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Monte Carlo studies of the Ising square lattice with competing interactions

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Abstract. We use improved Monte-Carlo algorithms to study the antiferromagnetic 2D-Ising model with competing interactions J_1 on nearest neighbour and J_2 on next-nearest neighbour bonds. The finite-temperature phase diagram is divided by a critical point at $J_2 = J_1/2$ where the groundstate is highly degenerate. To analyse the phase boundaries we look at the specific heat and the energy distribution for various ratios of J_2/J_1 . We find a first order transition for small $J_2 > J_1/2$ and the transition temperature suppressed to $T_C = 0$ at the critical point.

1. Introduction

The antiferromagnetic J_1 - J_2 spin-1/2 Heisenberg model [1, 2, 3, 4] and related bosonic models on the square lattice [5, 6, 7, 8] with hopping t_i and repulsion terms J_i on nearest neighbour (NN) and next-nearest neighbour (NNN) bonds have been intensively studied over recent years via different approaches. The treatment of the bosonic model via Quantum Monte-Carlo (QMC) algorithms suffers from freezing problems in the intermediate regime at $J_2 = J_1/2$ which can be traced to a groundstate degeneracy of the static limit with hopping terms $t_i = 0$. This motivated us to restudy the 2D-Ising model with competing interactions and solve these freezing problems via improved classical Monte-Carlo (MC) algorithms. The 2D-Ising model has a long history and is still a topic of discussion [9, 10, 11, 12, 13, 14]; especially the character of the phase boundary for $J_2 > J_1/2$ is an open question [15, 16, 17, 18]. There are two scenarios discussed: Landau and Binder as well as Malakis et al [14, 16] used MC methods to infer a second order transition for all $J_2 > J_1/2$ with non universal exponents. In contrast Lopez et al and Anjos et al use variational methods [15, 18] and find a first order transition for small $J_1 \gtrsim J_2 > J_1/2$ and a continuous transition only for larger J_2 . Our simulation strengthens the latter scenario [19].

We outline the model and the methods in section 2 and 3 and present our results in section 4. We end with a short discussion and outlook.

2. Model

The model of hardcore bosons on a square lattice with competing interactions on NN bonds and NNN bonds is described by the hamiltonian:

$$H_{\text{boson}} = -t_1 \sum_{\text{NN}} (b_i^\dagger b_j + b_j^\dagger b_i) - t_2 \sum_{\text{NNN}} (b_i^\dagger b_j + b_j^\dagger b_i) + V_1 \sum_{\text{NN}} n_i n_j + V_2 \sum_{\text{NNN}} n_i n_j \quad (1)$$

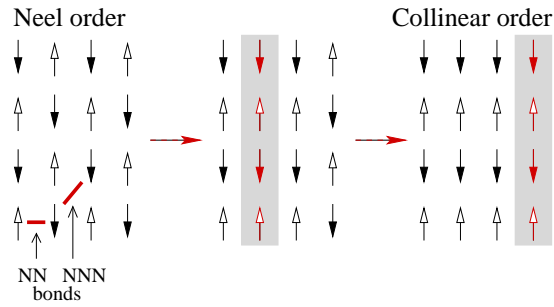


Figure 1. Sketched are both ordered phases and a third groundstate configuration at $J_2 = J_1/2$ (middle). Shaded areas mark flipped lines.

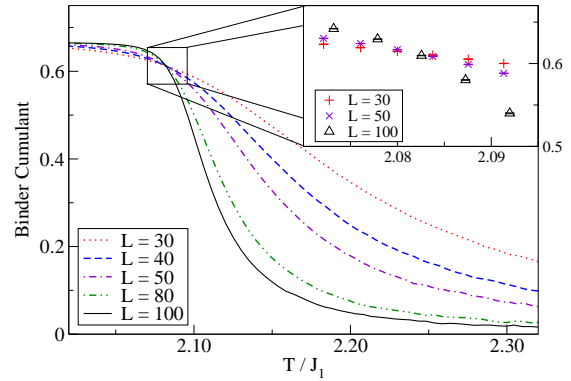


Figure 2. Binder cumulants depending on temperature and L for $J_2 = J_1$. In the inset the intersection area of the cumulants with errorbars gives $T_C/J_1 = 2.082 \pm 0.005$.

