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Abstract

We used the modified decoupled cell method (mDCM) of the quantum Monte Carlo simulation to calculate the thermodynamic properties and spin configurations of the frustrated J_1–J_2 model on a square lattice by increasing the frustration parameter $\alpha = J_2/J_1$ from 0 to 1. The size N of the system used in the Monte Carlo simulation in this study is 32×32. For small values of α the Néel state is a ground state spin configuration of this model system, and for $\alpha > 0.6$ a collinear state is the ground state configuration instead of the Néel state.

Since the discovery of high T_c superconductors the two-dimensional quantum spin ($s = \frac{1}{2}$) system has received much attention experimentally as well as theoretically (for a review see Ref. [1]). Particularly the frustrated J_1–J_2 model on the square lattice (hereafter we call it the J_1–J_2 model) has attracted much interest because of the suggestion that the effect of hole doping in high T_c superconductors may be simulated by the introduction of frustrations into the antiferromagnetic Heisenberg model with nearest neighbor interaction [2]. And this model is also expected to exhibit interplay between the frustration and the quantum fluctuation, an important problem in low-dimensional quantum spin systems. The main problem is which is the ground state spin configuration when the frustration parameter $\alpha = J_2/J_1$ increases from 0 to 1.

In the case of the classical J_1–J_2 model the ground state is the Néel-ordered state for $\alpha < 0.5$, and the continuously degenerate four-sublattice state for $\alpha > 0.5$. At $\alpha = 0.5$, the two classical states are degenerate. In the quantum case the Néel order is believed to be the stable ground state for $\alpha \ll 0.5$. The nonexistence of the twisted ordered state has been proved [3]. For the case where α is near 1, it is supposed that collinear states are the ground state spin configuration [4]. In the region, in which α is near 0.5, the ground state configuration still remains to be solved. For theoretical studies the spin wave theory, ordinary as well as modified [5,6], Schwinger-boson mean-field theory [7], finite lattice study [8] and series expansions [9] are to be noted. However, their results for the ground state spin configuration are different from each other. For example some works predicted a disordered or spin liquid state at around $\alpha = 0.5$, and others claimed that the classical Néel state is a ground state configuration even in the quantum mechanical J_1–J_2 model. Numerical studies of finite lattices based on the exact diagonalization method gave results showing that at 0 K the Néel state gradually decreases with the increase of α and at about $\alpha = 0.6$ this state disappears. However, the number of lattice sites included in those

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studies were at most 36 and this is not enough to extract definite conclusions about the physical quantities of the system in the thermodynamic limit.

To overcome this difficulty and to extend the study to finite temperatures, a quantum Monte Carlo calculation was used by invoking the generalized Trotter formula (Suzuki–Trotter formula), giving information about the magnetic properties of this model [10]. However, there exists a serious negative sign problem there and the lattice sizes used there were also small. Therefore it is desirable to invoke a quantum Monte Carlo method free from the negative sign problem and also able to extend the lattice size easily. The modified decoupled cell method (mDCM) is free from these problems [11,12].

It is the purpose of this short note to study the quantum J_1–J_2 model on a square lattice by applying the mDCM and to show the results obtained. The basic ingredients and detailed procedures of the Monte Carlo calculation of the mDCM are described in Refs. [11,12].

The Hamiltonian of the quantum J_1–J_2 model is defined as

$$H = 2J_1 \sum_{i,j}^{nn} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + 2J_2 \sum_{i,j}^{nnn} \boldsymbol{S}_i \cdot \boldsymbol{S}_j . \tag{1}$$

Here J_1 and J_2 are the nearest-neighbor and next-nearest-neighbor interactions, both are antiferromagnetic ($J_1, J_2 > 0$) on a square lattice. $\boldsymbol{S}_i$ is the quantum spin operator ($S = \frac{1}{2}$) of the ith lattice site. The Hamiltonian is isotropic, so that we take the z-axis as the axis of diagonal representation. The thermodynamic quantities we calculate here are the internal energy, specific heat, total magnetization, susceptibility of the total system and also spin configurations at various temperatures for a given frustration parameter α. We did not calculate staggered magnetizations and susceptibilities, for at present we do not know the spin configuration of the Hamiltonian for a given α. The size of the decoupled cell (DC) used here is depicted in Fig. 1, where the interaction on each edge is $\frac{1}{2}J_1$ instead of J_1. This arises because the coupling constants on the edge of the DC are split equally into two neighboring DC in the cell (DC) decomposition of the Hamiltonian. The number n of lattice sites included in the DC of Fig. 1 is nine. The total number N of lattice points in the system used in our Monte Carlo calculations are 32×32 with a periodic boundary condition.

