

# Zero Temperature Phases of the Frustrated $J_1$ – $J_2$ Antiferromagnetic Spin-1/2 Heisenberg Model on a Simple Cubic Lattice

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**Abstract** At zero temperature magnetic phases of the quantum spin-1/2 Heisenberg antiferromagnet on a simple cubic lattice with competing first and second neighbor exchanges ( $J_1$  and  $J_2$ ) is investigated using the non-linear spin wave theory. We find existence of two phases: a two sublattice Néel phase for small  $J_2$  (AF), and a collinear antiferromagnetic phase at large  $J_2$  (CAF). We obtain the sublattice magnetizations and ground state energies for the two phases and find that there exists a first order phase transition from the AF-phase to the CAF-phase at the critical transition point,  $p_c = 0.56$  or  $J_2/J_1 = 0.28$ . We also show that the quartic  $1/S$  corrections due spin-wave interactions enhance the sublattice magnetization in both the phases which causes the intermediate paramagnetic phase predicted from linear spin wave theory to disappear.

**Keywords** Magnetism · Frustrated magnetic spin systems · Quantum phase transition · Heisenberg spin systems

## 1 Introduction

Frustrated quantum Heisenberg magnets with competing nearest neighbor (NN) and next-nearest-neighbor (NNN) antiferromagnet (AF) exchange interactions,  $J_1$  and  $J_2$  respectively, have been under intense investigation both theoretically and experimentally in condensed matter physics for more than two decades [1]. At low temperatures these systems exhibit new types of magnetic order and novel quantum phases [1–3]. A well-known example is the quantum spin-1/2 antiferromagnetic  $J_1$ – $J_2$  model on a square lattice, which has been studied extensively by various analytical and numerical methods [4–14]. For this

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two-dimensional square lattice system with  $J_2 = 0$  the ground state is antiferromagnetically ordered at zero temperature. Addition of next nearest neighbor interactions induces a strong frustration and break the antiferromagnetic (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 disordered quantum spin liquid phase exists between  $p_{1c} \approx 0.38$  and  $p_{2c} \approx 0.60$ . For  $p < p_{1c}$  the square 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. The nature of phase transition from AF-ordered state to disordered state at  $p_{1c}$  is of second order and from the disordered state to the collinear state at  $p_{2c}$  is of first order.

The properties of quantum magnets depend strongly on the lattice dimensionality since the tendency to order is more pronounced in three dimensional (3D) systems than in the lower dimensional systems. Furthermore, in 3D the available phase space is more and we expect quantum fluctuations to play a lesser role as compared to 1D and 2D. In 1D and 2D the available phase space is limited and quantum fluctuations play a dominant role in determining the quantum critical points. Despite this fact a magnetically disordered phase has been observed in frustrated 3D systems such as the Heisenberg AF on the pyrochlore lattice [15] or on the stacked kagome lattice [16–19]. Studies on the Heisenberg AF on the pyrochlore lattice (a geometrically frustrated system) have revealed the existence of a spin liquid state [15]. On the other hand, for the 3D  $J_1$ – $J_2$  model on the body-centered cubic (BCC) lattice there are no signs of an intermediate quantum paramagnetic phase at zero temperature [20–22]. For the BCC lattice competing interactions and not lattice geometry generates the frustration. This comparison illustrates how the magnetic phase diagram may dramatically change based on whether the frustration is generated by *competing interactions* or by *geometry*.

Most of the efforts on quantum 3D magnets have primarily focused on geometrically frustrated lattices [1, 2]. There exists some computational [20, 21, 23–33] and very few analytical studies [22, 29, 34, 35] of the magnetic phase diagrams and magnetic order of spin-1/2 Heisenberg AF on 3D lattices where *competing interactions induce frustration* [20–35].

Very few analytical and numerical results exist for the frustrated  $J_1$ – $J_2$  isotropic Heisenberg model on a simple cubic lattice [14, 36–38]. In a recent work the critical properties of the 3D anisotropic quantum spin-1/2 model on a simple cubic (SC) lattice has been investigated within the framework of the differential operator technique and by using an effective field theory in a two-spin cluster [39]. The study revealed that at zero temperature there is a AF-lamellar (first order) phase transition. This work is sequel to our previously published work on the BCC lattice [22]. The motivation for the present work is to investigate the zero temperature phases of this model in the framework of non-linear spin wave theory (NLSWT) and to obtain the critical transition points of this model. Also we will compare our results from NLSWT with the prediction from the linear spin wave theory (LSWT).

The paper is organized as follows. In Sect. 2 we set-up the Hamiltonian for the spin-1/2 Heisenberg AF on the SC lattice. The classical ground state configurations of the model and the different phases are then discussed. In Sect. 3 we map the spin Hamiltonian to the Hamiltonian of interacting bosons and develop the NLSWT sublattice magnetization and energy expressions. The sublattice magnetizations and the ground state energies for the two phases are numerically calculated and the results are plotted and discussed in Sect. 4. Finally we summarize our findings in Sect. 5.