This hamiltonian can be mapped onto an equivalent spin model which coincides with the J_1 - J_2 spin-1/2 anisotropic Heisenberg model apart from the sign in front of the hopping terms t_i . Taking the static limit $t_i = 0$ the hamiltonian reduces to that of the Ising model with competing antiferromagnetic interactions $J_i > 0$:

$$H_{\text{Ising}} = J_1 \sum_{\text{NN}} S_i S_j + J_2 \sum_{\text{NNN}} S_i S_j, \quad S_i = \pm 1. \quad (2)$$

We will study square lattices of linear extent L with periodic boundary conditions.

For $J_2 < J_1/2$ the groundstate of (2) is Néel-ordered (see Fig. 1, left) with energy:

$$E_{\text{Néel}} = -2N(J_1 - J_2), \quad N = L^2. \quad (3)$$

For $J_2 > J_1/2$ the system orders in the collinear (or superantiferromagnetic) phase (see Fig. 1, right). In this state every spin has two parallel and two antiparallel aligned nearest neighbours. Thus, the energy depends only on the antiparallel diagonal bonds:

$$E_{\text{Coll}} = -2NJ_2. \quad (4)$$

At the critical point $J_2 = J_1/2$ separating these two phases the transition temperature is suppressed and the groundstate is highly degenerate of order $2^{L+1} - 2$ (one of these states is shown in the middle panel of Fig. 1). Due to this groundstate degeneracy the free energy is characterised by many local minima. This leads to freezing problems for simple importance sampling MC simulations.

3. Methods

In order to compute the transition temperature T_C for ratios of J_2/J_1 very close to the critical point $J_2 = J_1/2$ we used parallel tempering [20, 21, 22, 23] MC methods with additional line flip updates [19].

To detect the finite temperature phase transitions we use the Binder cumulant (reduced fourth order cumulant) $U_4 = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$ [24, 25, 14] of the order parameter $M(\vec{q}) = \sqrt{S(\vec{q})/N}$, where

$$S(\vec{q}) = \frac{1}{N} \sum_{i,j} e^{i\vec{q} \cdot (\vec{x}_i - \vec{x}_j)} \langle S_i S_j \rangle \quad (5)$$

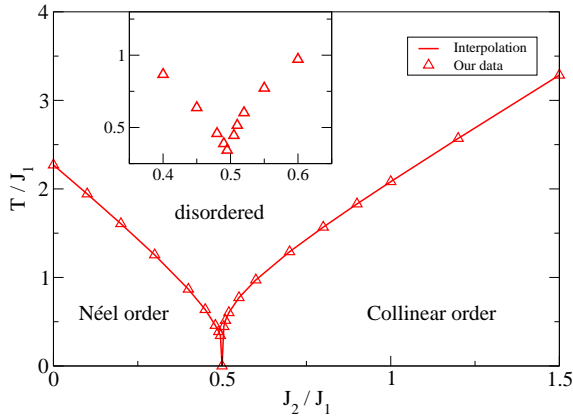


Figure 3. Plotted is T_C over the ratio J_2/J_1 . Data were produced by *parallel tempering MC simulations*.

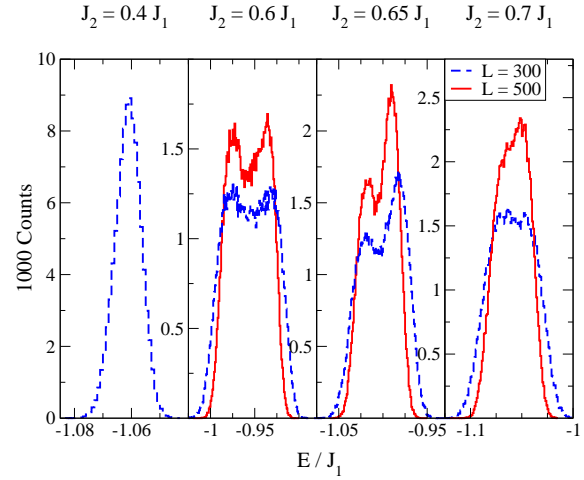


Figure 4. Energy histogram for several ratios of J_2/J_1 at T_C depending on given L .