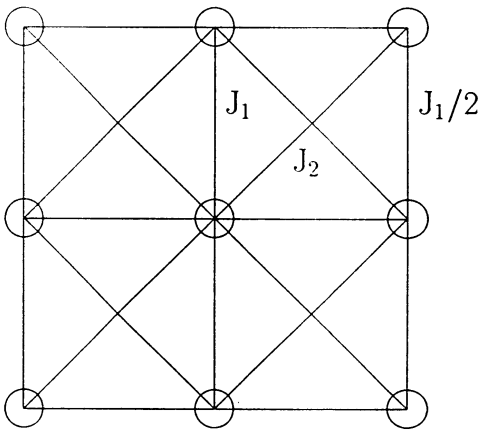

Fig. 1. Size of a decoupled cell (DC).

The calculations were performed using the Metropolis Monte Carlo procedure. The run was taken at $k_B T = 2.0J_1$, starting from a random configuration. The first 1000 Monte Carlo steps (MCS) were used to stabilize the system in thermal equilibrium and the following 10000 MCS were used to calculate the thermodynamic quantities and the spin configurations. The system is then cooled in steps down to $k_B T = 0.1J_1$. For each temperature the initial configuration was taken from the final configuration of the previous temperature and the first 1000 MCS were used to get thermal equilibrium.

In calculating the energy of the system we have used the following expression,

$$\epsilon = \frac{\langle H \rangle}{N} = \frac{1}{Nr(n)} \sum_{j=1}^{r(n)} \left(\sum_{k} \langle H_n(j,k) \rangle \right), \tag{2}$$

where $\langle\ \rangle$ denotes average with respect to the cell Hamiltonian $H_n(j,k)$ and $r(n)$ means the number of different decompositions. The sum over k and j means sum of the cells over a whole lattice and sum over all different decompositions. For the DC depicted in Fig. 1 $r(n = 9)$ is 4. The specific heat c is calculated as

$$c = \frac{\Delta\epsilon}{\Delta T}. \tag{3}$$

The total magnetization M_z along the z-axis is

$$M_z = \left\langle \sum_i S_i^z \right\rangle. \tag{4}$$

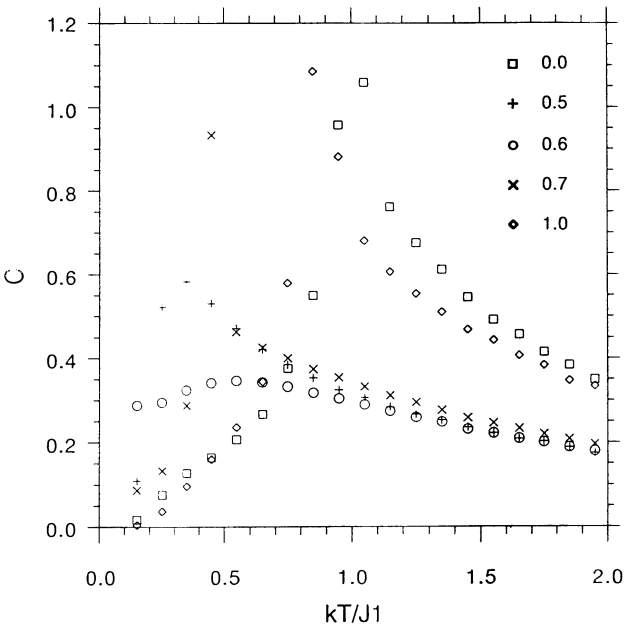

Fig. 2. Specific heat of the quantum J_1–J_2 model (J_1–J_2 model), where the numerical values represent the value of α.

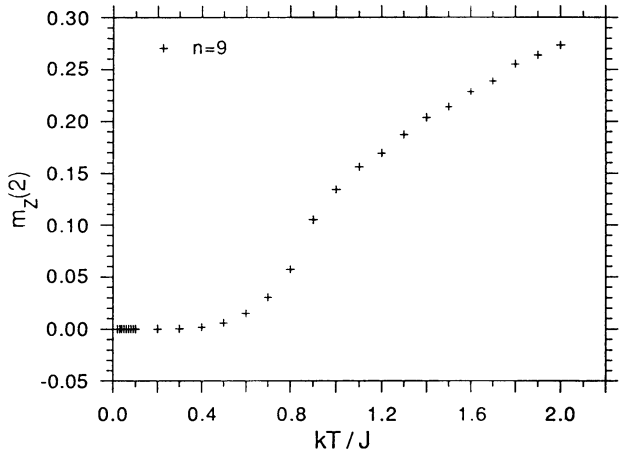

Fig. 3. Mean square magnetization $m_z(2)$ of the J_1–J_2 model.