## 2 Classical Ground State Configurations

The Hamiltonian for a spin-1/2 Heisenberg antiferromagnet with first and second neighbor interactions on a simple cubic (SC) lattice is

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

$J_1$  is the NN and  $J_2$  is the frustrating NNN (which are along the face diagonals of the cube) exchange constants. Both couplings are considered antiferromagnetic, i.e.  $J_1, J_2 > 0$ . For the SC lattice the number of nearest and next-nearest neighbors are  $z_1 = 6$  and  $z_2 = 12$ .

The limit of infinite spin,  $S \rightarrow \infty$ , corresponds to the classical Heisenberg model. We assume that classically the spin configurations of the system are 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. The classical ground state energy of the lattice in terms of the frustration parameter,  $p$ , is given by

$$E_{\mathbf{k}}/N J_1 = \frac{1}{2} S^2 z_1 [\gamma_{1\mathbf{k}} + p \gamma_{2\mathbf{k}}], \quad (2)$$

with the structure factors

$$\gamma_{1\mathbf{k}} = \frac{1}{3} [\cos(k_x) + \cos(k_y) + \cos(k_z)], \quad (3)$$

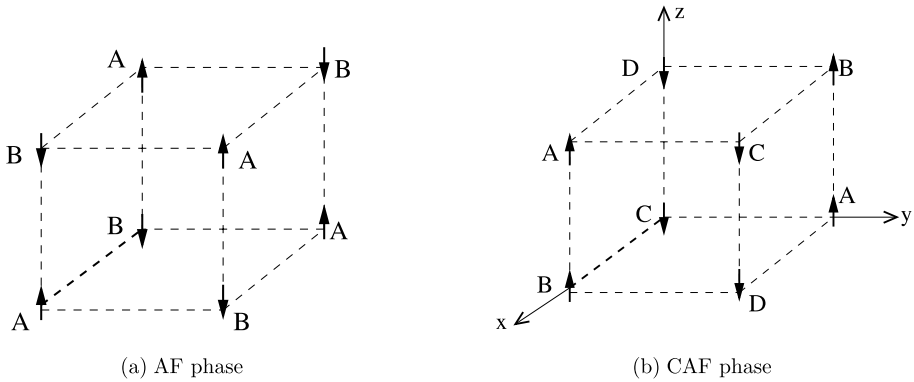
$$\gamma_{2\mathbf{k}} = \frac{1}{3} [\cos(k_x) \cos(k_y) + \cos(k_y) \cos(k_z) + \cos(k_z) \cos(k_x)], \quad (4)$$

where we define the parameter of frustration as  $p = z_2 J_2 / z_1 J_1$ .<sup>1</sup> The wave-vectors along the  $x$ ,  $y$ , and  $z$  directions are denoted by  $k_x$ ,  $k_y$ , and  $k_z$ . The number of lattice sites are given by  $N$  and we have set the lattice spacing  $a = 1$ .

At zero temperature the classical ground state (GS) for the SC lattice can be characterized by the values of  $p$ .  $p = 0$  corresponds to the unfrustrated case (only AF interactions between NN). For  $p < 1/2$  or  $J_2/J_1 < 1/4$ , there is a single minimum in energy  $E_0/N J_1 = -3S^2(1-p)$  for the wave-vectors  $(\pm\pi, \pm\pi, \pm\pi)$ . They correspond to the classical two sublattice Néel state (AF phase) where spins in A and B-sublattices point in opposite directions [Fig. 1(a)].

For  $p > 1/2$  apart from the global rotation the classical ground state has another infinite degeneracy—the frustration is uniformly distributed on all the spins, causing a non-collinear GS with very large degeneracy. In general, the GS for  $p > 1/2$  can be decomposed into two NNN tetrahedra. The spin configurations in each of these two NNN tetrahedra can be characterized by two angles  $\theta$  and  $\phi$ . This results in a four sublattice  $A, B, C, D$  [Fig. 1(b)] antiferromagnetic structure. Out of these infinite possibilities there are three collinear configurations (one line up, one line down). The wave-vectors corresponding to these collinear states are  $(\pi, \pi, 0)$ ,  $(\pi, 0, \pi)$ ,  $(0, \pi, \pi)$ . The classical GS energy for these states is  $E_0/N J_1 = -S^2(1+p)$ . Thermal or quantum fluctuations lift these degeneracies and select specific discrete states and it has been conjectured that thermal or quantum disorder favors collinear states (*order by disorder*) [1, 2, 40, 41]. The four fold rotational symmetry

<sup>1</sup>Note that  $p$  defined here differs by a factor  $z_2/z_1$  with the definition of  $p$  in the introduction.



**Fig. 1** AF and collinear antiferromagnetic (CAF) ordered phases of the SC lattice. In the AF phase all  $A$ -sublattice spins point in the direction of an arbitrary unit vector while  $B$ -sublattice spins point in the opposite direction. For the CAF phase the spin configurations (lines of spins up and down) of the four sublattices  $A, B, C,$  and  $D$  are shown in the figure. There are two other equivalent configurations with lines along the two other directions of the cubic lattice

of the lattice is spontaneously broken in this state. By employing a spin wave theory based on the general four sublattice mean field ground state it has been shown that the quantum fluctuations stabilize a collinear spin ordering [42]. Quantum Monte Carlo simulations on the frustrated SC lattice for  $p > 1/2$  also confirm this conjecture [36]. In the present article, for  $p > 1/2$ , we consider the system to be in one of these three collinear configurations (collinear antiferromagnet or CAF).

