Dimensional crossover in the quasi-two-dimensional Ising-O(3) model

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Abstract. We study the Ising-O(3) model on two-dimensional (2D) and quasi-2D lattices. This is an unfrustrated effective model for the stacked square-lattice \( J_1 - J_2 \) Heisenberg model where the nearest neighbor \( (J_1) \) and next-nearest neighbor \( (J_2, J_2 \gg J_1/2) \) exchange interactions are frustrated. By means of Monte Carlo simulation we show that this model has an Ising ordered phase where the O(3) spins remain disordered in a moderate quasi-2D region. We obtain a first-order transition in a region with a sufficiently large inter-layer coupling. Our results provide a qualitative explanation of the experiments on ferropnictides, namely the observed sequence and the orders of the structural and magnetic transitions as a function of the ratio between the inter-layer and intra-layer couplings.

1. Introduction

The square-lattice \( J_1 - J_2 \) Heisenberg model is a prototypical example of a frustrated spin system. This model is believed to have a nontrivial ground state and finite temperature properties due to the combination of frustration and low-dimensionality [1]. The corresponding single-layer Hamiltonian is

\[
H = J_1 \sum_{\text{n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\text{n.n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j,
\]

where the nearest neighbor \( (J_1) \) and next-nearest neighbor \( (J_2) \) couplings are frustrated. Here we consider a stacked square lattice by introducing a finite inter-layer coupling. It is known that the ground state of the \( H \) (1) has Néel ordering for \( J_2/J_1 \lesssim 0.4 \) while it exhibits a two-sublattice collinear antiferromagnetic (CAF) ordering for \( J_2/J_1 \gtrsim 0.65 \) (Fig. 1). The intervening region \( J_2 \sim J_1/2 \) is still controversial [2].

Both theoretical and experimental efforts have been extensively devoted to understanding the phase diagram of this Hamiltonian [1]. Recently, the discovery of high-\( T_c \) superconductivity in ferropnictides has revived this interest [3]. The local moment picture is most likely inadequate for a microscopic description of the metallic ferropnictides. However, in this work we show that this simple model provides a qualitative understanding of almost universal features in the structural and magnetic transitions observed in ferropnictides. Particularly, although lattice degrees of freedom are not included in the model, the electronically driven Ising-like ordering shown in Fig. 1 will necessarily trigger the observed structural transition (\( C_4 \) symmetry breaking) [4, 5].

The model may be related to ferropnictides in the CAF region. More specifically, we are interested in the 1111-family of quasi-2D compounds \( R \text{FeAsO} \), where \( R \) is a rare earth ion [6, 7]
and 122-type 3D compounds $\text{AFe}_2\text{As}_2$ with alkaline earth elements $\text{A}$ [8]. Different experiments have confirmed the following features for the undoped ground states of these ferropnictides [3]: (i) spin-density-wave (SDW) order at $(\pi, 0)$ and (ii) orthorhombic lattice structure, distorted from high-$T$ tetragonal structure. Interestingly, the tetragonal-orthorhombic structural transition occurs at a temperature ($T_{c1}$) that is either the same as the Néel temperature ($T_{c2}$), as in the 3D 122-type undoped compounds [8], or slightly higher than $T_{c2}$, as in the more quasi-2D 1111-type compounds [6, 7]. Experiments also confirmed first-order features such as hysteresis in the undoped 122 compounds [8], while the separate transitions in the 1111 compounds seem to be of second order or very weakly first order [7]. The proximity of these transitions is evidence in favor of a relevant magneto-elastic coupling. This was also confirmed by density functional calculations in Ref. [9]. As it was suggested in Ref. [10], it seems that there is a correlation between the sequence of the transition(s) and the magnitude of the inter-layer coupling. Finally, $T_{c1} \geq T_{c2}$ seems to be a universal feature among ferropnictides.

Several authors have argued that these almost universal characteristics of ferropnictides can be qualitatively explained by using an oversimplified $J_1-J_2$ Heisenberg model in the CAF region [4, 5]. In this picture, the structural transition is identified with the Ising-like order that emerges from an order-by-disorder effect [11], while the SDW order is identified with the magnetic transition that breaks $O(3)$ spin rotational symmetry as well as the translational symmetry. The ordering wave-vectors are $(\pi, 0)$ or $(0, \pi)$ [4, 5]. The inequality $T_{c1} \geq T_{c2}$ immediately follows from this picture because the Ising order is described by a composite order parameter in terms of spins [4, 5]. Furthermore, according to Mermin-Wagner theorem [12, 13], only the Ising order can survive at $T > 0$ in $d = 2$: $T_{c1}^{2D} > T_{c2}^{2D} = 0$. This result was confirmed by a Monte Carlo study [14]. This also implies that the Ising order without magnetic order will be present in some quasi-2D region of the phase diagram even in the presence of a finite inter-layer coupling [5]. However, the precise form of the phase diagram of the $J_1-J_2$ Heisenberg model as a function of the inter-layer coupling is still unknown. This is the main motivation of our numerical study.

