Cluster mean-field theory study of $J_1$–$J_2$ Heisenberg model on a square lattice

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Abstract
We study the spin-1/2 $J_1$–$J_2$ Heisenberg model on a square lattice using the cluster mean-field theory. We find a rapid convergence of phase boundaries with increasing cluster size. By extrapolating the cluster size $L$ to infinity, we obtain accurate phase boundaries $J_1^2 \approx 0.42$ (between the Néel antiferromagnetic phase and non-magnetic phase), and $J_2^2 \approx 0.59$ (between non-magnetic phase and the collinear antiferromagnetic phase). Our results support the second-order phase transition at $J_2^1$ and the first-order one at $J_2^2$. For the spin-anisotropic $J_1$–$J_2$ model, we present its finite temperature phase diagram and demonstrate that the non-magnetic state is unstable towards the first-order phase transition under intermediate spin anisotropy.

Keywords: $J_1$–$J_2$ Heisenberg model, quantum phase transition, cluster mean-field theory

(Some figures may appear in colour only in the online journal)

1. Introduction

It was suggested by Anderson [1] that low spin, low spatial dimension, and high frustration are the three main factors which favor the melting of magnetic long-range order (LRO) and lead to exotic spin liquid ground state. Such a state was closely related to the appearance of high temperature superconductivity in Cu-based oxides upon doping [2]. The spin-1/2 $J_1$–$J_2$ Heisenberg model in a two-dimensional square lattice is such a model that bears all the three factors, hence its ground state is a promising candidate for the exotic spin liquid state [3]. Besides the interest for spin liquid, this model in the large $J_2/J_1$ regime is relevant to materials such as Li$_2$VOSiO$_4$ [4, 27], and the $S > 1/2$ version is relevant to the parent material of iron-based high temperature superconductors [5].

The Hamiltonian of the antiferromagnetic (AFM) $J_1$–$J_2$ model reads

$$\hat{H} = J_1 \sum_{\langle i, j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle i, j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $\mathbf{S}_i$ is the spin $\frac{1}{2}$ operator on site $i$, and $J_1$ and $J_2$ are the nearest neighbor and the next-nearest-neighbor coupling coefficients, respectively. In the following, we set $J_1 = 1$ as the unit of energy. For the next-nearest-neighbor coupling $J_2$, we confine ourself to the AFM case $J_2 > 0$.

This model has been the subject of numerous studies in the past two decades, using various methods including exact diagonalization (ED) [6–11], series expansion [12–16], coupled cluster [17, 18], spin wave approximation [3, 19], Green’s function method [20], density-matrix renormalization group (DMRG) [21, 22], matrix-product or tensor-network based algorithms [23–26], high temperature expansion [27], resonating valence bond approaches [28–32], bond operator formalism [33, 34], mean-field theories [12, 35, 36], and field theoretical methods [37–39]. It has been established that in the regime $0 < J_2/J_1 \lesssim 0.4$, the ground state of the $J_1$–$J_2$ model is an AFM phase with Néel order. In $J_2/J_1 \gtrsim 0.6$, an AFM phase with collinear LRO is stable, due to the dominance of the next-nearest-neighbor coupling $J_2$. One of the most controversial regimes is the intermediate regime $0.4 \lesssim J_2/J_1 \lesssim 0.6$ where the ground state is non-magnetic.
and hence the $SU(2)$ symmetry is not broken. The nature of this intermediate non-magnetic ground state is still a much debated issue. The possible candidates of this ground state, as proposed by various authors, include dimerized valence bond solid (VBS) which breaks both the translation and the rotation symmetries of the lattice [8, 12–14], the plaquette VBS which breaks only the translation symmetry [33, 38, 36], the nematic spin liquid which breaks only the rotational symmetry [39], and the gapped [21, 26, 29] or gapless [31] spin liquid which conserves all the symmetries of the lattice. The difficulty of this issue lies in that there is no unbiased and accurate method to study the ground state of the $J_1–J_2$ model in the thermodynamical limit. Most of the numerical studies heavily rely on the extrapolation of the finite size results to the thermodynamical limit. In cases where there is little guidance from analytical knowledge, this practice may have uncertainties [40, 24], as demonstrated by a recent study on the J–Q model [41].