$p = 1/2$  corresponds to the case where both  $J_1$  and  $J_2$  compete—causing frustration in the system. This critical value  $p_{\text{class}} = 0.5$  is the classical phase transition point where a phase transition from AF to CAF phase occurs. In this work we will investigate the role of quantum fluctuations in the two different phases (AF and CAF) of the model and how these fluctuations shift the critical transition point.

### 3 Self-consistent Non-linear Spin Wave Theory

The Hamiltonian in (1) can be mapped into an equivalent Hamiltonian of interacting bosons by transforming the spin operators to bosonic operators  $a, a^\dagger$  and  $b, b^\dagger$  using the well-known Holstein-Primakoff transformations. For the AF-phase ( $J_2 < J_1$ ) the operators  $a, a^\dagger$  and  $b, b^\dagger$  are for the  $A$  and  $B$  sublattices. On the other hand for the CAF phase ( $J_2 > J_1$ ) we have used the operators  $a, a^\dagger$  and  $b, b^\dagger$  for the up and down spin configurations.

$$\begin{aligned}
 S_{Ai}^+ &\approx \sqrt{2S} \left(1 - \frac{a_i^\dagger a_i}{4S}\right) a_i, & S_{Ai}^- &\approx \sqrt{2S} a_i^\dagger \left(1 - \frac{a_i^\dagger a_i}{4S}\right), \\
 S_{Ai}^z &= S - a_i^\dagger a_i, \\
 S_{Bj}^+ &\approx \sqrt{2S} b_j^\dagger \left(1 - \frac{b_j^\dagger b_j}{4S}\right), & S_{Bj}^- &\approx \sqrt{2S} \left(1 - \frac{b_j^\dagger b_j}{4S}\right) b_j, \\
 S_{Bj}^z &= -S + b_j^\dagger b_j.
 \end{aligned}
 \tag{5}$$

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

$$a_i = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}}, \quad b_j = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_j} b_{\mathbf{k}},$$

the real space Hamiltonian is transformed to the  $\mathbf{k}$ -space Hamiltonian. In the following two sections we study the cases  $J_2 < J_1$  and  $J_2 > J_1$  separately.

### 3.1 $J_2 < J_1$ : AF Phase

In this phase the classical ground state is the two-sublattice Néel state [Fig. 1(a)]. For the NN interaction, spins in  $A$  sublattice interacts with spins in  $B$  sublattice and vice versa. On the other hand the NNN exchange  $J_2$  connects spins on the same sublattice,  $A$  with  $A$  and  $B$  with  $B$ . Substituting (5) into (1), the  $\mathbf{k}$ -space Hamiltonian takes the form:

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

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

$$H^{(0)} = -\frac{1}{2} N J_1 S^2 z_1 (1 - p), \quad (7)$$

$$H^{(2)} = J_1 S z_1 \sum_{\mathbf{k}} \left[ A_{0\mathbf{k}}^{(1)} (a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}}) + B_{0\mathbf{k}}^{(1)} (a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}} b_{\mathbf{k}}) \right]. \quad (8)$$

with the coefficients  $A_{0\mathbf{k}}^{(1)}$  and  $B_{0\mathbf{k}}^{(1)}$  defined as

$$A_{0\mathbf{k}}^{(1)} = 1 - p(1 - \gamma_{2\mathbf{k}}), \quad (9)$$

$$B_{0\mathbf{k}}^{(1)} = \gamma_{1\mathbf{k}}. \quad (10)$$

The quartic terms in the Hamiltonian  $H^{(4)}$  involve interactions between  $A$ - $B$  (for NN terms) and  $A$ - $A$ ,  $B$ - $B$  (for NNN terms) sublattices. The Hamiltonian for these interactions are stated in Appendix A, (A.1). These terms are evaluated by applying the Hartree-Fock decoupling process. The contributions of the decoupled quartic terms to the harmonic Hamiltonian in (8) are to redefine the values of  $A_{0\mathbf{k}}^{(1)}$  and  $B_{0\mathbf{k}}^{(1)}$  which are now

$$A_{\mathbf{k}}^{(1)} = \left( 1 - \frac{u_1 + v_1}{S} \right) - p[1 - \gamma_{2\mathbf{k}}] \left( 1 - \frac{u_1 - w_1}{S} \right), \quad (11)$$

$$B_{\mathbf{k}}^{(1)} = \gamma_{1\mathbf{k}} \left( 1 - \frac{u_1 + v_1}{S} \right), \quad (12)$$

$$\omega_{\mathbf{k}}^{(1)} = \sqrt{(A_{\mathbf{k}}^{(1)})^2 - (B_{\mathbf{k}}^{(1)})^2}. \quad (13)$$

The coefficients  $u_1$ ,  $v_1$  and  $w_1$  are in Appendix A. They are evaluated self-consistently from equations (11), (12), (A.2)–(A.4).

