Numerical Experiments on Frustrated Quantum Spin Systems

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Abstract. Thermodynamic properties of the antiferromagnetic Heisenberg model with frustration on the square lattice are investigated using quantum simulation based on the decoupled cell Monte Carlo method. The effect of frustration is introduced through an additional next-nearest neighbor antiferromagnetic interaction J_2. With increasing J_2, certain spin ordering was observed at low temperatures.

The discovery of high T_c superconductivity renewed the interest in two- dimensional quantum spin systems [1]. Among these systems the antiferromagnetic Heisenberg model with frustration on the square lattice (FAFH) is an important one due to its relation to the doped oxide superconductors. The frustration is introduced through an additional next-nearest neighbor exchange interaction along the diagonal of the plaquettes of the lattice. In this short note, we study the thermodynamic properties of the spin-1/2 FAFH on the square lattice, defined by the Hamiltonian

$$H = 2J_1 \sum_{i,\epsilon} S_i S_{i+\epsilon} + 2J_2 \sum_{i,\delta} S_i S_{i+\delta} \qquad (1)$$

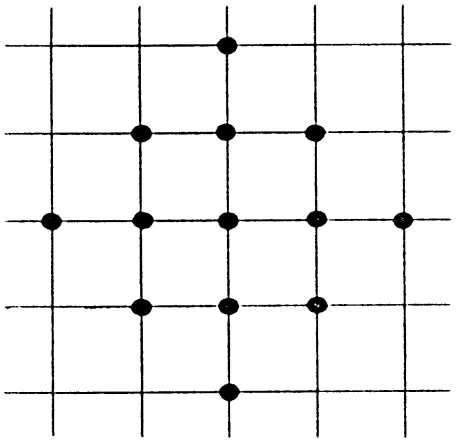

Fig.1

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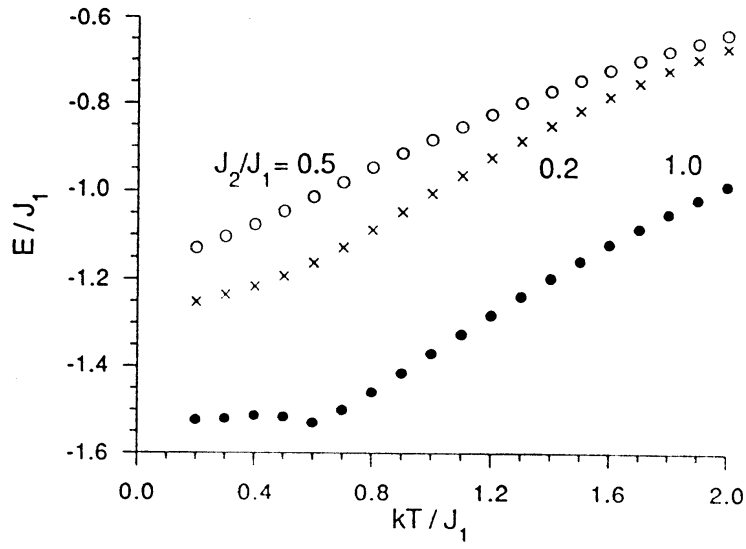

Fig.2

Here, i denotes a site of the square lattice, while ϵ are vectors along x or y directions, and δ are along the diagonals of a plaquette. The energy scale is fixed by setting $J_1 = 1$. We performed a quantum Monte Carlo simulation based on the decoupled cell Monte Carlo method (DCM) [2]. The basic ingredient of DCM is to calculate transition probabilities from a spin state to another one on a cell of finite size, where the central spin of the cell makes a transition from up(down) to down(up). Transition probabilities thus derived generate a sample of the Markov chain. The time average of this Markov chain gives relevant thermodynamic quantities. We calculated energy E, uniform magnetic susceptibilty χ and spin pair correlation function $C(\mathbf{r})$, defined by:

$$E = \frac{1}{N} < H >, \quad \chi = \frac{1}{NT} < (\sum_{\mathbf{i}} S^z_{\mathbf{i}})^2 >, \quad C(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{i}} < S^z_{\mathbf{i}} S^z_{\mathbf{i+r}} > \quad (2)$$

where $< \Omega >$ denotes the canonical average of Ω. The decoupled cell (DC) here includes 13 spins, with free boundaries, as depicted in Fig. 1. In DC, the central spin is flipped with all the remaining spins being fixed. The total numbers N of lattice sites are 32 X 32 and 64 X 64, with periodic boundary conditions. The simulation begins at $T = 2.0J_1$ from a random initial spin configuration. The system is then cooled in steps of $\Delta T = 0.1J_1$.

We now present results for the 64 X 64 system. In Fig. 2 we show the temperature dependence of E for various values of J_2. For $J_2 = 0.5$, the results of frustration are so strong that they prevent formation of some spin ordering. For $J_2 = 1.0$ we obtain nonuniform behavior of E near $kT/J_1 \simeq 0.6$, resulting in negative specific heat. At the present time, we do not have conclusions whether this is due to finitness of DC or an indication of the formation of spin ordering depicted in Fig. 4, which is observed below $KT/J_1 = 0.5$ for $J_2 = 1.0$ in our calculation. In Fig. 3 we show the dependence of χ on J_2. With increasing J_2, χ decreases. We could not find a nonuniform behavior of the susceptibility in the temperature region of our simulations. Present work is a preliminary one, and further, more detailed calculations will be published in the near future.

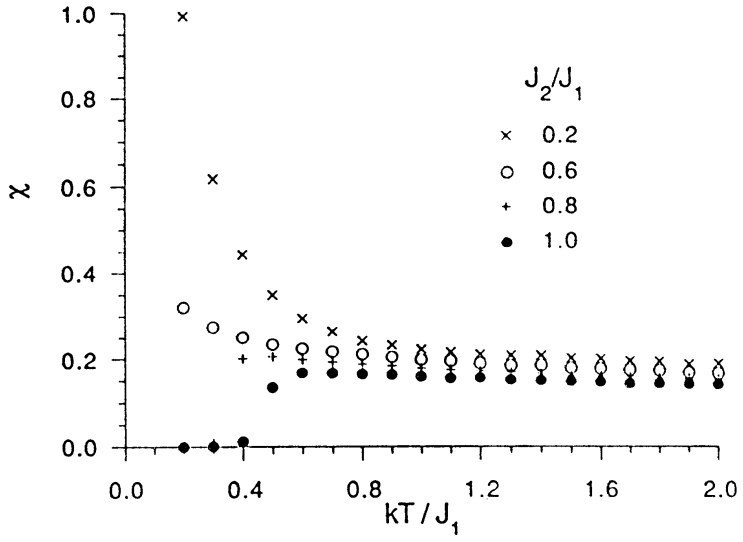

Fig.3

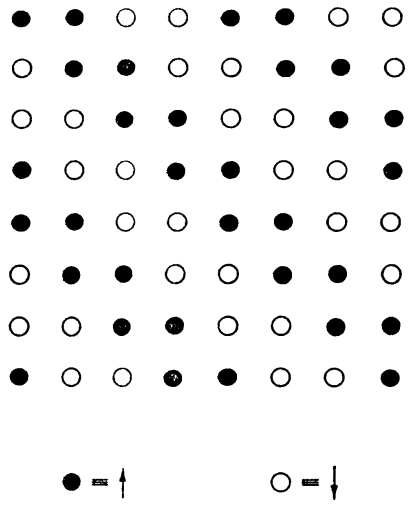

Fig.4

References

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[2] S. Homma, H. Matsuda, and N. Ogita, Prog. Theor. Phys. **75**, 1058 (1986).