Besides the nature of the non-magnetic state, there are other important issues under various physical contexts. Previous studies show that the AFM Néel phase transits into the non-magnetic state at $J_2/J_1 \approx 0.4$ through a continuous quantum phase transition. If the intermediate region actually possesses a VBS order, this transition is an abnormal one, as a continuous transition between two phases without the group–subgroup symmetries violates the conventional ‘Landau rule’. A ‘deconfined’ quantum critical point was proposed to exist between the Néel and the VBS states [42].

For the parameter regime $J_2/J_1 \gtrsim 0.6$, this model also invoked much interest since lots of real materials are related to this parameter regime, such as the La–O–Cu–As iron-based superconductors [43, 44] and Li$_2$VOSiO$_4$ [4, 27]. Another interesting issue in this parameter regime is the possible finite temperature symmetry breaking. For this model, although the spin $SU(2)$ symmetry cannot be broken spontaneously at finite temperature due to the Mermin–Wagner theorem [45], symmetry breaking of the lattice $C_4$ symmetry could occur below a finite $T < T_c$ [37, 46, 47]. However, there is also a different opinion on this issue [15].

The effect of spin anisotropy in the $J_1–J_2$ model is also an interesting issue, given that the anisotropy is quite common in real materials. Theoretical studies on this issue are rare [48, 49].

In this paper, we focus on the phase boundary of the $J_1–J_2$ model and attempt to present accurate critical values $J_1^c$ and $J_2^c$. We use the cluster mean-field theory (CMFT), which is the cluster extension of the Weiss mean-field theory [50, 51]. We obtained the Néel AFM phase, the collinear AFM phase, and the non-magnetic phase. Using the reshaping method for plotting multiple-valued curves [52], we studied the fine structure of the first-order phase transition between the non-magnetic phase and the collinear AFM phases, including the stable, meta-stable and unstable phases. This information is important when the system is under external influence but has often been neglected in previous studies. The critical values $J_1^c$ and $J_2^c$ are found to converge very fast with increasing cluster size, allowing us to obtain an accurate estimation of them. We also study the effect of spin anisotropy, producing the finite temperature phase diagram and analyzing the stability of the non-magnetic phase under the spin anisotropy.

The rest of this paper is organized as follows. In section 2, we introduce the CMFT and the method we used to obtain the fine structure of the first-order phase transition. In section 3, we first present the zero temperature results, including the phase diagram and magnetic susceptibility. Then, the effect of the spin anisotropy is considered and the phase diagram at finite temperature is given.

2. Method

The simplest mean-field theory for spin systems is Weiss’s single-site mean-field theory [50]. In this theory, the influence of surrounding spins to a central spin is approximated by an effective static field, which is then determined self-consistently. The Weiss mean-field theory thus neglects the spatial fluctuations and often overestimates the stability of LRO. Based on a similar idea, Bethe–Peierls–Weiss (BPW) [54–56] and Oguchi [57] improved the approximation by mapping the lattice model into clusters subjected to self-consistently determined effective fields. Interactions inside a cluster are treated exactly while interactions between clusters are approximated by mean fields. Since the short-range spatial fluctuations inside a cluster are taken into account, the results are expected to improve as cluster size increases.

In this work, we study the $J_1–J_2$ model on a square lattice using the cluster extension of Weiss mean-field theory. Although being simple, this theory produces surprisingly accurate boundaries between various phases, as compared to results from the more sophisticated methods. We first divide the lattice into identical clusters of $L$ sites. To separate the spin couplings inside a cluster from those between clusters, the Hamiltonian of $J_1–J_2$ model is rewritten as

$$
\hat{H} = \sum_{c_n} \left[ J_1 \sum_{\langle ij \rangle} \mathbf{S}_{i,c_n} \cdot \mathbf{S}_{j,c_n} + J_2 \sum_{\langle \langle ij \rangle \rangle} \mathbf{S}_{i,c_n} \cdot \mathbf{S}_{j,c_n} \right] + \sum_{c_n \neq c_m} \left[ J_1 \sum_{\langle ij \rangle} \mathbf{S}_{i,c_n} \cdot \mathbf{S}_{j,c_m} + J_2 \sum_{\langle \langle ij \rangle \rangle} \mathbf{S}_{i,c_n} \cdot \mathbf{S}_{j,c_m} \right].
$$

(2)