The quartic corrections to the ground state energy is calculated from the four-boson averages. In the leading order they are decoupled into the bilinear combinations (A.2)–(A.4) using Wick's theorem. The corresponding four boson terms are,

$$\langle a_i^\dagger a_i b_j^\dagger b_j \rangle = u_1^2 + v_1^2, \quad \langle a_i^\dagger b_j^\dagger b_j b_i \rangle = 2u_1 v_1,$$

$$\begin{aligned}\langle a_i^\dagger a_i a_j b_j \rangle &= 2u_1 v_1, & \langle a_i^\dagger a_i a_j^\dagger a_j \rangle &= u_1^2 + w_1^2, \\ \langle a_i a_j^\dagger a_j^\dagger a_j \rangle &= 2u_1 w_1, & \langle a_i^\dagger a_i a_i a_i^\dagger \rangle &= 2u_1 w_1.\end{aligned}\quad (14)$$

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

$$\delta E^{(4)} = -\frac{1}{2} N J_1 z_1 [(u_1 + v_1)^2 - p(u_1 - w_1)^2]. \quad (15)$$

Adding all the corrections together the ground state energy takes the form

$$\begin{aligned}E/NJ_1 &= -\frac{1}{2} z_1 S(S+1)(1-p) + \frac{1}{2} z_1 S \left[ \frac{2}{N} \sum_{\mathbf{k}} \omega_{\mathbf{k}}^{(1)} \right] \\ &+ \frac{1}{2} z_1 [(u_1 + v_1)(1 - u_1 - v_1) - p(u_1 - w_1)(1 - u_1 + w_1)]\end{aligned}\quad (16)$$

and the average sublattice magnetization  $\langle S_\alpha \rangle$  is given by

$$\langle S_\alpha \rangle = S \left[ 1 - \frac{1}{2S} \left\{ \frac{2}{N} \sum_{\mathbf{k}} \frac{A_{\mathbf{k}}^{(1)}}{\omega_{\mathbf{k}}^{(1)}} - 1 \right\} \right]. \quad (17)$$

Using (11)–(13), we numerically evaluate  $E/NJ_1$  and  $\langle S_\alpha \rangle$ .

### 3.2 $J_2 > J_1$ : CAF Phase

The classical ground state for  $J_2 > J_1$  is considered to be in one of the three collinear states [Fig. 1(b)]. For NN and NNN exchanges there are  $A$ - $B$ ,  $A$ - $C$ ,  $A$ - $D$ ,  $B$ - $C$ ,  $B$ - $D$ , and  $C$ - $D$  interactions between the four sublattices [See Fig. 1(b)]. Considering all their contributions together up to the quadratic terms the harmonic Hamiltonian takes the same form as before with

$$H^{(0)} = -\frac{1}{6} N J_1 S^2 z_1 (1+p), \quad (18)$$

$$A_{0\mathbf{k}}^{(2)} = \frac{1}{3} (1 + \cos k_z) + \frac{1}{3} p (1 + \cos k_x \cos k_y), \quad (19)$$

$$B_{0\mathbf{k}}^{(2)} = \frac{1}{3} (\cos k_x + \cos k_y) (1 + p \cos k_z). \quad (20)$$

The quartic terms in the Hamiltonian for this case are shown in Appendix B. These terms are decoupled and evaluated in the same way as before. The renormalized values of the coefficients  $A_{\mathbf{k}}^{(2)}$  and  $B_{\mathbf{k}}^{(2)}$  are

$$\begin{aligned}A_{\mathbf{k}}^{(2)} &= A_{0\mathbf{k}}^{(2)} + \frac{1}{3S} [(\bar{u} - \bar{w}_z)(1 - \cos k_z) - 2(\bar{u} + \bar{v}_1) \\ &+ p\{(\bar{u} - \bar{w}_1)(1 - \cos k_x \cos k_y) - 2(\bar{u} + \bar{v}_2)\}],\end{aligned}\quad (21)$$

$$B_{\mathbf{k}}^{(2)} = B_{0\mathbf{k}}^{(2)} - \frac{1}{3S} \{(\bar{u} + \bar{v}_1) + p(\bar{u} + \bar{v}_2) \cos k_z\} (\cos k_x + \cos k_y), \quad (22)$$

$$\omega_{\mathbf{k}}^{(2)} = \sqrt{(A_{\mathbf{k}}^{(2)})^2 - (B_{\mathbf{k}}^{(2)})^2}. \quad (23)$$

The coefficients  $\bar{u}, \bar{v}_1, \bar{v}_2, \bar{w}_1, \bar{w}_z$  are in Appendix B. As before these coefficients are calculated self-consistently from (21)–(23) and (B.2)–(B.8). The quartic correction to the ground state energy (following the same Hartree-Fock decoupling process as done in the AF-case) is

$$\delta E^{(4)} = -\frac{1}{6} N J_1 z_1 [2(\bar{u} + \bar{v}_1)^2 - (\bar{u} - \bar{w}_z)^2 + 2p(\bar{u} + \bar{v}_2)^2 - p(\bar{u} - \bar{w}_2)^2]. \tag{24}$$

Combining all these corrections, the ground state energy takes the following form:

