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2009 J. Phys.: Condens. Matter 21 406004

(http://iopscience.iop.org/0953-8984/21/40/406004)

J. Phys.: Condens. Matter **21** (2009) 406004 (5pp) doi:10.1088/0953-8984/21/40/406004

Non-linear spin wave theory results for the frustrated $S = \frac{1}{2}$ Heisenberg antiferromagnet on a body-centered cubic lattice

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Received 4 June 2009, in final form 13 August 2009
Published 14 September 2009
Online at stacks.iop.org/JPhysCM/21/406004

Abstract

At zero temperature the sublattice magnetization of the quantum spin-1/2 Heisenberg antiferromagnet on a body-centered cubic lattice with competing first and second neighbor exchange (J_1 and J_2) is investigated using the non-linear spin wave theory. The zero temperature phases of the model consist of a two sublattice Néel phase for small J_2 (AF_1) and a collinear phase at large J_2 (AF_2). We show that quartic corrections due to spin wave interactions enhance the sublattice magnetization in both the AF_1 and the AF_2 phase. The magnetization corrections are prominent near the classical transition point of the model and in the $J_2 > J_1$ regime. The ground state energy with quartic interactions is also calculated. It is found that up to quartic corrections the first order phase transition (previously observed in this model) between the AF_1 and the AF_2 phase survives.

1. Introduction

In recent years thermodynamic properties of frustrated quantum Heisenberg antiferromagnets have been of intense interest both theoretically and experimentally in condensed matter physics [1, 2]. The phase diagram of the quantum spin-1/2 Heisenberg antiferromagnetic (AF) model on two-dimensional (2D) lattices with nearest neighbor (J_1) and next nearest neighbor interactions (J_2) have been studied extensively by different methods [3–22]. For the square lattice with nearest neighbor (NN) exchange interaction only, the ground state is antiferromagnetically ordered at zero temperature. Addition of next nearest neighbor (NNN) interactions breaks the AF order. The competition between the NN and NNN interactions for the square lattice is characterized by the frustration parameter $p = J_2/J_1$. It has been found that a quantum spin liquid phase exists between $p_{1c} \approx 0.38$ and $p_{2c} \approx 0.60$. For $p < p_{1c}$ the lattice is AF ordered whereas for $p > p_{2c}$ a collinear phase emerges. In the collinear state the NN spins have a parallel orientation in the vertical direction and antiparallel orientation in the horizontal direction or vice versa.

Motivated by the results for the 2D lattices some work has been done by analytical and numerical techniques to understand the magnetic phase diagram of three-dimensional (3D) lattices [23–28]. Linear spin wave theory, exact diagonalization, renormalization group, and linked-cluster series expansions (at both zero and finite temperature) have been utilized to study the 3D quantum spin-1/2 Heisenberg AF on a body-centered-cubic (bcc) lattice [25, 26, 28]. It has been found that the lattice does not have a quantum disordered phase and a first-order phase transition from the AF phase (AF_1) to lamellar state (AF_2) occurs at $p_c = 0.53$ or $J_2/J_1 \approx 0.705$. The first-order nature of the phase transition from the AF_1 to the AF_2 phase in the model is inferred from a kink in the ground state energy of the system. In 1D and 2D due to reduced phase space quantum fluctuations play an important role in determining the quantum critical points of the system at low temperature. However, in 3D the phase space available is greater and quantum fluctuations play a lesser role, hence the absence of the quantum disordered phase for the BCC lattice.

In this work, we study the 3D quantum spin-1/2 AF on a bcc lattice using the non-linear spin wave theory where we

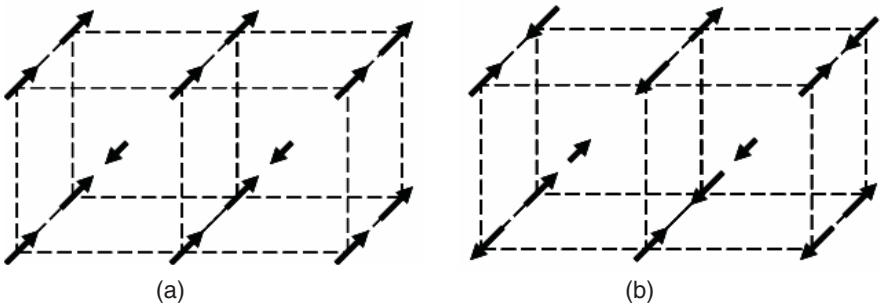

Figure 1. AF_1 and AF_2 ordered phases of the bcc lattice. (a) In the AF_1 phase all A-sublattice spins point in the direction of an arbitrary unit vector while B-sublattice spins point in the opposite direction. (b) For the AF_2 phase there are two interpenetrating Néel states, each living on the initial sublattices A and B.