The operator $\mathbf{S}_{i,c_n}$ denotes the spin operator on the $i$th site in the cluster $c_n$. The first term in equation (2) represents the Hamiltonian of decoupled clusters, while the second one represents interactions between clusters. We make the standard mean-field approximation for the interactions between two spins belonging to different clusters $c_n \neq c_m$,

$$
\mathbf{S}_{i,c_n} \cdot \mathbf{S}_{j,c_m} \approx \mathbf{S}_{i,c_n} \cdot \left( \langle \mathbf{S}_{j,c_m}^z \rangle \mathbf{S}_{j,c_m}^z \right) + \langle \mathbf{S}_{i,c_n}^z \rangle \mathbf{S}_{j,c_m}^z - \langle \mathbf{S}_{i,c_n}^z \rangle \langle \mathbf{S}_{j,c_m}^z \rangle. \tag{3}
$$

Here, the $z$-axis is chosen as the quantization axis. This approximation breaks both spin $SU(2)$ symmetry and spatial translation symmetry of the original Hamiltonian. Substituting it into the second term of equation (2) and neglecting a constant, we obtain the cluster-decoupled mean-field...
to become exact as \( L \) tends to infinity. Therefore, the results are expected to recover the Weiss mean-field theory. As the cluster size increases, larger and longer range correlations contained in the cluster are treated exactly. Therefore, the results are expected to become exact as \( L \) tends to infinity.

To solve the CMFT equations, we use the spatial translation symmetry of clusters to ensure \( \langle S^z_{i,c_n} \rangle = \langle S^z_{j,c_n} \rangle = m_i \). For a cluster with \( L \) sites, \( m_i \) \( ( i = 1, 2, \ldots, L ) \) are our magnetic order parameters that can characterize different magnetic orders. In this paper, we do not consider the possibility of LRO in the intermediate non-magnetic regime, as it is still an open issue how to incorporate the non-magnetic order parameters into the CMFT. With this notation, the effective field \( h_i \) reads

\[
\hat{h}_i = J_1 \sum_{\langle ij \rangle} m_\delta + J_2 \sum_{\langle\langle ij \rangle\rangle} m_\delta'.
\]

(5)

Here \( \delta, \delta' \in [1, L] \) denote the nearest neighbor site and the next-nearest neighbor site in the neighboring clusters of site \( i \), respectively. The CMFT equations are completed by solving \( m_i \) from a central cluster Hamiltonian \( \hat{H}_c \) in equation (4). In the limit of single-site cluster \( L = 1 \), the above approximation recovers the Weiss mean-field theory. As the cluster size increases, longer and longer range correlations contained in the cluster are treated exactly. Therefore, the results are expected to become exact as \( L \) tends to infinity.

To solve the CMFT equations, we use the spatial translation symmetry of clusters to ensure \( \langle S^z_{i,c_n} \rangle = \langle S^z_{j,c_n} \rangle = m_i \). For a cluster with \( L \) sites, \( m_i \) \( ( i = 1, 2, \ldots, L ) \) are our magnetic order parameters that can characterize different magnetic orders. In this paper, we do not consider the possibility of LRO in the intermediate non-magnetic regime, as it is still an open issue how to incorporate the non-magnetic order parameters into the CMFT. With this notation, the effective field \( h_i \) reads

\[
\hat{h}_i = J_1 \sum_{\langle ij \rangle} m_\delta + J_2 \sum_{\langle\langle ij \rangle\rangle} m_\delta'.
\]

(5)

3. Results and discussions

3.1. Zero temperature

In this work, we use the rectangular clusters of size \( L = L_x \times L_y \). To avoid odd number of spins in a cluster, we use even \( L_x \) and \( L_y \). The total number of spins \( L \) is confined as \( L \leq 16 \) due to the exponential increase of computational cost with \( L \). We choose \( 2 \times 2 \) and \( 4 \times 4 \) clusters for qualitative study, and use \( L_y = 2 \) and \( L_x = 2, 4, 6, 8 \) for quantitative size dependence analysis.

