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Magnetic properties of a quasi-two-dimensional Heisenberg antiferromagnetic model

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Abstract. On the basis of a two-sublattice approximation of antiferromagnets, it is obtained that ground states of quasi-two-dimensional Heisenberg antiferromagnets on simple cubic lattices are Néel states whose mean staggered spin is equivalent to 0.303–0.422 corresponding to $J_\perp/J_\parallel = 0$–1. The low-temperature mean magnetic moment and Néel temperature are calculated for various $J_\perp/J_\parallel$. There is no Néel ordering at any non-zero temperature in two-dimensional antiferromagnets. $J_\perp$ is necessary to maintain Néel ordering at finite temperatures.

$La_{2-x}(Ba, Sr)_xCuO_4$ ($x < 0.03$) and $RBa_2Cu_3O_{6+y}$ ($y < 0.4$) exhibit three-dimensional Néel antiferromagnetic (AFM) ordering with a staggered magnetic moment of about $0.6\mu_B$ (μ_B is the Bohr magneton), and their Néel temperatures are about 300 K and 450 K, respectively [1]. Coupling between CuO_2 planes is much weaker than in-plane coupling. Their two-dimensional (2D) excitations are spin waves with Heisenberg coupling constants J of 950 and 1300 K in La–(Ba, Sr)–Cu–O and R–Ba–Cu–O, respectively [2]. The cupric oxide materials can be described by a quasi-2D simple cubic Hubbard model with a large on-site Coulomb repulsion [3]. There are no dopants in ideal CuO_2 planes. This corresponds to La_2CuO_4 and $RBa_2Cu_3O_6$. In these cases the Hubbard models are half filled and are equivalent to the following AFM Heisenberg model on a simple cubic lattice because of the large Coulomb on-site repulsion:

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

$J_{ij} = J$ only when i and j are nearest-neighbour sites within a single CuO_2 plane, and $J_{ij} = \delta J$ when i and j are nearest-neighbour sites in the direction perpendicular to CuO_2 planes.

If $\delta = 0$, the Hamiltonian (1) reduces to a 2D Heisenberg AFM model on a square lattice:

$$H = J \sum_{\langle kl \rangle} \boldsymbol{S}_k \cdot \boldsymbol{S}_l \tag{2}$$

where $\langle kl \rangle$ are the nearest-neighbour sites within a 2D square lattice or a single CuO_2 plane.

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In [4] a 2+1-dimensional non-linear sigma model was used to approximate the 2D AFM Heisenberg model (2) and it was found that the correlation length had a renormalised classical behaviour $\kappa^{-1} = \exp(-A/T)$, where A/T is not equivalent to zero when T tends to zero. In [5] a mean-field method was used to investigate the model (2). The approach provided a Bose-liquid description of the excitations. In [6], making use of the Monte Carlo method, the Néel AFM ordered ground state of the 2D antiferromagnet (2) on 32×32 sites of a square lattice, whose staggered spin is 0.334 ± 0.001, was obtained.

However, the Mermin–Wagner [7] theorem excludes long-range magnetic ordering at finite temperatures in the Hamiltonian (2). In the 1960s and 1970s, to describe layer-like materials, workers usually introduced anisotropic fields or Ising-like anisotropy in their 2D models [8]. Lines [9] introduced a kind of interlayer coupling J' but concluded that 'for a given anisotropic field the existence of a non-zero J' always decreases T_N whether its sign is positive or negative'.

In this paper, we shall use the two-sublattice approximation to investigate the quasi-2D model (1). We obtain the Néel AFM ground states for all δ. The corresponding staggered moment is $0.606\ \mu_B$–$0.844\ \mu_B$. The low-temperature moment decreases with increasing square of the temperature, but the coefficients of the temperature-squared terms approach infinity when δ tends to zero. This means that 2D Heisenberg antiferromagnets have no Néel AFM ordering at any non-zero temperature, in agreement with the Mermin–Wagner [7] theorem. The Néel temperatures for various δ are calculated. The Néel temperatures 300 K and 450 K correspond to $\delta = 0.005$ and 0.008 for La_2CuO_4 and $RBa_2Cu_3O_6$, respectively. When δ tends to zero, the Néel temperature approaches zero as $1/\ln\delta$. $\delta > 0$ or $J_\perp > 0$ is necessary to keep Néel ordering at finite temperatures.

