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Classical Ground State Spin Ordering of the Antiferromagnetic J_1–J_2 Model *

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The classical frustrated antiferromagnetic J_1–J_2 model is considered in a description of the classical spin wave for a vector spin system. Its ground state (GS) spin ordering is analyzed by minimizing its energy. Our analytical derivations show that all the spins in the GS phase must lie in planes that are parallel to each other. When applying the derived formulations to concrete lattices such as the square and simple cubic lattices, we find that in the large J_2 region, a large continuous GS degeneracy concluded by a qualitative analysis is lifted, and collinear striped ordering is selected as the GS phase.

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In modern condensed matter physics, frustrated spin systems with competing interactions have been intensively studied in the last 30 years,[1,2] providing us a vast and intriguing world of physics with many novel and exotic magnetic phenomena, even at the classical level. In this research area, of great interest is the frustrated antiferromagnetic (AF) J_1–J_2 spin model with the Hamiltonian

$$H = \frac{1}{2}J_1 \sum_{<ij>} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{1}{2}J_2 \sum_{[ij]} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \qquad (1)$$

where J_1 and J_2 are the nearest-neighboring (NN) and the next-nearest-neighboring (NNN) exchange couplings, respectively, and both of them are considered to be AF, i.e., $J_1, J_2 > 0$.

In research of the ground state (GS) phases of this frustrated spin model, the subtle interplay between frustration and fluctuations is a fascinating subject. Frustration often tends to promote the degeneracy of the classical GS phases, while fluctuations can act strongly among the degenerate GS manifold, lift the degeneracy, and select certain spin ordering as the true and stable GS phase. This phenomenon has been called 'order by disorder'.[3–5]

A typical example is the discovery of collinear striped ordering in the region of large J_2 (or $J_1 \to 0$ and $J_2 \neq 0$). For the classical model, in this region, because $J_2 \gg J_1$, the system is often qualitatively and approximately decoupled into two interpenetrating sublattices with only NNN AF bonds. Thus the two sublattices for every order antiferromagnetically with their spin directions are independent of each other, and the energy of the system is independent of the NN exchange coupling J_1, which leads to a highly degenerate classical GS manifold including collinear and noncollinear spin orderings.[6] However, for the quantum model, when quantum fluctuations are considered, this degeneracy will be lifted, and the GS becomes magnetically ordered collinearly as a stripe phase.[6–10]

Studying the corresponding classical model is often the first step in studying the quantum spin model, so that influences of the quantum effect can be exhibited more distinctly by comparison. Furthermore, some research methods for the quantum spin model, such as the coupled cluster method,[9] the spin-wave theory[11] and the double-time Green's function method,[12] often recur to the GSs of the corresponding classical model as their reference state at the beginning of the research. Thus it is essential to make the properties of the corresponding classical model clear for the quantum model. However, for the frustrated AF J_1–J_2 model, in the large J_2 region, although the collinear striped ordering as the GS phase has been well accepted at the quantum level, it is still not obvious at the classical level.[13]

In this Letter, we restudy the GS of the frustrated AF J_1–J_2 model still at the classical level, but go beyond the qualitative analysis mentioned above. Resorting to a classical description of the spin wave for a vector spin system, we present detailed analytical derivations of the GS energy and its corresponding spin ordering. Our results show more information about the classical GS than the qualitative analysis did. Especially for the square and simple cubic lattices,[14–16] our results show that in the large J_2 region, the collinear striped ordering is obviously the GS phase at the classical level.

Here, at the classical level, the lattice spins are treated as classical vectors with length S, and their directions can continuously change in real space. According to the classical description of the spin wave,[17–19] we parameterize them by spherical coordinates

$$\begin{aligned} S_n^x &= S\sin\theta\cos\varphi_n, \\ S_n^y &= S\sin\theta\sin\varphi_n, \\ S_n^z &= S\cos\theta, \end{aligned} \qquad (2)$$

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where the orientation of the z-axis is arbitrarily chosen in real space, and the azimuthal angle φ_n is dependent on the lattice site, but the polar angle θ is not.