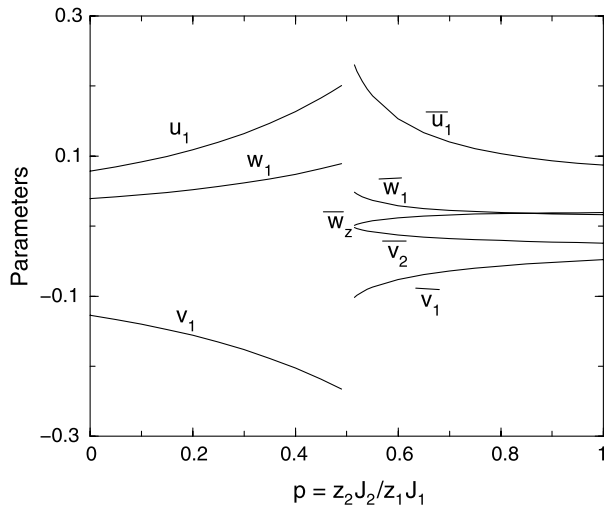
$$\begin{aligned} E/NJ_1 = & -\frac{1}{6} z_1 S(S+1)(1+p) + \frac{1}{2} z_1 S \left[ \frac{2}{N} \sum_{\mathbf{k}} \omega_{\mathbf{k}}^{(2)} \right] \\ & - \frac{1}{6} z_1 [(\bar{u} - \bar{w}_z) - 2(\bar{u} + \bar{v}_1) + p(\bar{u} - \bar{w}_1) - 2p(\bar{u} + \bar{v}_2)] \\ & - \frac{1}{6} z_1 [2(\bar{u} + \bar{v}_1)^2 - (\bar{u} - \bar{w}_z)^2 + 2p(\bar{u} + \bar{v}_2)^2 - p(\bar{u} - \bar{w}_2)^2]. \end{aligned} \tag{25}$$

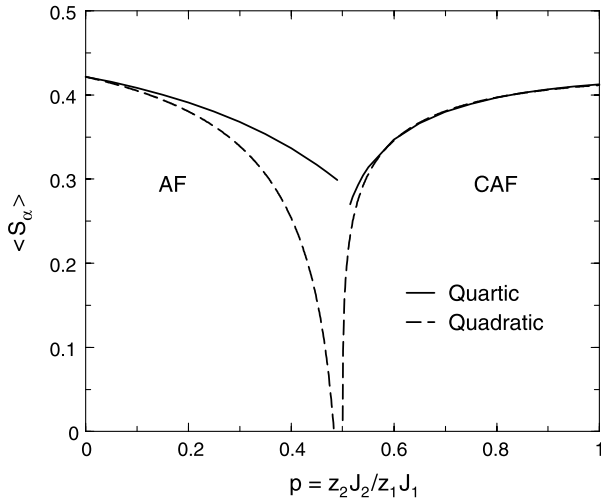
The sublattice magnetization and the ground state energy are then obtained numerically using (17) and (25).

### 4 Results

In Fig. 2 we show the self-consistent values of the different parameters  $u_1, v_1, w_1$  (AF phase) and  $\bar{u}_1, \bar{v}_1, \bar{v}_2, \bar{w}_1, \bar{w}_z$  (CAF phase) of our model. These parameters which provide the quartic corrections to our model do not appear in the LSWT calculations for the sublattice magnetization,  $\langle S_\alpha \rangle$  and the ground state energy,  $E$ . We see from Fig. 2 that most of these coefficients vary significantly with  $p$  especially as  $p$  approaches 0.5 from both ends. This demonstrates that non-linear corrections due to the spin-wave interactions play a significant role in determining the different phases of our model.

**Fig. 2** Self-consistent results for the different parameters,  $u_1, v_1, w_1$  (for the AF-phase) and  $\bar{u}_1, \bar{v}_1, \bar{v}_2, \bar{w}_1, \bar{w}_z$  (for the CAF phase) are plotted with the frustration parameter  $p = z_2 J_2 / z_1 J_1$  (for the SC lattice  $z_1 = 6$  and  $z_2 = 12$ ). These coefficients vary significantly with  $p$ , which shows that the quartic interaction terms play a significant role in determining the different phases of our model

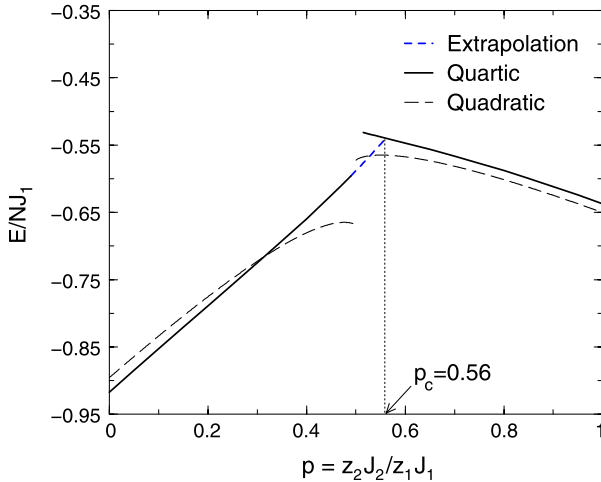




**Fig. 3** Average sublattice magnetization,  $\langle S_\alpha \rangle$ , is plotted with the frustration parameter  $p$  for AF and one of the three CAF phases with (solid lines) and without (dashed lines) quartic corrections. At zero temperature without the quartic  $1/S$  corrections (linear spin-wave theory)  $\langle S_\alpha \rangle \rightarrow 0$  at  $p_{c1} \approx 0.48$  indicating a phase transition from the AF-ordered state to the disordered paramagnetic state. At  $p_{c2} = 0.50$  there is a second phase transition from the collinear state to the disordered state for  $T = 0$ . Non-linear spin wave theory provides significant corrections to this phase diagram. With the quartic  $1/S$  corrections the disordered PM region disappears completely and we only obtain two phases: AF and CAF. There is no existence of any disordered state as predicted by the linear spin-wave theory (quadratic corrections). For both the phases the quartic corrections to the Hamiltonian enhance the magnetic order