Making use of the two-sublattice approximation, we divide the simple cubic lattice into two sublattices, labelled a and b. Every sublattice is a FCC lattice. We apply the definition that spins on sublattice a are up and spins on sublattice b are down.

After Holstein–Primakoff transformations of sublattices a and b, Hamiltonian (1) is transformed into momentum space (k_x, k_y, k_z) and then diagonalised (for details, see Callaway's book [10] or Anderson's paper [11]):

$$H = E_0 + \sum_k \varepsilon(k)(A_k^+ A_k + B_k^+ B_k) \tag{3}$$

where

$$E_0 = -NJZS^2\left(1 - \frac{2}{N}\sum_k \frac{[1 - r^2(k)]^{1/2}}{S}\right) \tag{4}$$

$$\varepsilon(k) = JZ\sqrt{1 - r^2(k)} \tag{5}$$

$$r(k) = (2\cos k_x + 2\cos k_y + 2\delta\cos k_z)/Z. \tag{6}$$

In the above equations, N is the total site number, $S = \frac{1}{2}$ is the spin on a single site, and $Z = 4 + 2\delta$ is the effective coordination number. Mean lattice a and b spin operators $S^3 = (2/N)\Sigma_j S_j^3$ can be expressed in terms of operators A_k and B_k:

$$S^3 = \frac{1}{2} - \frac{2}{N}\sum_k [\alpha_k^2 A_k^+ A_k + \beta_k^2 B_k B_k^+ + \alpha_k\beta_k(A_k B_k + B_k^+ A_k^+)]. \tag{7}$$

α_k and β_k satisfy $\alpha_k^2 - \beta_k^2 = 1$ and $\alpha_k^2 + \beta_k^2 = 1/\sqrt{1 - r^2(k)}$. The ground state $|\ \rangle$ is

Table 1. Some mean spins at zero temperature for different $\delta = J_\perp/J_\parallel$.

δ	1	0.5	0.1	0.05	0.01
S	0.422	0.412	0.371	0.355	0.327
δ	0.005	0.001	0.0005	0.0001	0
S	0.320	0.308	0.304	0.303	0.303

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

$$S_0^3 = \frac{1}{2} - \frac{2}{N}\sum_k \beta_k^2 = 1 - \frac{1}{N}\sum_k \frac{1}{[1 - r^2(k)]^{1/2}}. \tag{8}$$

The above k-summation can be changed into k-integration when N tends to infinity:

$$S_0^3 = 1 - (2\pi)^{-3} \int \frac{\mathrm{d}^3 k}{[1 - r^2(k)]^{1/2}}. \tag{9}$$

The integral region is the first Brillouin zone of the FCC lattice. Table 1 presents some S_0^3-values corresponding to different δ-values. As two special cases $S_0^3 = 0.422$ and 0.303 when $\delta = 1$ and 0, respectively, in agreement with the results of Anderson [11].

To investigate the quasi-2D antiferromagnet (1) at non-zero temperatures we shall use the thermodynamical Green function method in the following. This method was first developed by Bogoliubov *et al* [12] to investigate Heisenberg ferromagnets, but it was used effectively to investigate Heisenberg antiferromagnets as well [8, 9, 13]. The routine for quasi-2D Heisenberg antiferromagnets is as follows. The general routine can be found in [8, 9, 13].

Because of symmetry, we change the Hamiltonian (1) to

$$H = \sum_{\langle i_a j_b \rangle} J_{i_a j_b}[-S_{i_a}^3 S_{j_b}^3 + \tfrac{1}{2}(S_{i_a}^+ S_{j_b}^+ + S_{i_a}^- S_{j_b}^-)] \tag{10}$$

by means of the following transformation:

$$S_{j_b}^3 \to -S_{j_b}^3 \qquad S_{j_b}^{\pm} \to S_{j_b}^{\mp}. \tag{11}$$

i_a takes the value on lattice a, and j_b on lattice b.

The retarded and advanced thermodynamical Green functions are defined as

$$G^R(t - t') = \langle\langle A(t), B(t')\rangle\rangle_R = -i\theta(t - t')\langle[A(t), B(t')]\rangle \tag{12}$$

$$G^A(t - t') = \langle\langle A(t), B(t)\rangle\rangle_A = i\theta(t - t')\langle[A(t), B(t')]\rangle \tag{13}$$

where $\langle P\rangle = \mathrm{Tr}[\exp(-\beta H)P]/\mathrm{Tr}[\exp(-\beta H)]$ and $A(t) = \exp(iHt)\,A\,\exp(-iHt)$.