consider interactions between spin waves up to quartic terms in the Hamiltonian. We compute the effect of these higher-order terms on the sublattice magnetization (see figure 2). The corrections to the magnetization become important as the classical transition point is approached. Also, our calculations re-confirm the first-order nature of the phase transition found in [25, 26] up to quartic interactions (see figure 3).

The paper is organized as follows. In section 2 we begin with a brief description of the properties of the bcc lattice relevant to our calculations. We then set up the Hamiltonian for the Heisenberg spin-1/2 AF on the bcc lattice. The classical ground state configurations of the model and the different phases are then discussed. Next we map the spin Hamiltonian to the Hamiltonian of interacting bosons and the non-linear spin wave theory for the two phases is developed. The sublattice magnetizations and the ground state energies for the two phases are numerically calculated and the results are plotted and discussed in section 3. Finally, we summarize our results in section 4.

2. Formalism

The body-centered-cubic lattice consists of two interpenetrating, identical simple cubic lattices, each of which consists of two interpenetrating, identical face-centered lattices. This makes the bcc lattice a 3D bi-bipartite cubic lattice. The basis vectors of the bcc lattice connecting eight ($z_1 = 8$) nearest neighbors are (in units of simple cubic lattice spacing) $\mathbf{a_1} = (1, 1, -1), \mathbf{a_2} = (1, -1, 1), \mathbf{a_3} = (-1, 1, 1)$ and the lattice vectors connecting six ($z_2 = 6$) next nearest neighbors are $\mathbf{b_1} = (\pm 2, 0, 0), \mathbf{b_2} = (0, \pm 2, 0)$ and $\mathbf{b_3} = (0, 0, \pm 2)$. On such a lattice the Hamiltonian for a spin-1/2 Heisenberg AF with first and second neighbor interactions is

$$H = \tfrac{1}{2} J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \tfrac{1}{2} J_2 \sum_{[ij]} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (1)$$

where J_1 is the NN and J_2 is the frustrating NNN exchange constants. Both couplings are considered AF, i.e. $J_1, J_2 > 0$.

2.1. Classical ground state configurations

The limit of infinite spin, $S \to \infty$, corresponds to the classical Heisenberg model. We assume that the set of possible spin configurations of the system is described by $S_i = S\mathbf{u}e^{i\mathbf{q}\cdot\mathbf{r}_i}$, where $\mathbf{u}$ is a vector expressed in terms of an arbitrary orthonormal basis and $\mathbf{q}$ defines the relative orientation of the spins on the lattice [29]. The classical ground state energy of the system expressed as a function of the parameters J_1 and J_2 takes the form

$$E_{\mathbf{k}}/NJ_1 = \tfrac{1}{2} S^2 z_1 [\gamma_{1\mathbf{k}} + p\gamma_{2\mathbf{k}}], \qquad (2)$$

with the structure factors

$$\gamma_{1\mathbf{k}} = \cos(k_x)\cos(k_y)\cos(k_z), \qquad (3)$$

$$\gamma_{2\mathbf{k}} = [\cos(2k_x) + \cos(2k_y) + \cos(2k_z)]/3 \qquad (4)$$

where N is the number of sites on the lattice. For our study it is convenient to define the parameter of frustration $p = z_2 J_2 / z_1 J_1$.[3]

At zero temperature, the classical ground state for the bcc lattice has two phases. In the limit of small p or $J_2 \ll J_1$ three isolated minima in energy, $E_0/NJ_1 = -4S^2(1 - p)$, occur at the wavevectors $(\pm\pi, 0, 0)$, $(0, \pm\pi, 0)$ and $(0, 0, \pm\pi)$. They correspond to the classical two sublattice Néel state (AF_1 phase) where all A-sublattice spins point in the direction of an arbitrary unit vector $\hat{\mathbf{n}}$ while B-sublattice spins point in the opposite direction $-\hat{\mathbf{n}}$.