Taking Eq. (2) into Eq. (1), and rewriting the azimuthal angle by introducing a wave vector $\boldsymbol{q}$,

$$\varphi_n = \boldsymbol{q}\cdot\boldsymbol{r}_n, \tag{3}$$

we can finally obtain the energy of the model in a parameterized form

$$E_{\rm cl} = \frac{1}{2}Z_1J_1NS^2[\cos^2\theta(1+p)+\sin^2\theta(\gamma_{1\boldsymbol{q}}+p\gamma_{2\boldsymbol{q}})], \tag{4}$$

with the structure factors

$$\gamma_{i\boldsymbol{q}} = \frac{1}{Z_i}\sum_{\boldsymbol{\delta}_i}\cos(\boldsymbol{q}\cdot\boldsymbol{\delta}_i), \quad i=1,2, \tag{5}$$

where N is the total number of lattice sites, $p = (Z_2J_2)/(Z_1J_1)$ is the frustration parameter, Z_1 (Z_2) is the coordination number of the nearest (next-nearest) neighbors, and $\boldsymbol{\delta}_1$ and $\boldsymbol{\delta}_2$ are the lattice vectors connecting the NN and NNN sites, respectively.

In the expression of the classical energy, i.e., Eq. (4), there is a function $f(\theta) = A\cos^2\theta + B\sin^2\theta$ with $A = 1+p$ and $B = \gamma_{1\boldsymbol{q}}+p\gamma_{2\boldsymbol{q}}$ for $B \le A$ because of $\gamma_{1\boldsymbol{q}} \le 1$ and $\gamma_{2\boldsymbol{q}} \le 1$. The single minimum point of this function is $\theta = \pi/2$, thus we can obtain an upper limit of the classical GS energy by substituting $\theta = \pi/2$ into Eq. (4) and obtain

$$\bar{E}_{\rm cl} = \frac{1}{2}Z_1J_1NS^2(\gamma_{1\boldsymbol{q}}+p\gamma_{2\boldsymbol{q}}). \tag{6}$$

Because the orientation of the z-axis is arbitrarily selected, the polar angle $\theta = \pi/2$ means that all the spin vectors in real space must lie in planes that are parallel to each other. This result is independent of the frustration parameter p and applicable to all dimensions.

Let us consider the square lattice. For convenience, without loss of generality, the z-axis is set perpendicular to the square plane, and the x- and y-axes are set along the two edges of the primitive square plaquette, respectively. We have shown that the polar angle θ must be $\pi/2$ for the GS spin ordering, thus here all the spin vectors lie in the square plane (or x–y plane). Whether they are aligned collinearly or noncollinearly can be judged from the values of the azimuthal angles $\varphi_n, n = 1,2,\ldots$.

For a square lattice, the coordination numbers are $Z_1 = 4$ and $Z_2 = 4$. In the unit of lattice spacing ($a = 1$), the lattice vectors connecting four NN sites are $\boldsymbol{a}_1 = -\boldsymbol{a}_3 = (1,0,0)$, $\boldsymbol{a}_2 = -\boldsymbol{a}_4 = (0,1,0)$, and the ones connecting four NNN sites are $\boldsymbol{b}_1 = -\boldsymbol{b}_3 = (1,1,0)$, $\boldsymbol{b}_2 = -\boldsymbol{b}_4 = (-1,1,0)$. From Eq. (5), we obtain the structure factors for the square lattice