Here $\langle\Omega\rangle$ denotes canonical average of Ω. The mean square magnetization of a system, which is denoted by $m_z(2)$, is defined as

$$m_z(2) = \frac{1}{N}\left\langle\left(\sum_i S_i^z\right)^2\right\rangle. \tag{5}$$

Thus, the magnetic susceptibility χ of the system is calculated as

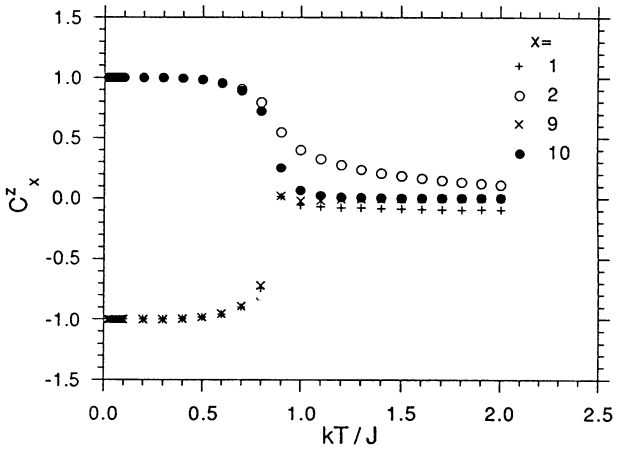

Fig. 4. The spin correlation function $C^z(r)$ along the x-axis, where the numerical values mean distance in units of lattice constant.

$$\chi = \frac{1}{Nk_BT}\left\langle\left(\sum_i S_i^z\right)^2\right\rangle = \frac{m_z(2)}{k_BT}. \tag{6}$$

The spin pair correlation function $C^z(r)$, which is defined as

$$C^z(r) = \langle S_i^z S_{i+r}^z\rangle, \tag{7}$$

was calculated along the x- and y-axis and also along the diagonal directions of the square lattice. In Fig. 2 we show the specific heat for various values of α.

There are two things to be noticed. The specific heat peak is sharp in the extreme cases of $\alpha = 0$ and 1, and appears in the high temperature side. This sharpening of the peaks might be interpreted as gradual ordering of the system into the Néel state and the collinear state, respectively. Second, the height and the position of the peaks at intermediate values of α become low and move to the low temperature region. Thus, the peak indicates that one does not expect any finite temperature transition. In Fig. 3 the result of $m_z(2)$ for $\alpha = 1$ is shown, from which we obtain χ. From the figure we see that χ is constant till $k_BT/J_1 = 1$, which is a little bit higher than the position of the peak of specific heat, and goes to zero with decreasing temperature. We have observed similar behaviors for different values of the frustration parameter α. For the total magnetization M_z we always observed zero as it should be.

The temperature dependence of the spin pair correlations $C^z(r)$ along the x- and y-direction for $\alpha = 1$ are shown in Figs. 4 and 5, respectively. In each figure

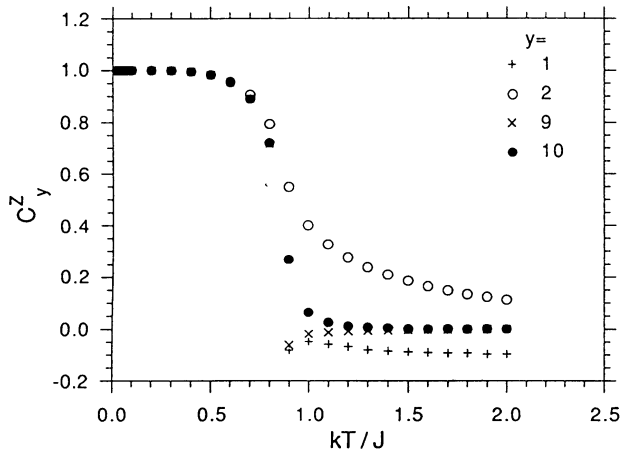

Fig. 5. The spin correlation function $C^z(r)$ along the y-axis, where the numerical values mean distance in units of lattice constant.

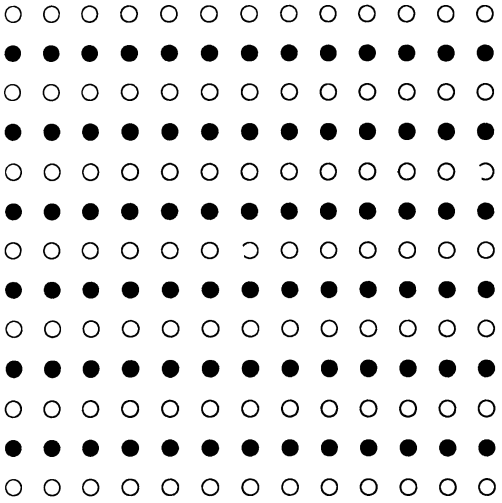

Fig. 6. The spin configuration of the J_1–J_2 model for $\alpha = 1.0$ at $k_BT = 0.1J_1$.

the numerical values indicate r in units of the nearest neighbor distance. From these figures we see that below $k_BT = 0.9J_1$ the collinear spin configuration dominates. This temperature corresponds to the position of the peak in the specific heat. From $C^z(r)$ we can depict the spin configuration, which is shown in Fig. 6 for the case of $\alpha = 1$ at $k_BT = 0.1J_1$, where the full and open circles mean up and down spin, respectively. In a similar way we are able to show the spin configurations of the J_1–J_2 model for a given frustration parameter α and temperature T.