In the other limit, for large p or $J_2 \gg J_1$, there is a single minimum in energy, $E_0/NJ_1 = -4S^2 p$, at $\mathbf{k} = (\pm\pi/2, \pm\pi/2, \pm\pi/2)$. In this case the classical ground state consists of two interpenetrating Néel states (AF_2 phase), each living on the initial sublattices A and B. The two phases are shown in figure 1.

The classical limit for the phase transition from AF_1 to AF_2 for the 3D model on the bcc lattice is at the critical value $p_c = 2z_2/3z_1 = 1/2$, i.e. when $J_2/J_1 = 2/3$. This is similar to the spin-1/2J_1–J_2 model on a 2D square lattice where the critical value of $p_c = 1/2$ or $J_2/J_1 = 1/2$.

2.2. Non-linear spin wave theory

The Hamiltonian in equation (1) can be mapped into an equivalent Hamiltonian of interacting bosons by transforming

[3] Note that p defined here differs by a factor z_2/z_1 with the definition of p in the introduction.

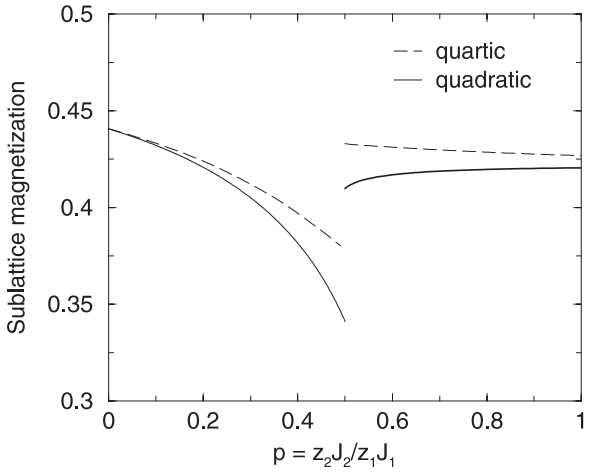

Figure 2. Sublattice magnetization, $\langle S_\alpha \rangle$, is plotted versus p for AF_1 and AF_2 ordered phases. In the AF_1 phase with increase in p the system aligns the spins antiferromagnetically along the horizontal and the vertical directions—thus decreasing the sublattice magnetization. In the AF_2 phase $\langle S_\alpha \rangle$ mostly stays the same and then shows a slight decrease (without quartic corrections) as p approaches the critical value $p_c = 0.5$ from above. However, with the quartic corrections $\langle S_\alpha \rangle$ remains almost constant at ≈0.43. In both cases quartic corrections to the Hamiltonian of the system enhance the magnetic order.

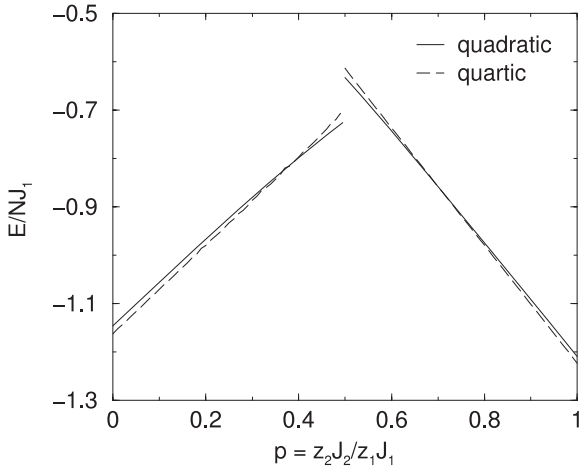

Figure 3. Ground state energy per site, E/NJ_1, is plotted as a function of the frustration parameter $p = z_2J_2/z_1J_1$ without (solid lines) and with (dashed lines) quartic corrections for both AF_1 ($p < 0.5$) and AF_2 ($p > 0.5$) ordered phases. For the bcc lattice $z_1 = 8$ and $z_2 = 6$. Spin wave theory becomes unstable at the classical transition point, i.e. $p \approx 0.5$. After extrapolation (not indicated in the figure above), we find that the two energies meet at $p \approx 0.53$ or $J_2/J_1 \approx 0.705$. The kink in the energy at this value of p indicates a first-order quantum phase transition from AF_1 to AF_2 phase.