Figure 3 shows the result for the average sublattice magnetization for the SC lattice for both AF and CAF phase without (dashed line) and with (solid line) quartic corrections.  $\langle S_\alpha \rangle$  is calculated using (17). In the AF 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  $p \approx 0.49$ . This gradual decrease in  $\langle S_\alpha \rangle$  with increase in  $p$  is expected as increasing strength of NNN interaction  $J_2$  disorders the antiferromagnetic spin alignments. With only quadratic terms in the Hamiltonian (linear spin wave theory) we find that  $\langle S_\alpha \rangle$  approaches zero as  $p \rightarrow p_{c1}$  where  $p_{c1} \approx 0.48$  indicating a order-disorder phase transition to a disordered paramagnetic (PM) state at this point. In the CAF phase with lines of spins up and down, LSWT calculations show that  $\langle S_\alpha \rangle$  decreases as  $p$  approaches 0.5 from above and at  $p = p_{c2} = 0.50$  there is an another phase transition from the CAF state to the disordered PM state. This is similar to the two dimensional AF-square lattice with Heisenberg spins where we have a line of quantum critical points between  $0.38 < p < 0.60$ . However, self-consistent calculations with quartic  $1/S$  corrections drastically alter the zero temperature phase diagram. We find that in the AF-phase with increase in  $p$  the system aligns the spins antiferromagnetically along the horizontal and vertical directions—thus decreasing the sublattice magnetization from  $\approx 0.42$  for  $p = 0$  to  $\approx 0.30$  for  $p = 0.49$ . In the CAF phase  $\langle S_\alpha \rangle$  steadily decreases from  $\approx 0.41$  for  $p = 1$  to  $\approx 0.27$  for  $p = 0.52$ . There is no existence of any disordered state as predicted by the linear spin-wave theory (quadratic corrections). The disordered PM region disappears completely and we only obtain two phases: AF and CAF. This is one of our main findings in the present work. This significant change due to the quartic corrections is due to the enhancement of order by quantum fluctuations.





**Fig. 4** Zero temperature ground state energy per site,  $E/NJ_1$ , is plotted versus  $p$  without (*dashed lines*) and with (*solid lines*) quartic corrections for both AF ( $p < 0.5$ ) and CAF ( $p > 0.5$ ) ordered phases. Spin wave theory becomes unstable close to the classical transition point ( $p_{\text{class}} \approx 0.5$ ) between the two phases. After extrapolation (shown by the *dotted line*), we find that the two energies meet at the quantum transition point,  $p_c \approx 0.56$  or  $J_2/J_1 \approx 0.28$ . This kink in the energy indicates a first-order quantum phase transition from the AF to CAF phase. Compared to the results without quartic corrections (*long dashed lines*) we find that the quartic corrections provide significant corrections to the ground state energy especially near the AF-CAF phase transition point

At  $p = 0$  (no frustration) there is no quartic corrections to  $\langle S_\alpha \rangle$ . This can be observed from (11)–(13) as the correction factor  $(1 - (u_1 + v_1)/S)$  cancels out in (17). Our non-linear spin wave theory calculations become unstable close to the classical transition point  $p_{\text{class}} = 0.5$  since the coefficient  $A_{\mathbf{k}}^1$  becomes equal to  $B_{\mathbf{k}}^1$ .

We have also applied the NLSWT technique to compute the quartic corrections in the spin-1/2 Heisenberg AF on a body-centered lattice [22]. The LSWT calculation for the BCC lattice does not predict any intermediate disordered state and the quartic corrections play a role in stabilizing the sublattice magnetization (see Fig. 2 of [22]). However, the effect of quartic corrections is more pronounced in the SC lattice where the intermediate disordered phase disappears.

In Fig. 4 we show the ground state energy per site,  $E/NJ_1$ , for the AF and the CAF phases with (solid line) and without (dashed line) quartic corrections as a function of the frustration parameter  $p$ .  $E/NJ_1$  is calculated from (16) and (25). Classically  $p_{\text{class}} = 0.5$  or  $J_2/J_1 = 0.25$  is the critical point where a phase transition from the AF phase to one of the three CAF phases occur. With increase in frustration (as  $p$  approaches 0.5 from both sides) we expect the GS energy to increase as the system goes from an energetically favored ordered state to a more disordered state. However, linear spin-wave theory calculation fails to capture this. Especially when  $p$  is close to 0.5 we find a slight downward turn in energy. This has been reported in [38]. On the other hand, NLSWT calculation correctly produces the expected energy increase. At  $p = 0$  the calculated energy with the quartic corrections is slightly lower than the energy obtained without the quartic corrections. This small decrease from the LSWT calculation is due to the ground state energy correction, which is negative (as seen in (15))—these terms originate from the self-energy Hartree diagrams). As our spin-wave theory calculation becomes unstable in the regime  $0.49 < p < 0.52$  we used a spline