$$\gamma_{1\boldsymbol{q}} = \frac{1}{2}(\cos q_x + \cos q_y), \tag{7}$$

$$\gamma_{2\boldsymbol{q}} = \cos q_x \cos q_y. \tag{8}$$

In the region of small J_2 (or $p \ll 1$), the main contribution to the classical energy $\bar{E}_{\rm cl}$ in Eq. (6) comes from the NN structure factor $\gamma_{1\boldsymbol{q}}$. From Eq. (7), we find that the minimum of $\gamma_{1\boldsymbol{q}}$ occurs at the following wave vectors

$$\boldsymbol{q} = \pi(m,n,C), \quad \text{with odd } m,\ n, \tag{9}$$

where C is an arbitrary constant. This form of wave vectors leads to GS spin ordering with the relative azimuthal angles between the NN spins and between the NNN spins as

$$\begin{cases} \Delta\varphi_1 = \boldsymbol{q}\cdot\boldsymbol{a}_i = k\pi, \text{ with odd } k \\ \Delta\varphi_2 = \boldsymbol{q}\cdot\boldsymbol{b}_i = k\pi, \text{ with even } k \end{cases}, \text{ for } i = 1,2,3,4, \tag{10}$$

which means that all the nearest neighbors (next-nearest neighbors) of a given spin are aligned exactly antiparallel (parallel) to it. This is the classical two-sublattice Néel ordering phase, as shown in Fig. 1(a).

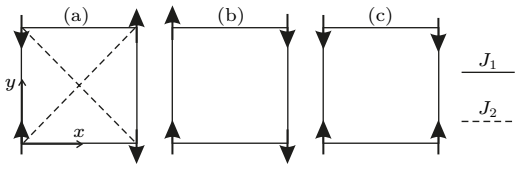


Fig. 1. Classical GS phases of the square lattice: (a) Néel ordering for small J_2; (b) and (c) the two degenerate collinear striped orderings for large J_2.

Substituting Eq. (9) into Eq. (6), we obtain the classical GS energy of the Néel phase

$$E_0^{\rm N}({\rm square}) = -\frac{1}{2}Z_1J_1NS^2(1-p). \tag{11}$$

In the region of large J_2 (or $p \gg 1$), the main contribution to the classical energy $\bar{E}_{\rm cl}$ in Eq. (6) comes from the NNN structure factor $\gamma_{2\boldsymbol{q}}$. From Eq. (8), we find that the minimum of $\gamma_{2\boldsymbol{q}}$ occurs at the following wave vectors

$$\boldsymbol{q} = \pi(m,n,C), \text{ with odd } m \text{ and even } n, \text{ or vice versa}, \tag{12}$$

where C is an arbitrary constant. If we choose odd m and even n, this form of wave vectors will lead to GS spin ordering with the relative azimuthal angles between the NN spins as

$$\Delta\varphi_1 = \boldsymbol{q}\cdot\boldsymbol{a}_i = k\pi, \quad \text{with odd } k \text{ for } i = 1,\ 3, \quad \text{with even } k \text{ for } i = 2,\ 4, \tag{13}$$

and the ones between the NNN spins as

$$\Delta\varphi_2 = \boldsymbol{q}\cdot\boldsymbol{b}_i = k\pi, \text{ with odd } k \text{ for i=1, 2, 3, 4.} \tag{14}$$

The expression of $\Delta\varphi_1$ in Eq. (13) means that the NN spins along the x-axis are aligned exactly antiparallel to each other, while the ones along the y-axis are

aligned parallel to each other. The expression of $\Delta\varphi_2$ in Eq. (14) means that all the NNN spins are aligned exactly antiparallel to each other. This spin ordering is a collinear striped ordering, as shown in Fig. 1(b).

Going back to Eq. (12), if we choose even m and odd n, we can obtain nothing but a degenerate collinear striped ordering of the former, with the NN spins along the y-axis aligned antiparallel to each other, whereas those along the x-axis are aligned parallel to each other, as shown in Fig. 1(c).