In figure 2, we show \(|m| \) versus \( J_z \) for three successively larger clusters. \(|m| \) is measured on the center site of the cluster. For all the clusters we used, the Néel order is stable for small \( J_z \) regime. As \( J_z \) increases, \(|m| \) decreases and vanishes continuously at a critical value \( J_z^{c1} \approx 0.41-0.42 \), which indicates a second-order transition to a non-magnetic phase. As \( J_z \) increases above \( J_z^{c2} \approx 0.6-0.7 \), \(|m| \) jumps from zero to a finite value, with a collinear magnetic pattern. In both Néel and collinear phases, \(|m| \) decreases with increasing \( L \), showing that more and more quantum fluctuations are taken into account by using large clusters, and hence the increasing
quality of our results. The exact value $m = 0.307 \ [53]$ for $J_2 = 0$ is only asymptotically approached in the \( L = \infty \) limit. It is interesting to observe that from $L = 4$ to $L = 16$, the $|m| - J_2$ curve always vanishes continuously and the critical point $J_{2c1}$ does not change much. Although it is difficult to numerically distinguish a second-order phase transition from a weak first-order one, the rapid convergence of results with $L$ supports the second-order nature of the transition at $J_{2c1}$. Taking the $L = 16$ result as our estimation for the thermodynamical limit, we obtain $J_{2c1} \approx 0.42$. Compared to other methods such as the ED \([8, 9]\), series expansion \([12, 14]\) and DMRG \([21]\), CMFT is surprisingly accurate and simple in producing the ground state phase boundaries.

In figure 3(a), we take a closer look at the fine structure of the $|m| - J_2$ curve near $J_{2c2}^2$, where the transition between the non-magnetic phase and collinear AFM phase occurs. It is obtained by the ‘stretching trick’ mentioned above. In order to see the systematic cluster size dependence, we fix $L_x = 2$ and increase $L_y$ from 2 to 8. We always obtain continuous curves with $S$-shaped structures which contain the stable, meta-stable, and the unstable phases and are generic features of the first-order phase transition. The width of the coexistence region $W$ decreases as $L_y$ increases. As shown in the inset of figure 3(a), $W$ is found to scale with $1/L_y$ as $W \propto a e^{-\beta L_y}$ for the calculated cluster size. Fitting of the data gives $\alpha = 0.038$ and $\beta = 0.42$. $\alpha = 0.038 > 0$ means that the first-order phase transition still exists even if we use a cluster $L_x = 2, L_y = \infty$. This seems to be a strong support to the first-order phase transition between non-magnetic phase and collinear AFM phase in the thermodynamical limit. For a more convincing conclusion, one should extrapolate $L_x$ and $L_y$ to infinity simultaneously. However, due to the rapid increase of the numerical cost, this is not done in our present study.

In figure 3(b), the ground state energy per site versus $J_2$ is plotted for the Néel AFM, non-magnetic, and the collinear AFM phases. We show the result obtained using $2 \times 2$ cluster for demonstration purpose. As $J_2$ increases up to 0.42 (marked by arrow ‘a’), the energy of Néel AFM continuously approaches that of the non-magnetic phase from below, consistent with the scenario of a second-order transition. The transition between the non-magnetic phase and the collinear AFM phase occurs at the energy crossing point marked by the arrow ‘b’ in figure 3(b), which we denote as $J_{2c2}^2$. In the coexistence region, a third collinear AFM solution has the highest energy. It corresponds to the unstable solution with negative $|m| - J_2$ slope in figure 3(a). In this first-order transition, a continuous transition does exist at the meta-stable level, between collinear AFM and non-magnetic phases (marked by arrow ‘c’).

This scenario is common in first-order phase transitions described by mean-field equations, as disclosed by the dynamical mean-field theory study for the correlated electron systems \([52]\). Extrapolating $L_y$ to infinity, we get $J_{2c2}^2 \approx 0.59$, which should be very close to the exact value in the thermodynamical limit. This value agrees quite well with the more sophisticated calculations such as DMRG \([21]\) (see table 1) and resonating valence bond trial wavefunction method \([32]\). It is noted that our energy curve agree quantitatively with the result from the hierarchical mean-field approach (HMFA) on a $2 \times 2$ cluster \([36]\) (solid lines in figure 3(b)). Although HMFA is based on the sophisticated Schwinger boson representation and mean-field approximation, the quantitative agreement makes us believe that the HMFA is equivalent to the cluster mean-field method that we have used here, at least for the case of the $2 \times 2$
Various candidate ground states were proposed based on these ED calculations, including the dimerized state and the chiral state. Since in CMFT the translation symmetry of the original lattice is broken by hand, we cannot answer this question directly. In the non-magnetic phase, the effective fields of CMFT become zero and $H_{mf}$ describes uncorrelated clusters. Then CMFT is equivalent to ED on a cluster with open boundary condition. Previously, ED studies have been carried out for clusters up to 40 sites with periodic boundary condition [7–9]. Various candidate ground states were proposed based on these ED calculations, including the dimerized state and the chiral state [8], and the twisted magnetic LRO [7]. However, due to the severe finite size effect, it is difficult to draw definite conclusion from these studies. It is the same situation for our study here on clusters up to 16 sites. In contrast to the periodic boundary condition used in previous ED studies, here the open boundary condition will induce nonzero VBS order parameter in small clusters. For an example, the operator of plaquette order parameter reads [58]