the spin operators to bosonic operators $a, a^\dagger$ for the A sublattice and $b, b^\dagger$ for the B sublattice using the well known Holstein–Primakoff transformations [30]

$$S^+_{Ai} \approx \sqrt{2S}\Big(1 - \frac{a_i^\dagger a_i}{4S}\Big)a_i, \qquad S^-_{Ai} \approx \sqrt{2S}a_i^\dagger\Big(1 - \frac{a_i^\dagger a_i}{4S}\Big),$$
$$S^z_{Ai} = S - a_i^\dagger a_i, \qquad S^+_{Bj} \approx \sqrt{2S}b_j^\dagger\Big(1 - \frac{b_j^\dagger b_j}{4S}\Big),$$
$$S^-_{Bj} \approx \sqrt{2S}\Big(1 - \frac{b_j^\dagger b_j}{4S}\Big)b_j, \qquad S^z_{Bj} = -S + b_j^\dagger b_j. \tag{5}$$

In these transformations we have kept terms up to the order of $1/S$. Next using the Fourier transforms

$$a_i = \sqrt{\frac{2}{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R_i}}a_{\mathbf{k}}, \qquad b_j = \sqrt{\frac{2}{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R_j}}b_{\mathbf{k}},$$

the real space Hamiltonian is transformed to the **k**-space Hamiltonian. The reduced Brillouin zone contains $N/2$ **k** vectors as the unit cell is a magnetic supercell consisting of an A site and a B site. In the following two sections we study the cases $J_2 < J_1$ and $J_2 > J_1$ separately.

2.2.1. $J_2 < J_1$: AF_1 phase. In this phase the classical ground state is the two sublattice Néel state (see figure 1). For the NN interaction, spins in the A sublattice interact with spins in the B sublattice and vice versa. On the other hand, for the NNN exchange J_2 connects spins on the same sublattice, A with A and B with B. Substituting equations (5) into (1), expanding the radical, and restricting to terms only up to the anharmonic quartic terms, we obtain the **k**-space Hamiltonian

$$H = H^{(0)} + H^{(2)} + H^{(4)}. \tag{6}$$

The classical ground state energy $H^{(0)}$ and the quadratic terms $H^{(2)}$ are

$$H^{(0)} = -\tfrac{1}{2}NJ_1S^2z_1(1-p) \tag{7}$$
$$H^{(2)} = J_1Sz_1\sum_{\mathbf{k}}[A_{0\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}) + B_{0\mathbf{k}}(a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}}b_{\mathbf{k}})], \tag{8}$$

with the coefficients $A_{0\mathbf{k}}$ and $B_{0\mathbf{k}}$ defined as

$$A_{0\mathbf{k}} = 1 - p(1-\gamma_{2\mathbf{k}}), \tag{9}$$
$$B_{0\mathbf{k}} = \gamma_{1\mathbf{k}}. \tag{10}$$

The quartic terms in the Hamiltonian $H^{(4)}$ are

$$H^{(4)} = -J_1\sum_{\langle ij\rangle}[a_i^\dagger a_i b_j^\dagger b_j + \tfrac{1}{4}(a_i b_j^\dagger b_j b_j + a_i^\dagger a_i a_i b_j + \text{h.c.})] + \tfrac{1}{2}J_2\sum_{[ij]}[a_i^\dagger a_i a_j^\dagger a_j - \tfrac{1}{4}(a_i a_j^\dagger a_j^\dagger a_j + a_i^\dagger a_i a_i a_j^\dagger + \text{h.c.}) + a \leftrightarrow b]. \tag{11}$$