Substituting Eq. (12) into Eq. (6), we can obtain the classical GS energy of this collinear striped ordering phase

$$E_0^{\rm S}({\rm square}) = -\frac{1}{2}Z_1J_1NS^2p. \tag{15}$$

Interestingly, because $p = (Z_2J_2)/(Z_1J_1)$, this energy is in fact independent of the NN coupling J_1, the same as the energy from the qualitative analysis that neglects J_1 at the beginning. However, our analysis shows that the GS phase is collinear striped ordering, which is a result beyond the qualitative analysis.

For a simple cubic (SC) lattice, it is convenient to set the x, y, z-axes along the three edges of the primitive cube, respectively. The coordination numbers are $Z_1 = 6$ and $Z_2 = 12$. In the unit of lattice spacing ($a = 1$), the lattice vectors connecting six NN sites are $\boldsymbol{a}_1 = -\boldsymbol{a}_4 = (1,0,0)$, $\boldsymbol{a}_2 = -\boldsymbol{a}_5 = (0,1,0)$, $\boldsymbol{a}_3 = -\boldsymbol{a}_6 = (0,0,1)$, and the ones connecting twelve NNN sites are $\boldsymbol{b}_1 = -\boldsymbol{b}_7 = (1,1,0)$, $\boldsymbol{b}_2 = -\boldsymbol{b}_8 = (-1,1,0)$, $\boldsymbol{b}_3 = -\boldsymbol{b}_9 = (1,0,1)$, $\boldsymbol{b}_4 = -\boldsymbol{b}_{10} = (-1,0,1)$, $\boldsymbol{b}_5 = -\boldsymbol{b}_{11} = (0,1,1)$, $\boldsymbol{b}_6 = -\boldsymbol{b}_{12} = (0,-1,1)$. Taking these lattice vectors into Eq. (5), we obtain the structure factors for the SC lattice,

$$\gamma_{1\boldsymbol{q}} = \frac{1}{3}[\cos q_x + \cos q_y + \cos q_z], \tag{16}$$

$$\gamma_{2\boldsymbol{q}} = \frac{1}{3}[\cos q_x \cos q_z + \cos q_x \cos q_y + \cos q_y \cos q_z]. \tag{17}$$

The subsequent analyses are similar to those for the square lattice, thus we give only the results and some necessary discussions in the following.

In the region of small J_2, the minimum of classical energy for this case occurs at the following wave vectors

$$\boldsymbol{q} = \pi(l,m,n), \text{ with } l,\ m,\ n \text{ all odd}, \tag{18}$$

and the relative pitch angles between NN spins and between NNN spins are

$$\begin{aligned}&\Delta\varphi_1 = \boldsymbol{q}\cdot\boldsymbol{a}_i = k\pi, \text{ with odd } k \text{ for } i = 1,\ 2, \cdots, 6\\ &\Delta\varphi_2 = \boldsymbol{q}\cdot\boldsymbol{b}_i = k\pi, \text{ with even } k \text{ for } i = 1,\ 2,\ \cdots, 12,\end{aligned} \tag{19}$$

which also lead to the Néel phase, as shown in Fig. 2(a). The corresponding classical GS energy is

$$E_0^{\rm N}({\rm SC}) = -\frac{1}{2}Z_1J_1NS^2(1-p). \tag{20}$$

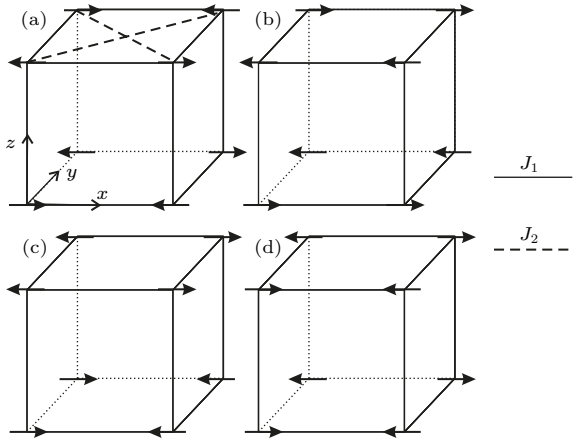


Fig. 2. Classical GS phases of the SC lattice: (a) Néel ordering for small J_2; (b), (c) and (d) the three degenerate collinear striped orderings. The direction of the (0,0,0) site spin vector is assumed to be along the x-axis.