fit for the AF-phase energy data points and then extrapolated the line so that it intersects the CAF-phase energy line. The extrapolated curve is shown by dotted lines (color online) in the figure. After extrapolation, we find that the two energies meet at  $p_c \approx 0.56$  or  $J_2/J_1 \approx 0.28$ . The symmetries of the two phases are different:  $\text{SO}(3)/\text{SO}(2)$  for the AF phase and  $Z_3 \times \text{SO}(3)/\text{SO}(2)$  for the CAF phase [1]. Due to the different symmetries of the two phases the transition is of first order. This is confirmed by the kink in the energy at  $p_c \approx 0.56$ . Our obtained value from our self-consistent NLSWT calculations for the quantum critical point is  $J_2/J_1 \approx 0.28$ . This is another major finding of our work.

Using the variational spin-wave theory the authors in [38] obtained an upper bound of 0.27 for the ground state energy. However, their variational calculation slightly overestimates the value of GS energy. This is quite noticeable at  $p = 0$ , where their energy value is higher than the LSWT prediction. We have found the  $p = 0$  energy value to be slightly less than the LSWT prediction. This is due to the quartic corrections explained earlier. However, the shape of the quartic corrections in [38] is essentially same as ours. By extensive standard and histogram classical Monte-Carlo simulations Diep et al. [36] obtained the transition point to be around 0.26. However, it should be noted that the MC simulations were done for classical spins. Our result is in excellent agreement with the results obtained from the variational spin-wave theory calculations (our  $p_c$  differs by less than 3.5% from the variational spin-wave theory prediction).

## 5 Conclusion

In this work we have investigated the zero temperature phases of a spin-1/2 Heisenberg frustrated AF on a SC lattice by considering the quartic  $1/S$  corrections due to the spin-wave interactions. We have compared our results obtained from NLSWT calculations with the predictions from LSWT. It is known that LSWT predicts the existence of three phases: a two sublattice Néel phase for smaller values of the NNN exchange  $J_2$ , an intermediate paramagnetic phase, and a collinear phase for larger values of  $J_2$ . At zero temperature there are two quantum phase transitions—one from the AF-state to the disordered paramagnetic state and the other from the disordered state to one of the three collinear states. Both these transitions occur at the quantum critical point  $p_c \approx 0.5$  or  $J_2/J_1 \approx 0.25$ . We have found that quartic corrections significantly alter this phase diagram as intermediate paramagnetic phase disappears. We find the existence of two phases at zero temperature: a two sublattice AF phase for small  $J_2$  and a collinear phase for large  $J_2$ . With the inclusion of quartic interactions the intermediate paramagnetic phase completely disappears. Due to the different symmetries of the two phases (AF and CAF) the transition between the two phases is of first order and we find that the critical point for transition to be 0.28. Results from variational spin-wave theory agree with our obtained results.

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## Appendix A: Quartic Terms for the AF Phase

The quartic terms for the AF phase from the NN interactions involve  $A$ – $B$  interactions and for the NNN interactions involve  $A$ – $A$  and  $B$ – $B$  type interactions. Considering all these

interactions the quartic Hamiltonian takes the form:

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

In the harmonic approximation the following Hartree-Fock averages are non-zero for the SC-lattice Heisenberg antiferromagnet:

$$u_1 = \langle a_i^\dagger a_i \rangle = \langle b_i^\dagger b_i \rangle = \frac{1}{2} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{A_{\mathbf{k}}^{(1)}}{\omega_{\mathbf{k}}^{(1)}} - 1 \right], \quad (\text{A.2})$$

$$v_1 = \langle a_i b_j \rangle = \langle a_i^\dagger b_j^\dagger \rangle = -\frac{1}{2} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\gamma_{1\mathbf{k}} B_{\mathbf{k}}^{(1)}}{\omega_{\mathbf{k}}^{(1)}} \right], \quad (\text{A.3})$$

$$w_1 = \langle a_i^\dagger a_j \rangle = \langle b_i^\dagger b_j \rangle = \frac{1}{2} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\gamma_{2\mathbf{k}} A_{\mathbf{k}}^{(1)}}{\omega_{\mathbf{k}}^{(1)}} \right], \quad (\text{A.4})$$

where  $\omega_{\mathbf{k}}^{(1)} = \sqrt{(A_{\mathbf{k}}^{(1)})^2 - (B_{\mathbf{k}}^{(1)})^2}$ .