These terms are evaluated by applying the Hartree–Fock decoupling process [31]. In the harmonic approximation the following Hartree–Fock averages are non-zero for the bcc lattice Heisenberg AF:

$$u = \langle a_i^\dagger a_i\rangle = \langle b_i^\dagger b_i\rangle = \frac{1}{2}\Big[\frac{2}{N}\sum_{\mathbf{k}}\frac{A_{0\mathbf{k}}}{\omega_{0\mathbf{k}}} - 1\Big], \tag{12}$$

$$v = \langle a_i b_j\rangle = \langle a_i^\dagger b_j^\dagger\rangle = -\frac{1}{2}\Big[\frac{2}{N}\sum_{\mathbf{k}}\frac{\gamma_{1\mathbf{k}}B_{0\mathbf{k}}}{\omega_{0\mathbf{k}}}\Big], \tag{13}$$

$$w = \langle a_i^\dagger a_j\rangle = \langle b_i^\dagger b_j\rangle = \frac{1}{2}\Big[\frac{2}{N}\sum_{\mathbf{k}}\frac{\gamma_{2\mathbf{k}}A_{0\mathbf{k}}}{\omega_{0\mathbf{k}}}\Big], \tag{14}$$

where $\omega_{0\mathbf{k}} = \sqrt{A_{0\mathbf{k}}^2 - B_{0\mathbf{k}}^2}$.

The contributions of the decoupled quartic terms to the harmonic Hamiltonian in equation (8) are to renormalize the values of $A_{0\mathbf{k}}$ and $B_{0\mathbf{k}}$, which are now

$$A_{\mathbf{k}} = \Big(1 - \frac{u+v}{S}\Big) - p[1-\gamma_{2\mathbf{k}}]\Big(1 - \frac{u-w}{S}\Big), \tag{15}$$

$$B_{\mathbf{k}} = \gamma_{1\mathbf{k}}\Big(1 - \frac{u+v}{S}\Big), \tag{16}$$

$$\omega_{\mathbf{k}} = \sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}. \tag{17}$$

The quartic correction to the ground state energy is calculated from the four boson averages. In the leading order they are decoupled into the bilinear combinations (equations (12)–(14)) using Wick's theorem. The corresponding four boson terms are

$$\begin{aligned} &\langle a_i^\dagger a_i b_j^\dagger b_j\rangle = u^2 + v^2, \qquad \langle a_i^\dagger b_j^\dagger b_j b_j\rangle = 2uv, \\ &\langle a_i^\dagger a_i a_i b_j\rangle = 2uv, \qquad \langle a_i^\dagger a_i a_j^\dagger a_j\rangle = u^2 + w^2, \\ &\langle a_i a_j^\dagger a_j^\dagger a_j\rangle = 2uw, \qquad \langle a_i^\dagger a_i a_i a_j^\dagger\rangle = 2uw. \end{aligned} \tag{18}$$

This yields the ground state energy correction from the quartic terms,

$$\delta E^{(4)} = -\tfrac{1}{2} N J_1 z_1 [(u+v)^2 - p(u-w)^2]. \tag{19}$$

Summing all the corrections together, the ground state energy takes the form

$$\begin{aligned} E/NJ_1 = &-\frac{1}{2} z_1 S(S+1)(1-p) + \frac{1}{2} z_1 S\Big[\frac{2}{N}\sum_{\mathbf{k}} \omega_{\mathbf{k}}\Big] \\ &+ \tfrac{1}{2} z_1 [(u+v)(1-u-v) - p(u-w)(1-u+w)] \end{aligned} \tag{20}$$

and the sublattice magnetization $\langle S_\alpha\rangle$ at zero temperature is given by

$$\langle S_\alpha\rangle = S\Big[1 - \frac{1}{2S}\Big\{\frac{2}{N}\sum_{\mathbf{k}} \frac{A_{\mathbf{k}}}{\omega_{\mathbf{k}}} - 1\Big\}\Big]. \tag{21}$$

Using equations (15)–(17), we numerically evaluate E/NJ_1 and $\langle S_\alpha\rangle$. For the bcc lattice the $\mathbf{k}$-sum is replaced by an integral over the Brillouin zone [32],

$$\frac{2}{N}\sum_{\mathbf{k}} \to \frac{1}{\pi^3}\int_0^\pi \int_0^\pi \int_0^\pi \mathrm{d}k_x\, \mathrm{d}k_y\, \mathrm{d}k_z. \tag{22}$$