$$Q_{\alpha\beta\gamma\delta} = 2((S_{\alpha} \cdot S_{\beta})(S_{\gamma} \cdot S_{\delta}) + (S_{\alpha} \cdot S_{\delta})(S_{\beta} \cdot S_{\gamma})$$

$$- (S_{\alpha} \cdot S_{\gamma})(S_{\beta} \cdot S_{\delta}) + \frac{1}{2}(S_{\alpha} \cdot S_{\beta} + S_{\gamma} \cdot S_{\delta}$$

$$+ S_{\alpha} \cdot S_{\delta} + S_{\beta} \cdot S_{\gamma} + S_{\alpha} \cdot S_{\gamma} + S_{\beta} \cdot S_{\delta} + \frac{1}{2}).$$

Here $\alpha, \beta, \gamma, \delta$ denote the four sites of a plaquette clockwise. At $J_2 = 0.5$, the plaquette order parameter is evaluated on a $2 \times 2$ cluster as $Q_{\alpha\beta\gamma\delta} \approx 0.988$, very close to its saturated value 1.0. Evaluating $Q_{\alpha\beta\gamma\delta}$ on a larger cluster also gives nonzero result. However, this is the boundary effect of the cluster and does not support a true VBS state. It is an interesting open question how to incorporate the order parameter of various VBS state into the mean-field approximation. If such a mean-field theory does exist, considering that it tends to exaggerate the LRO, a negative result about the existence of VBS may rule out the possibility of VBS in the intermediate parameter regime.

| Reference | Met. | ED | SE | DMRG | CC | HMFT | VMC | CMFT |
|-----------|------|----|----|------|----|------|-----|------|
| $J_2^{1}$ | 0.35 | 0.41 | 0.41 | 0.44 | 0.42 | 0.45 | 0.42 |
| $J_2^{2}$ | 0.66 | 0.64 | 0.62 | 0.59 | 0.66 | 0.60 | 0.59 |

Table 1. Comparison of $J_2^{1}$ and $J_2^{2}$ from various works. The methods are abbreviated as ED (exact diagonalization), SE (series expansion), DMRG (density-matrix renormalization group), HMFT (hierarchical mean-field theory), VMC (variational Monte Carlo), and CMFT (cluster mean-field theory).

The critical values of $J_2$ have been obtained in many works, using different methods with varied sophistication. In table 1, we summarize some of the previous results and compare them with ours. Note that a similar CMFT study on the $J_1$–$J_2$ model was carried out in [12], but the cluster size effect was not analyzed systematically.

A central issue in the study of the $J_1$–$J_2$ model concerns the properties of the intermediate non-magnetic phase. The key open question is whether it is a spin liquid or a state which spontaneously breaks some symmetry of the original model, such as the lattice translation and/or rotation symmetry. However, due to the severe finite size effect, it is difficult to draw definite conclusion from these studies. It is the same situation for our study here on clusters up to 16 sites. In contrast to the periodic boundary condition used in previous ED studies, here the open boundary condition will induce nonzero VBS order parameter in small clusters. For an example, the operator of plaquette order parameter reads [58]

$$Q_{\alpha\beta\gamma\delta} = 2((S_{\alpha} \cdot S_{\beta})(S_{\gamma} \cdot S_{\delta}) + (S_{\alpha} \cdot S_{\delta})(S_{\beta} \cdot S_{\gamma})$$

$$- (S_{\alpha} \cdot S_{\gamma})(S_{\beta} \cdot S_{\delta}) + \frac{1}{2}(S_{\alpha} \cdot S_{\beta} + S_{\gamma} \cdot S_{\delta}$$

$$+ S_{\alpha} \cdot S_{\delta} + S_{\beta} \cdot S_{\gamma} + S_{\alpha} \cdot S_{\gamma} + S_{\beta} \cdot S_{\delta} + \frac{1}{2}).$$