Defining

$$\langle B(t')A(t)\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} J(\omega) \exp[-\mathrm{i}\omega(t-t')] \tag{14}$$

$$G^{\mathrm{A,R}}(t,t') = \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{2\pi} G^{\mathrm{A,R}}(E) \exp[-\mathrm{i}E(t-t')]. \tag{15}$$

$G^{\mathrm{A}}(E)$ and $G^{\mathrm{R}}(E)$ can be incorporated into one single Green function $G(E)$:

$$G(E) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} J(\omega) \frac{\exp(\beta\omega)-1}{E-\omega}. \tag{16}$$

$\langle B(t')A(t)\rangle$ can be expressed in terms of $G(E)$:

$$\langle B(t')A(t)\rangle = \mathrm{i}\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{G(\omega+\mathrm{i}0^+) - G(\omega-\mathrm{i}0^+)}{\exp(\beta\omega)-1} \exp[-\mathrm{i}\omega(t-t')]. \tag{17}$$

$\langle\langle S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle$ and $\langle\langle S_{i_\mathrm{b}}^-(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle$ have the following equations of motion:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle = \delta(t-t')\langle[S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')]\rangle + \left\langle\left\langle \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')\right\rangle\right\rangle$$

$$= 2\delta(t-t')\delta_{i_\mathrm{a}j_\mathrm{a}}\langle S_{i_\mathrm{a}}^3\rangle + \sum_{j_\mathrm{b}} J_{i_\mathrm{a}j_\mathrm{b}}\langle\langle S_{i_\mathrm{a}}^+(t)S_{j_\mathrm{b}}^3(t) + S_{i_\mathrm{a}}^3(t)S_{j_\mathrm{b}}^-(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle \tag{18}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle S_{i_\mathrm{b}}^-(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle = -\sum_{i_\mathrm{a}} J_{i_\mathrm{a}i_\mathrm{b}}\langle\langle S_{i_\mathrm{a}}^3(t)S_{i_\mathrm{b}}^-(t) + S_{i_\mathrm{a}}^+(t)S_{i_\mathrm{b}}^3(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle. \tag{19}$$

Making the cut-off approximation the above two equations reduce to the following two equations:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle = 2\delta(t-t')\delta_{i_\mathrm{a}j_\mathrm{a}}\langle S_{i_\mathrm{a}}^3\rangle$$

$$+ J\langle S_{i_\mathrm{a}}^3\rangle\left(Z\langle\langle S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle + \sum_{i_\mathrm{b}} \langle\langle S_{i_\mathrm{b}}^-(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle\right) \tag{20}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\langle\langle S_{i_\mathrm{b}}^-(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle = -J\langle S_{i_\mathrm{a}}^3\rangle\left(Z\langle\langle S_{i_\mathrm{b}}^-(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle + \sum_{i_\mathrm{a}} \langle\langle S_{i_\mathrm{a}}^+(t), S_{j_\mathrm{a}}^-(t')\rangle\rangle\right). \tag{21}$$

Solving equations (20) and (21), we obtain

$$\langle\langle S_{i_\mathrm{a}}^+, S_{j_\mathrm{a}}^-\rangle\rangle = 2\langle S^3\rangle \sum_k \exp[\mathrm{i}k(i-j)]$$

$$\times \frac{[E(k) + ZJ\langle S^3\rangle]/[E-E(k)] + [E(k) - ZJ\langle S^3\rangle]/[E+E(k)]}{E(k)}$$

$$E(k) = ZJ\langle S^3\rangle[1-r^2(k)]^{1/2} \qquad \langle S^3\rangle = \langle S_{i_\mathrm{a}}^3\rangle. \tag{22}$$

Because of equation (17), we have

Table 2. Some C and T_N/J for different $\delta = J_\perp/J_\parallel$.