2. Model

We consider an unfrustrated classical effective model, called the Ising-$O(3)$ model [5], adequate for describing the $J_1-J_2$ Heisenberg model in the CAF region. The Hamiltonian of this model is defined by

$$H_{I-O(3)} = -\sum_{\langle i,j \rangle} J_{ij} (1 + \sigma_i \sigma_j) \mathbf{S}_i \cdot \mathbf{S}_j,$$
where $\sigma_i$ and $\mathbf{S}_i$ denote the classical Ising and Heisenberg spins respectively. We consider a 2D square lattice and a quasi-2D cubic lattice. For the latter we assume that the coupling constant $J_{ij}$ is spatially anisotropic in such a way that:

$$J_{ij} = \begin{cases} J & \text{if } (i, j) \text{ are on the same layer} \\ J_z & \text{if } (i, j) \text{ are on the nearest neighbor layers}, \end{cases}$$

where $0 < J_z \lesssim J$. We use the unit $J \equiv 1$ below. The following effective Hamiltonian can be derived by introducing auxiliary O(3) fields $\phi_A \sim \mathbf{S}$ and $\phi_B \sim \sigma \mathbf{S}$:

$$H_{\text{eff}} = \int d^d x \left[ \sum_{a=A,B} \left( \frac{1}{2} |\nabla \phi_a|^2 + r|\phi_a|^2 + u|\phi_a|^4 \right) + u_{AB} |\phi_A|^2 |\phi_B|^2 + \lambda (\phi_A \cdot \phi_B)^2 \right],$$

where $\lambda < 0$. It was argued that an effective field theory of the $J_1$-$J_2$ Heisenberg model can also be written in this form when $J_2 \gtrsim J_1/2$ [5]. In that case, $\phi_A$ and $\phi_B$ are Néel order parameters of the $\sqrt{2} \times \sqrt{2}$ sublattices. Therefore, a comparison between $H_{\text{Ising}}$ and the effective Hamiltonian (4) suggests that $\sigma_i$ in the Ising-O(3) model represents a degree of freedom that specifies whether the local spin configuration is “vertical” or “horizontal” (see Fig. 1).

3. Numerical results

We simulated the Ising-O(3) model (2) on the square and the anisotropic cubic lattices by employing the cluster Monte Carlo method where the Ising and O(3) spins are updated alternatively. When $J_z \neq 0$, we combine the cluster update with a local update. In this case, we also use a semi-global cluster update where the clusters are allowed to expand only within a given layer.

3.1. 2D case

First, we show the results in $d = 2$. The non-negativity of $J_{ij} (1 + \sigma_i \sigma_j)$ favours a parallel alignment of the O(3) spins at any temperature. This implies that the effective coupling between the Ising spins is also ferromagnetic because, at the mean-field level, it is given by $J_{ij} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$. This cooperative relation leads to a finite-$T$ transition of the 2D system where only the Ising spins become critical. A standard finite-size scaling analysis strongly indicates that the transition belongs to the 2D Ising universality class [15].

3.2. Quasi-2D case

Here we show the results for the quasi-2D region ($J_z \neq 0$). The inter-layer coupling stabilizes the O(3) spin order at $T > 0$. It also makes the Ising order 3D. In particular, we are interested in a region where the Ising and O(3)-like transitions occur at different temperatures because this may be related to the separate transitions observed in the 1111 compounds [6]. We also note that previous analytical studies suggested different scenarios when these transitions are close to each other: a large-$N$ approximation predicted always two separate second-order transitions [4] whereas a mean-field theory predicted a phase diagram with richer structure [16].

We obtained two transitions for $J_z = 0.01$ (Fig. 2). Naturally, the separation between both transitions increases for a smaller inter-layer coupling [5, 15]. The lattice that we simulated has a tetragonal shape $L \times L \times rL$ with aspect ratio $r = 1/12$. The value of $r$ was determined in such a way that $G^m(L_x/2, 0, 0) \approx G^m(0, 0, L_z/2)$ and $G^r(L_x/2, 0, 0) \approx G^r(0, 0, L_z/2)$, where $G^m(r)$ ($G^r(r)$) is the correlation function of the O(3) (Ising) order parameter. We studied system sizes that range from $L = 48$ to $L = 120$.