## Appendix B: Quartic Terms for the CAF Phase

The quartic terms for the collinear phase from the NN interactions involve interactions between the sublattices  $B-C$  and  $A-D$  along the  $x$  axis,  $A-C$  and  $B-D$  along the  $y$  axis, and  $A-B$  and  $C-D$  along the  $z$  axis. For the NNN interactions spin-spin interactions are between sublattices  $A-B$  and  $C-D$  (in the  $xy$ -plane),  $A-C$  and  $B-D$  (in the  $xz$ -plane), and  $A-D$  and  $B-C$  (in the  $yz$ -plane) as shown in Fig. 1(b). Adding all the contributions together yield

$$H^{(4)} = -J_1 \sum_{\langle ijx \rangle} \left[ a_i^\dagger a_i b_{j_x}^\dagger b_{j_x} + \frac{1}{4} (a_i b_{j_x}^\dagger b_{j_x} b_{j_x} + a_i^\dagger a_i a_i b_{j_x} + \text{h.c.}) \right] \\ - J_1 \sum_{\langle i jy \rangle} \left[ a_i^\dagger a_i b_{j_y}^\dagger b_{j_y} + \frac{1}{4} (a_i b_{j_y}^\dagger b_{j_y} b_{j_y} + a_i^\dagger a_i a_i b_{j_y} + \text{h.c.}) \right] \\ + \frac{1}{2} J_1 \sum_{\langle ijz \rangle} \left[ a_i^\dagger a_i a_{j_z}^\dagger a_{j_z} - \frac{1}{4} (a_i a_{j_z}^\dagger a_{j_z}^\dagger a_{j_z} + a_i^\dagger a_i a_i a_{j_z}^\dagger + \text{h.c.}) + a \leftrightarrow b \right] \\ + \frac{1}{2} J_2 \sum_{\langle ijxy \rangle} \left[ a_i^\dagger a_i a_{j_{xy}}^\dagger a_{j_{xy}} - \frac{1}{4} (a_i a_{j_{xy}}^\dagger a_{j_{xy}}^\dagger a_{j_{xy}} + a_i^\dagger a_i a_i a_{j_{xy}}^\dagger + \text{h.c.}) + a \leftrightarrow b \right] \\ - J_2 \sum_{\langle ijyz \rangle} \left[ a_i^\dagger a_i b_{j_{yz}}^\dagger b_{j_{yz}} + \frac{1}{4} (a_i b_{j_{yz}}^\dagger b_{j_{yz}} b_{j_{yz}} + a_i^\dagger a_i a_i b_{j_{yz}} + \text{h.c.}) \right] \\ - J_2 \sum_{\langle ijxz \rangle} \left[ a_i^\dagger a_i b_{j_{xz}}^\dagger b_{j_{xz}} + \frac{1}{4} (a_i b_{j_{xz}}^\dagger b_{j_{xz}} b_{j_{xz}} + a_i^\dagger a_i a_i b_{j_{xz}} + \text{h.c.}) \right]. \quad (\text{B.1})$$

Above  $j_x, j_y, j_z$  are NN lattice sites along  $x, y, z$  axes and  $j_{xy}, j_{yz}, j_{xz}$  connects one lattice site with a NNN corner lattice sites on the  $xy, yz, xz$  planes. The different coefficients that originate from Hartree-Fock decoupling process are

$$\bar{u} = \langle a_i^\dagger a_i \rangle = \langle b_i^\dagger b_i \rangle = \frac{1}{2} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{A_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} - 1 \right], \quad (\text{B.2})$$

$$\bar{v}_{1x} = \langle a_i b_{j_x} \rangle = \langle a_i^\dagger b_{j_x}^\dagger \rangle = -\frac{1}{6} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\cos k_x B_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} \right], \quad (\text{B.3})$$

$$\bar{v}_{1y} = \langle a_i b_{j_y} \rangle = \langle a_i^\dagger b_{j_y}^\dagger \rangle = -\frac{1}{6} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\cos k_y B_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} \right], \quad (\text{B.4})$$

$$\bar{v}_{2yz} = \langle a_i b_{j_{yz}} \rangle = \langle a_i^\dagger b_{j_{yz}}^\dagger \rangle = -\frac{1}{6} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\cos k_y \cos k_z B_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} \right], \quad (\text{B.5})$$

$$\bar{v}_{2xz} = \langle a_i b_{j_{xz}} \rangle = \langle a_i^\dagger b_{j_{xz}}^\dagger \rangle = -\frac{1}{6} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\cos k_x \cos k_z B_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} \right], \quad (\text{B.6})$$

$$\bar{w}_z = \langle a_i^\dagger a_{j_z} \rangle = \langle b_i^\dagger b_{j_z} \rangle = \frac{1}{6} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\cos k_z A_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} \right], \quad (\text{B.7})$$

$$\bar{w}_1 = \langle a_i^\dagger a_{j_{xy}} \rangle = \langle b_i^\dagger b_{j_{xy}} \rangle = \frac{1}{6} \left[ \frac{2}{N} \sum_{\mathbf{k}} \frac{\cos k_x \cos k_y A_{\mathbf{k}}^{(2)}}{\omega_{\mathbf{k}}^{(2)}} \right], \quad (\text{B.8})$$

where  $\omega_{\mathbf{k}}^{(2)} = \sqrt{(A_{\mathbf{k}}^{(2)})^2 - (B_{\mathbf{k}}^{(2)})^2}$ . By symmetry  $\bar{v}_{1x} = \bar{v}_{1y} = \bar{v}_1$  and  $\bar{v}_{2yz} = \bar{v}_{2xz} = \bar{v}_2$ .

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