In Figs. 7–9 we show the spin configurations for $\alpha = 0.5$, 0.6 and 0.7 at temperature $k_BT = 0.1J_1$. From

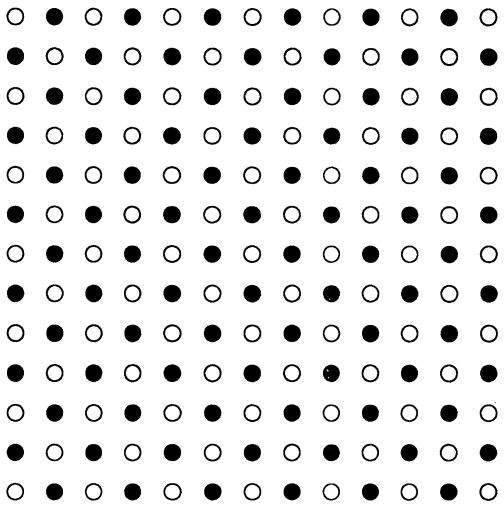

Fig. 7. The spin configuration of the J_1–J_2 model for $\alpha = 0.5$ at $k_BT = 0.1J_1$.

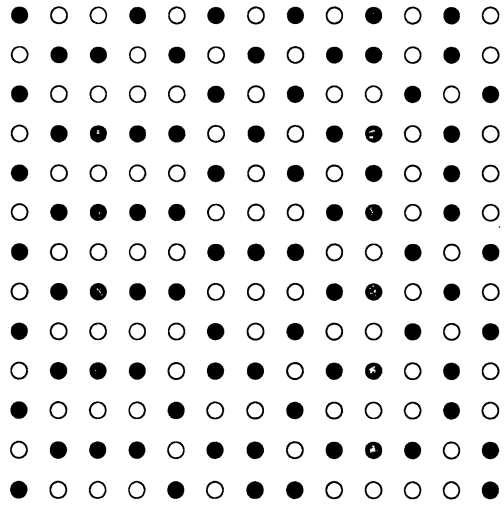

Fig. 8. The spin configuration of the J_1–J_2 model for $\alpha = 0.6$ at $k_BT = 0.1J_1$.

these figures we see that at $\alpha = 0.5$ the Néel state might be the ground state spin configuration, whereas at $\alpha = 0.7$ the collinear state seems to be the stable one. At $\alpha = 0.6$ we see, from Fig. 8, the beginning of an increase of the collinear structure.

At present it is not certain that at 0 K there exists phase transition from the Néel state to a collinear state when the frustration parameter α is increased. In order to obtain a definite conclusion about the behavior of the system near $\alpha = 0.6$ in the low temperature region, we have to enlarge the size of the DC as well as the size of the system. This problem will be studied in

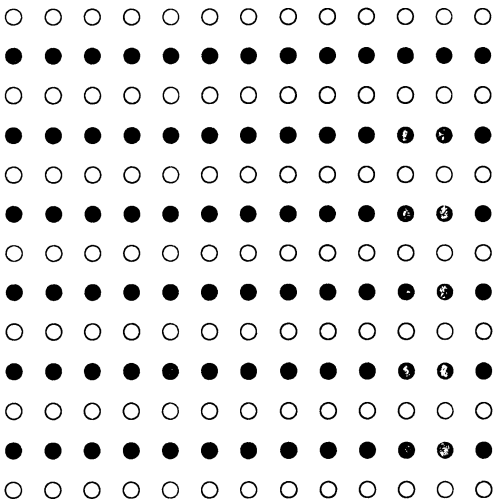

Fig. 9. The spin configuration of the J_1–J_2 model for $\alpha = 0.7$ at $k_B T = 0.1 J_1$.

the future.

In this study we have applied the mDCM, which is free from negative sign problem, to the quantum J_1–J_2 model on a square lattice and have calculated thermodynamic quantities such as internal energy, specific heat and magnetic susceptibility as well as spin configurations at various values of frustration parameter α and temperature T.

We have obtained the result that for small values of α the spin configuration is the Néel ordered state and at $\alpha = 0.5$, for which the spin configuration is degenerate in the classical case, it is still the Néel state. For $\alpha > 0.6$ we have observed that the spin configuration in the low temperature region is collinear. Our results at finite temperature seem to indicate the existence of long-range order. However this is an artifact arising from the finiteness of the system sizes used in the present Monte Carlo calculations.

Detailed results of the present work will be published elsewhere.

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