δ	1	0.5	0.1	0.05	0.01	0.009
C	1.516	1.560	1.900	2.107	2.762	2.813
T_N/J	0.989	0.801	0.553	0.476	0.364	0.357
δ	0.008	0.007	0.006	0.005	0.001	0.0005
C	2.893	2.944	3.056	3.220	6.48	9.2
T_N/J	0.347	0.341	0.328	0.311	0.154	0.11

$$\langle S_{j_a}^- S_{j_a}^+ \rangle = \mathrm{i} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\langle\langle S_{j_a}^+, S_{j_a}^- \rangle\rangle(\omega + \mathrm{i}0^+) - \langle\langle S_{j_a}^+, S_{j_a}^- \rangle\rangle(\omega - \mathrm{i}0^+)}{\exp(\beta\omega) - 1} = 2\langle S^3 \rangle W \tag{23}$$

where

$$W = \frac{1}{N} \sum_k \left[\frac{ZJ\langle S^3 \rangle}{E(k)} \coth\left(\frac{\beta E(k)}{2} \right) - 1 \right]. \tag{24}$$

As a result we obtain

$$\langle S^3 \rangle = \tfrac{1}{2}(1 + 2W)^{-1} \simeq \tfrac{1}{2} - W. \tag{25}$$

Equations (24) and (25) can be used to determine the mean staggered spin $\langle S^3 \rangle$ at any non-zero temperature $T = 1/k\beta$.

When T is very small, we have $\langle S^3 \rangle = \frac{1}{2}$ as our zeroth approximation. Letting $\langle S^3 \rangle = \frac{1}{2}$ on the right-hand side of equation (25), we have as the first approximation

$$\langle S^3 \rangle = S_0^3(\delta) - \nu(\delta)(T/JZS)^2 + \mathrm{O}(T/JZS)^4. \tag{26}$$

The zero-temperature mean spins $S_0^3(\delta) = \frac{1}{2} - W_0(\delta)$ are presented in table 1. $\nu(\delta) = (2 + \delta)^{3/2}/6\sqrt{\delta}$ and $\nu(1) = \sqrt{3}/2$, which are in agreement with the spin-wave theory of Oguchi and Kubo [14]. $\nu(\delta)$ increases with decreasing δ. ν approaches infinity when $\delta \to 0$. This means that there is no Néel AFM ordering at any non-zero temperature for $\delta = 0$, or 2D antiferromagnets, in agreement with the Mermin–Wagner [7] theorem.

When the temperature approaches the Néel temperature T_N, $\langle S^3 \rangle$ should tend to zero. Therefore the right-hand side of equation (25) can be expanded in terms of $\langle S^3 \rangle$. In this way, we solve equations (25) and (24) from

$$\langle S^3 \rangle = [3T(1 - T/T_N)/4CT_N]^{1/2} \tag{27}$$

where T_N and c are expressed as follows:

$$T_N = JZ/4C \tag{28}$$

$$C = \frac{2}{N} \sum_k \frac{1}{1 - r^2(k)}. \tag{29}$$

Table 2 presents some c- and T_N/J-values corresponding to different δ-values. We observe that $c = \infty$ when $\delta = 0$. Again we come to conclusion that there is no Néel AFM ordering at any non-zero temperature for 2D antiferromagnets.

La_2CuO_4 has $T_N/J = 300/950 \simeq 0.316$. This value corresponds to $\delta \simeq 0.005$. For $RBa_2Cu_3O_6$ we have $T_N/J = 450/1300 \simeq 0.346$, which corresponds to $\delta \simeq 0.008$. We conclude that the coupling between CuO_2 planes in $RBa_2Cu_3O_6$ is stronger than that in

La_2CuO_4. Therefore, the staggered magnetic moments observed at low temperatures should be $0.64\mu_B$ and $0.65\mu_B$ for La_2CuO_4 and $Ba_2Cu_3O_6$, respectively. This is in agreement with experimental data [1].

In summary, we make use of the two-lattice approximation method to investigate the quasi-2D Heisenberg antiferromagnets (1) on a simple cubic lattice, which are believed to describe the magnetic properties of the cupric oxide materials without dopants. The ground states of the models are Néel AFM ordering states whose staggered spins vary from 0.422 to 0.303, corresponding to $\delta = J_\perp/J_\parallel = 1\text{–}0$. The low-temperature magnetic moments and Néel temperatures are calculated for various δ-values. There is no Néel AFM ordering at any non-zero temperature in 2D Heisenberg antiferromagnets. Comparison with the experimental Néel temperature leads to the conclusion that $J_\perp/J_\parallel = 0.008$ and 0.005 in La_2CuO_4 and $RBa_2Cu_3O_6$.

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