2.2.2. $J_2 > J_1$: AF_2 phase. The classical ground state for $J_2 > J_1$ corresponds to a four sublattice state where each of the A and B sublattices is itself antiferromagnetically ordered (see figure 1). For the NN exchange there are four A–A, four B–B, and eight A–B type interactions between the sublattices. In case of NNN exchanges there are a total of 12 A–B type interactions. Adding all their contributions together up to the quadratic terms the harmonic Hamiltonian takes the same form as equation (8) with

$$H^{(0)} = -\tfrac{1}{2} N J_1 S^2 z_1 p, \tag{23}$$

$$A_{0\mathbf{k}} = \tfrac{1}{2}(\gamma_{1\mathbf{k}} + 2p), \tag{24}$$

$$B_{0\mathbf{k}} = \tfrac{1}{2}(\gamma_{1\mathbf{k}} + 2p\gamma_{2\mathbf{k}}). \tag{25}$$

The quartic terms in the Hamiltonian for this case are

$$\begin{aligned} H^{(4)} = &-J_1 \sum_{\langle ij\rangle} [a_i^\dagger a_i b_j^\dagger b_j + \tfrac{1}{4}(a_i b_j^\dagger b_j b_j \\ &+ a_i^\dagger a_i a_i b_j + \text{h.c.})] + \tfrac{1}{2} J_1 \sum_{\langle ij\rangle} [a_i^\dagger a_i a_j^\dagger a_j - \tfrac{1}{4}(a_i a_j^\dagger a_j^\dagger a_j \\ &+ a_i^\dagger a_i a_i a_j^\dagger + \text{h.c.}) + a \leftrightarrow b] - J_2 \sum_{\langle ij\rangle} [a_i^\dagger a_i b_j^\dagger b_j \\ &+ \tfrac{1}{4}(a_i b_j^\dagger b_j b_j + a_i^\dagger a_i a_i b_j + \text{h.c.})]. \end{aligned} \tag{26}$$

These terms are decoupled and evaluated in the same way as before. The renormalized values of the coefficients $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are

$$A_{\mathbf{k}} = \frac{1}{2}\Big[\gamma_{1\mathbf{k}}\Big(1 - \frac{u-\bar{w}}{S}\Big) - \frac{v+\bar{w}}{S} + 2p\Big(1 - \frac{u+\bar{v}}{S}\Big)\Big], \tag{27}$$

$$B_{\mathbf{k}} = \frac{1}{2}\Big[\gamma_{1\mathbf{k}}\Big(1 - \frac{u+v}{S}\Big) + 2p\gamma_{2\mathbf{k}}\Big(1 - \frac{u+\bar{v}}{S}\Big)\Big], \tag{28}$$

where

$$\bar{v} = -\frac{1}{2}\Big[\frac{2}{N}\sum_{\mathbf{k}} \frac{\gamma_{2\mathbf{k}} B_{0\mathbf{k}}}{\omega_{0\mathbf{k}}}\Big], \tag{29}$$

$$\bar{w} = \frac{1}{2}\Big[\frac{2}{N}\sum_{\mathbf{k}} \frac{\gamma_{1\mathbf{k}} A_{0\mathbf{k}}}{\omega_{0\mathbf{k}}}\Big]. \tag{30}$$

In equations (27) and (28) u, v have the same form as in equations (12) and (13) but they are evaluated with the coefficients $A_{0\mathbf{k}}$ and $B_{0\mathbf{k}}$ in equations (24) and (25). The quartic correction to the ground state energy is

$$\delta E^{(4)} = \tfrac{1}{2} N J_1 z_1 \{(u-\bar{w})^2 - (u+v)^2 - p(u+\bar{v})^2\}. \tag{31}$$

Combining all these corrections, the ground state energy is

$$\begin{aligned} E/NJ_1 = &-\frac{1}{2} z_1 S(S+1)p + \frac{1}{2} z_1 S\Big[\frac{2}{N}\sum_{\mathbf{k}} \omega_{\mathbf{k}}\Big] \\ &+ \tfrac{1}{4} z_1 [(v+\bar{w})(1-2u-v+\bar{w}) \\ &+ 2p(u+\bar{v})(1-u-\bar{v})]. \end{aligned} \tag{32}$$

The sublattice magnetization and ground state energy are then obtained numerically using equations (21), (27), (28), and (32).