Here $\alpha, \beta, \gamma, \delta$ denote the four sites of a plaquette clockwise. At $J_2 = 0.5$, the plaquette order parameter is evaluated on a $2 \times 2$ cluster as $Q_{\alpha\beta\gamma\delta} \approx 0.988$, very close to its saturated value 1.0. Evaluating $Q_{\alpha\beta\gamma\delta}$ on a larger cluster also gives nonzero result. However, this is the boundary effect of the cluster and does not support a true VBS state. It is an interesting open question how to incorporate the order parameter of various VBS state into the mean-field approximation. If such a mean-field theory does exist, considering that it tends to exaggerate the LRO, a negative result about the existence of VBS may rule out the possibility of VBS in the intermediate parameter regime.

We also investigate the Néel as well as the collinear magnetic susceptibility at zero temperature. These susceptibilities are defined as

$$\chi_n = \lim_{h \to 0^+} \frac{\text{Tr}[e^{-\beta(H - hM_n)}M_n]}{h \text{Tr}[e^{-\beta(H - hM_n)}]}.$$  

Figure 4. Zero temperature Néel susceptibility $\chi_n$ (squares on the guiding line) and collinear susceptibility $\chi_c$ (dots on the guiding line) as functions of $J_2$. The data are obtained by numerical derivation with the applied field $h = 0.01$.

Here, the Néel susceptibility $\chi_n$ and collinear susceptibility $\chi_c$ are defined using staggered magnetization $M_n$ and $M_c$, respectively. For the $2 \times 2$ cluster shown in figure 1, $M_n = S_1^z - S_2^z + S_3^z - S_4^z$ and $M_c = S_1^z + S_2^z - S_3^z - S_4^z$. We apply a small staggered field $h$ and evaluate $\chi_n$ and $\chi_c$ using numerical derivation. The results obtained are shown in figure 4.

The continuously diverging behavior of $\chi_n$ at $J_2 \approx 0.42$ confirms the continuous transition from Néel AFM phase to non-magnetic phase. In contrast, near the collinear transition $J_2^{2}$, an abrupt jump of $\chi_c$ is observed, being consistent with a first-order phase transition. Note that both $\chi_n$ and $\chi_c$ are much larger in the non-magnetic phase than in their corresponding long-range ordered regime. This shows that the intermediate non-magnetic ground state is rich of short-range spin fluctuations at various momentums, and different types of spin correlation compete strongly with each other. This leads to the notorious difficulty in the study of the non-magnetic state.

The mean-field approximation used in our study introduces a symmetry breaking term $H' = \sum_{i=1}^{L} h_i S_i^z$, which breaks the $SU(2)$ symmetry of the original Hamiltonian. For CMFT calculation using a finite cluster, this term effectively suppresses the quantum fluctuation and tends to exaggerate the stability of LRO in the ground state. As a result, the obtained $|m|$ is larger than the exact value (as checked in the $J_2 = 0$ case). The region of the magnetic LRO is enlarged and the non-magnetic region suppressed. Here, to phenomenologically study the effects of enhancing or reducing quantum fluctuations, we introduce artificial fluctuations by multiplying a tunable factor $\lambda$ to the mean-field term $H'$. The total Hamiltonian becomes $H_{\text{eff}} = H_n + \lambda H'$. $\lambda < 1$ enhances the fluctuation of $H_{\text{eff}}$, and it mimics the effects of larger cluster or smaller...
spin. \( \lambda > 1 \) reduces the fluctuation of \( H_{\text{eff}} \) and it mimics the effects of anisotropy or larger spin. Figure 5 shows a phase diagram in the \( \lambda - J_2 \) plane. For larger \( \lambda \), the LRO region is enlarged and the non-magnetic region shrinks. At \( \lambda = 1.4 \), the non-magnetic region diminishes, leading to a direct first-order transition between Néel phase and collinear phase. At this point the phase diagram resembles that of the \( J_1 - J_2 \) Ising model where quantum fluctuation disappears. For smaller \( \lambda \), the non-magnetic region enlarges and for sufficiently small \( \lambda \), the LRO regime will disappear. This phase diagram resembles the phase diagram of anisotropic Heisenberg model [48]. Note that this artificial fluctuation does not influence the width of the coexistence region, showing that the first-order phase transition at \( J_2^2 \) is robust against quantum fluctuations.