Figure 2 shows the specific heat $C = N^{-1} \beta^2 \left[ \langle H_{\text{LO}(3)} \rangle^2 - \langle H_{\text{LO}(3)} \rangle^2 \right]$ where $N \equiv rL^3$. The double peak structure that develops for $L = 120$ suggests two separate transitions. This
observation is also supported by the behavior of Binder parameters $U_m = \langle m^4 \rangle / \langle m^2 \rangle^2$ with $m = N^{-1} \sum_i S_i$ and $U_\sigma = \langle \sigma^4 \rangle / \langle \sigma^2 \rangle^2$ ($\sigma = N^{-1} \sum_i \sigma_i$). Figure 3 shows their finite-size scaling plots. Based on symmetry arguments we assume that the higher-$T$ (lower-$T$) transition is in the 3D Ising (Heisenberg) universality class and we use critical exponents available in the literature: $\eta_\text{Is} = 0.03639(15)$ and $\nu_\text{Is} = 0.63012(16)$ for the 3D Ising universality class [17] and $\eta_\text{H} = 0.0375(5)$ and $\nu_\text{H} = 0.7112(5)$ for the 3D Heisenberg universality class [17]. Although there are large finite-size effects, there is an asymptotic tendency towards data collapse that supports our assumptions for the universality classes. From these results we obtain $T_{c1} = 1.0610(8)$ and $T_{c2} = 1.0575(5)$. As for the sizable sub-leading corrections observed in these scaling plots, it appears that they are largely due to (i) the proximity of the two transitions and (ii) the spatially anisotropic correlations [15]. A more comprehensive finite-size scaling study including other dimensionless parameters and the correlation functions will be discussed elsewhere [15].

3.3. 3D case with weak spatial anisotropy

Finally, we move on to the 3D region with a larger inter-layer coupling. We simulated the system for $J_z = 0.1$, 0.0625, 0.04, 0.0278 and 0.0204, and aspect ratios of the lattice that turned out to be $r = 1/3$, 1/4, 1/5, 1/6 and 1/7, respectively. We obtained a bimodal structure of the internal energy distribution for all of these parameters [15], which is an unambiguous sign of a first-order transition. We also found that the first-order feature is stronger for a larger inter-layer coupling [15]. We also confirmed the diverging behavior in the Binder parameters of both of order parameters for all the inter-layer couplings listed above except for $J_z = 0.0204$ [15]. This means that the first-order transition takes place between the paramagnetic phase and the lowest-$T$ phase, where $\langle m \rangle \neq 0$ and $\langle \sigma \rangle \neq 0$. The intervening region including $J_z = 0.0204$ is currently under investigation. Figure 4 shows the phase diagram that summarizes our results.

4. Conclusion

In summary, we studied the Ising-O(3) model on 2D and quasi-2D lattices. This is an effective model of the $J_1$-$J_2$ Heisenberg model with $J_2 \lesssim J_1/2$. By solving this effective model we
Figure 3. Finite-size scaling plots of the Binder parameters (a) $U_m$ and (b) $U_\sigma$ for $J_z = 0.01$. The insets show explicit relations between the scaled temperatures $t_{1,2} \equiv (T - T_{c1,2})/T_{c1,2}$ and the real temperature $T$. The lines are guides to the eye.

Figure 4. Phase diagram of the quasi-2D Ising-O(3) model. The Ising ordered phase retaining full O(3) symmetry exists in a region with a weak inter-layer coupling $J_z \lesssim 0.01$. The line that separates the Ising ordered phase and the lowest-$T$ phase is a schematic one. The other lines are guides to the eye.

identified the region where the O(3)-symmetric Ising ordered phase exists. For sufficiently large inter-layer coupling, we found that a single first-order transition occurs between the paramagnetic and lowest-$T$ ordered phase. The other subtle features discussed in the context of a mean-field theory [16] have not been reproduced but may need further investigation.

Our results provide a qualitative explanation for the sequence and the orders of transitions observed in ferropnictides as a function of the ratio between the inter-layer and intra-layer exchange couplings. This suggests that the separate structural and SDW transitions observed in the quasi-2D 1111 compounds [6, 7] are due to the fragility of the SDW order against fluctuations, which makes it more sensitive to the magnitude of the inter-layer coupling. The first-order nature of the simultaneous structural and SDW transition observed in the more 3D 122 parent...
compounds [8] is also consistent with our results. Despite the oversimplified nature of our local-moment model for the microscopic description of ferropnictides, we obtained a qualitatively correct phase diagram. This result indicates that the $J_1$-$J_2$ Heisenberg model and the related Ising-O(3) model are good starting points for describing universal properties of these compounds.

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