (1989).

[7]K. Kumagai, Y. Nakamichi, I. Watanabe, Y. Nakamura, H. Nakajima, and N. Wada, Phys. Rev. Lett. **60**, 724 (1988).

[8]J. Callaway, *Quantum Theory of the Solid State* (Academic, New York, 1976).

[9]P. W. Anderson, Phys. Rev. **86**, 694 (1952).

[10]N. N. Bogoliubov *et al.*, Dokl. Acad. Nauk. SSSR **126**, 53 (1959) [Sov. Phys. Dokl. **4**, 589 (1959)].

[11]Q.-Q. Zheng and F.-C. Pu, Wuli Xuebao (J. Phys.) **20**, 624 (1964); J-H. Chai *et al.*, *Green's Function Theory of Quantum Statistics* (Science, Beijing, 1982) (in Chinese).

[12]T. Oguchi, Phys. Rev. **117**, 117 (1960); R. Kubo, *ibid.* **87**, 568 (1952).