### 3.2. Effect of anisotropic coupling

In this section, we study the effect of spin-anisotropic coupling which breaks the \( SU(2) \) symmetry of the original \( J_1 - J_2 \) Heisenberg Hamiltonian. It is expected that the spin anisotropy strongly suppresses the quantum fluctuations. Studying the effect of spin anisotropy can help us understand the role of quantum fluctuations in stabilizing the non-magnetic ground state. Also, the anisotropy will induce a finite temperature phase transition even in two-dimensions. A similar study of the spin anisotropy has been carried out for the \( J_1 - J_2 - J_3 \) model [48]. In the following, we study the spin-anisotropy effect using the following Hamiltonian:

\[
\hat{H}_{\text{ani}} = (1 - \delta) J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + (1 - \delta) J_2 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\
+ \delta J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i^z \mathbf{S}_j^z + \delta J_2 \sum_{\langle i,j \rangle} \mathbf{S}_i^z \mathbf{S}_j^z.
\]

Here, the parameter \( \delta \) is used to tune the strength of the spin anisotropy in this Hamiltonian. For \( \delta = 0 \), \( H_{\text{ani}} \) reduces to the isotropic \( J_1 - J_2 \) model. For \( \delta = 1 \), it becomes the Ising model.

In figure 6, we show the phase diagram in the \( T - J_2 \) plane for an intermediate spin anisotropy \( \delta = 0.5 \). The solid line is the Ising model for \( \delta = 0 \). For larger \( \delta \), the ground state changes from Néel AFM into collinear AFM through a first-order phase transition, accompanied by a coexistence regime in \( 0.53 < J_2 < 0.77 \). Upon increasing temperature, the Néel AFM in the small \( J_2 \) regime and the collinear AFM in the large \( J_2 \) regime extend up to a finite critical temperature where they disappear continuously. Although the \( 2 \times 2 \) CMFT tends to overestimate the transition temperature, the finite critical temperature is qualitatively reasonable considering that the Mermin–Wagner theorem does not apply in this case. Meanwhile a precise Monte Carlo calculation shows that even small anisotropy will significantly enhance transition temperature in the non-frustrated antiferromagnetic model [58]. For the intermediate \( J_2 \) value, the coexistence region shrinks as \( T \) increases. Above the critical point \( (J_{2c} = 0.653, T_c = 0.4) \), the first-order phase transition changes into the second-order one. In a small temperature window just below \( T_c \), the coexistence occurs between the PM phase and the collinear AFM phase. The whole phase diagram is similar to that of the anisotropic \( J_1 - J_2 \) model studied in [48] using the effective field theory. Our results show that strong quantum fluctuations are crucial for the existence of the non-magnetic phase in the \( J_1 - J_2 \) Heisenberg model.

It is noted that for the isotropic \( J_1 - J_2 \) model, a finite temperature phase transition in regime \( J_2 > J_2^c \) may exist to break the \( C_4 \) rotation symmetry of the lattice, according to Chandra et al [37, 46, 47]. However, what we obtained in figure 6 has nothing to do with this transition. It would be interesting to develop our CMFT for further study of this novel Ising transition. We leave this issue for the future.
4. Summary

In summary, we use the cluster mean-field theory to study the $J_1 - J_2$ Heisenberg model on a square lattice. For small, intermediate, and large $J_2/J_1$ regime, we obtain the Néel AFM phase, the non-magnetic phase, and the collinear AFM phase, respectively. The Néel-to-non-magnetic transition is found to be of second order, and the non-magnetic-to-collinear transition is of first order. The respective critical values $J_1^c$ and $J_2^c$ are found to converge rapidly with increasing $L$. From the largest $4 \times 4$ cluster we obtain $J_2^c \approx 0.42$, which is very close to the results of the $2 \times 2$ cluster 0.41. Extrapolating the cluster size to infinity, we obtain $J_2^c \approx 0.59$. Both $J_1^c$ and $J_2^c$ agree with the previous results very well. We also investigate the finite temperature phase diagram of the spin-anisotropic $J_1 - J_2$ model. It is demonstrated that with sufficiently strong Ising coupling, the non-magnetic ground state is unstable towards a first-order phase transition. Above the critical temperature $T_c$, the first-order phase transition changes into a second-order transition. Our results show that the cluster mean-field theory is not only a very useful tool for studying classical phase transitions [51], but can also give surprisingly accurate ground state phase boundaries for the frustrated quantum magnet.

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