is the respective structure factor (for an example see Fig. 2). To determine the critical exponent ν we calculate the derivative of U_4 with respect to T which is proportional to $L^{1/\nu}$ [14]. The behaviour of the specific heat and energy histograms [26, 27, 28, 29] for various ratios of J_2/J_1 provides further details to analyse the character of the given finite temperature phase boundaries and the transition at the critical point $J_2 = J_1/2$.

4. Results

In Fig. 3 we present the finite temperature phase diagram for the classical Ising model (solid line) for various ratios $|J_2/J_1 - 0.5| \geq 0.005$ very close to the critical point. The data is in good agreement with MC results from Landau and Binder for $|J_2/J_1 - 0.5| \geq 0.1$ [12, 10] and for $J_2 = J_1$ ($T_C/J_1 = 2.082 \pm 0.005$ as shown in Fig. 2) with the recent result $T_C/J_1 = 2.0823 \pm 0.0017$ [16].

Calculating lattice sizes up to $L = 300$ we find the critical exponent $\nu = 1.002 \pm 0.010$ for $J_2 = 0.3J_1$. This and a slowly emerging peak in the specific heat confirms the assumption that for $J_2 < J_1/2$ the phase transition lies in the Ising universality class [30, 31]. For $J_2 > J_1/2$ the character of the phase transition is an open subject. We used a histogram method [26, 27, 28] to verify a first order transition [29] for small $J_2 > J_1/2$. The slowly emerging double peak in the energy distribution for $J_2 = 0.6 J_1$ and $J_2 = 0.65 J_1$ in Fig. 4 compared to the single gaussian peak for $J_2 < J_1/2$ indicates a first order transition. For larger J_2 the shape of the energy distribution only shows a broadened peak for the simulated lattice sizes. The calculation of ν for $J_2 > J_1/2$ strongly depends on the lattice size because of large crossover scales near the critical point and above. For $J_2 > J_1$ we find the critical exponent $\nu \approx 1$ ($\nu = 1.02 \pm 0.02$ for $J_2 = 1.2 J_1$, $\nu = 0.96 \pm 0.02$ for $J_2 = 1.5 J_1$) for large lattice sizes which indicates that an Ising-like second order phase transition is recovered for $J_2 \gtrsim J_1$. So we believe that the character of the phase transition varies with J_2 and is transferred from a first order transition for $J_1/2 < J_2 \lesssim J_1$ to a continuous transition for larger J_2 with universal exponents. At the critical point $J_2 = J_1/2$ the finite size scaling analysis of the specific heat [19, 27] suggests a suppression of the transition temperature to $T_C = 0$.

5. Discussion

We used substantially enhanced MC methods to determine transition temperatures and characterise the phase boundaries of the frustrated 2D-Ising model. We solved the freezing

problems which arise near the critical point at $J_2 = J_1/2$ due to a groundstate degeneracy and calculated critical temperatures in the direct vicinity. We found the phase transition for $J_2 < J_1/2$ to be continuous and Ising-like. For $J_2 = J_1/2$ the phase transition is suppressed to zero temperature. The character of the phase boundary on the right hand side of the phase diagram was discussed via histograms. We decide the discussion about the character in favour of a first order transition for small $J_2 > J_1/2$ and find strong indications that the transition is transferred into a continuous one with universal Ising exponents for large $J_2 > J_1$. However, this is complicated to show via MC simulations because of large crossover scales and the need for very large lattices. Next we want to introduce finite hopping terms t_i and study the bosonic model given in (1) using parallel tempering QMC simulations [32].

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