3. Results

In figure 2 we show the results for the sublattice magnetization, $\langle S_\alpha\rangle$, obtained numerically from equation (21) for both AF_1 and AF_2 phases with (dashed line) and without (solid line) quartic corrections. In the AF_1 ordered phase or the two sublattice Néel phase where A and B sublattice spins point in the opposite directions, sublattice magnetization decreases monotonically with increase in p until $p \approx 0.5$. The curve starts at ≈0.44 for $p = 0$ and ends at ≈0.34 for $p = 0.5$. The gradual decrease in $\langle S_\alpha\rangle$ is expected with increase in p as increasing strength of NNN interaction J_2 aligns the spins antiferromagnetically along the horizontal and the vertical directions. The quartic corrections produce a change in the

sublattice magnetization, $\langle S_\alpha \rangle$, which becomes significant as one approaches the classical transition point $p_c = 0.5$ (see figure 2). With quartic corrections the magnetization curve starts at ≈0.44 for $p = 0$ and ends at ≈0.38 for $p = 0.49$. At $p = 0$ (no frustration) there is no quartic corrections to $\langle S_\alpha \rangle$. This can be observed from equations (15)–(17), (21) as the correction factor $(1 - (u + v)/S)$ cancels out in equation (21). At the wavevector $\mathbf{k} = (\pm\pi/2, \pm\pi/2, \pm\pi/2)$ spin wave theory calculations become unstable (at $p_c \approx 0.5$) since the coefficient $A_\mathbf{k}$ becomes equal to $B_\mathbf{k}$.

In the AF_2 ordered phase or the lamellar phase with two interpenetrating Néel states, sublattice magnetization stays mostly flat except for a slight decrease (without quartic corrections) as p approaches the critical value p_c from above. The curve starts at ≈0.42 for $p = 1$ and ends at ≈0.41 for $p = 0.5$. However, with quartic corrections the curve has a very small upward turn. This upward curve has been observed in previous numerical works on this model [25, 26]. For the AF_2 phase, quartic fluctuations produce an overall enhancement of the magnetization over the high-p values (0.5–1), but for low p (0–0.5) with increase in frustration quantum spin fluctuations play a dominant role, as seen in figure 2.

In figure 3 we plot the ground state energy per site, E/NJ_1, for the AF_1 and AF_2 phases with and without quartic corrections as a function of the frustration parameter $p = z_2 J_2/z_1 J_1$. $p_c = 0.5$ is the classical transition point where a phase transition from the AF_1 phase to the AF_2 phase occurs. The quadratic calculation agrees well with the results of [25, 26]. The quartic corrections to the energy are shown by the dashed lines in figure 3. At $p = 0$ the calculated energy with the quartic correction is slightly lower than the energy calculated without the quartic interaction terms. This small decrease from the linear spin wave theory calculation is due to the ground state energy correction, which is negative (as seen in equation (19)) from the quartic terms (self-energy Hartree diagrams). This trend for low p continues until $p \approx 0.38$, after which the energy with quartic corrections becomes dominant. For large p, we find the energy with quartic corrections to be lower than the energy calculated without the quartic interactions in the interval ≈0.70–1. In both the phases quantum spin fluctuations tend to maintain the magnetic order by lowering the ground state energies. As p approaches the critical value p_c from both phases, frustration increases, causing the ground state energies to increase. Then $1/S$ corrections due to spin fluctuations play a lesser role. As mentioned in the magnetization calculation, our non-linear spin wave analysis becomes unstable at the classical transition point $p_c = 0.5$. After extrapolation of the ground state energy curve from the AF_1 phase in the regime where non-linear spin wave theory breaks down, we find that the energies from the two phases meet at $p \approx 0.53$.[4] The kink at this point signals that a first-order phase transition occurs from AF_1 to AF_2 phase.

4. Conclusions

In this work we have investigated the zero temperature $1/S$ corrections to the sublattice magnetization and ground state energy of a spin-1/2 Heisenberg frustrated antiferromagnet on a bcc lattice using the framework of non-linear spin wave theory. We have found that $1/S$ corrections due to spin wave interactions cause noticeable changes to the sublattice magnetization for both the two sublattice Néel phase (small NNN interaction J_2) and the AF_2 phase or the lamellar phase (large J_2). As non-linear spin wave theory calculations become unstable close to the classical transition point we are unable to analyze the nature of the phase transition using this method. We also confirm that up to quartic corrections the system undergoes a first-order phase transition, as indicated by a kink in the energy calculation.

[4] To avoid confusion we have not shown the extrapolated line in figure 3.

Acknowledgment

One of us (KM) thanks O Starykh for helpful discussions.

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