In the region of large J_2, the minimum of classical energy for this case occurs at the following wave vectors

$$\boldsymbol{q} = \pi(l,m,n), \text{ with only one of } l,\ m,\ n \text{ even}. \tag{21}$$

If we choose even l, the relative pitch angles between NN spins and between NNN spins are

$$\begin{aligned}&\Delta\varphi_1 = \boldsymbol{q}\cdot\boldsymbol{a}_i = k\pi,\\ &\text{with even } k \text{ for } i = 1,\ 4,\\ &\text{with odd } k \text{ for } i = 2,\ 3,\ 5,\ 6,\end{aligned} \tag{22}$$

$$\begin{aligned}&\Delta\varphi_2 = \boldsymbol{q}\cdot\boldsymbol{b}_i = k\pi,\\ &\text{with even } k \text{ for } i = 5,\ 6,\ 11,\ 12,\\ &\text{with odd } k \text{ for } i = 1,\ 2,\ 3,\ 4,\ 7,\ 8,\ 9,\ 10,\end{aligned} \tag{23}$$

which lead to the following spin ordering: the NN spins along the x-axis are all aligned parallel to each other, while the NN spins along the y- and z-axes are all aligned antiparallel to each other. This is also a kind of collinear striped ordering, as shown in Fig. 2(b).

If we choose even m or even n, we will obtain the other two collinear striped ordering phases which are degenerate with the former, as shown in Figs. 2(c) and 2(d).

Substituting Eq. (21) into Eq. (6), we can obtain the classical energy of the stripe ordered phase

$$E_0^{\rm S}({\rm SC}) = -\frac{1}{6}Z_1J_1NS^2(1+p). \tag{24}$$

It is noticed that this form of energy is dependent on the NN coupling J_1, which is different from the case of the square lattice.

In summary, it has been widely accepted that collinear striped spin ordering is the GS phase of the quantum frustrated AF J_1–J_2 spin model in the large J_2 region. However, for the classical model, it is not

obvious whether the case is the same. At the classical level, when $J_2 \gg J_1$, the system is often qualitatively and approximately decoupled into two independent sublattices with NNN bonds only, which leads a highly degenerate GS manifold including collinear and noncollinear spin orderings.

In this study, going beyond the qualitative and approximate treatment mentioned above, we have restudied the classical model resorting to a classical description of the spin wave for a vector spin system. From the analytical derivation for the classical GS energy and its corresponding spin ordering, we conclude firstly that in the GS phase, all the spins must lie in planes that are parallel to each other. Then for square and SC lattices, we further conclude that in the large J_2 region, the spin ordering in the GS phase must be collinear and striped. Thus for the classical model, our results show that in a classical spin wave description, the collinear striped ordering can also be selected as the true GS phase from the highly degenerate GS manifold.

Finally, we are obliged to point out that our derivations are not suitable for the region near the critical frustration parameter denoted by $p_{\rm c} = J_{2{\rm c}}/J_1$, where the frustration is so strong that it causes the system to be in a magnetic disordered phase between the Néel phase and the stripe ordered phase. If we solve the equation $E_0^{\rm N} = E_0^{\rm S}$, we can obtain $p_{\rm c} = 1/2$ for the square lattice and $p_{\rm c} = 1/4$ for the SC lattice, which are just the classical critical frustration parameters of the AF J_1–J_2 model on these two lattices, respectively.[6] Thus our derivations and results are effective far outside of the region $J_2/J_1 \sim p_{\rm c}$ where the frustration is weak.

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