Monte-Carlo Calculation of Quantum $J_1 - J_2$ Model on the Square Lattice

S. Miyazawa and S. Homma

Faculty of Engineering, Gunma University, Kiryu 376, Japan

Abstract: We used the modified Decoupled Cell method (mDCM) of quantum Monte Carlo simulation to calculate the thermodynamic properties and spin configurations of the frustrated $J_1 - J_2$ model on the square lattice by increasing the frustration parameter $\alpha = \frac{J_2}{J_1}$ from 0 to 1. The size N of a system used in Monte Carlo simulation in this study is 32×32. We found that for small values of α the Neel state is a ground state spin configutation of this model system, whereas for $\alpha > 0.6$ a collinear state is its ground state configuration instead of the Neel state.

1. Introduction

Since the discovery of high T_c-superconductor the two-dimensional quantum spin ($s = \frac{1}{2}$) system have received much attention experimentally as well as theoretically [1]. Particularly the frustrated $J_1 - J_2$ model on the square lattice (hereafter we call it $J_1 - J_2$ model) have attracted much interest because of the suggestion that the effect of the hole doping in the high T_c superconductor may be simulated by the introduction of frustrations into the antiferromagnetic Heisenberg model with the nearest neighbor interaction [2]. In addition it is expected that this model exhibits the interplay between the frustration and the quantum fluctuation, an important problem in the low-dimensional quantum spin systems. The main problems there are which is the ground state spin configuration, and how are the thermodynamic propeties such as the specific heat, magnetic susceptibility and the spin pair correlation functions when the frustration parameter α increases from 0 to 1.

In the case of the classical $J_1 - J_2$ model the ground state is the Neel-ordered state for $\alpha < 0.5$, and is 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 Neel order is believed to be the stable ground state for $\alpha \ll 0.5$. It has been proved that the nonexistence of the twisted ordered state [3]. For the case where α is near 1, it is supposed that a collinear state is the ground state spin configuration [4]. In the region, in which α is near 0.5 the ground state configuration is still remained to be solved. For the theoretical studies the spin wave theory, ordinary as well as modified [5-6], Schwinger-boson mean-field theory [7], finite lattice study [8-13] and series expansions [14-15] are to be noted. However their results for the ground state spin configuration are different to each other. For example some works predicted a disordered or spin liquid state at around $\alpha = 0.5$, and the others claimed that the classical Neel 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 the results that at 0 K the Neel state gradually decreases with an increase of α and at about $\alpha = 0.6$ this state disappear [16]. However the number of lattice sites included in those studies were at most 36 and is not enough to

Springer Proceedings in Physics, Vol. 80
Computer Simulation Studies in Condensed-Matter Physics VIII
Editors: D.P. Landau · K.K. Mon · H.-B. Schüttler

extract definite conclusions of the physical quantities of the system in the thermodynamic limit.

To overcome this difficulty and to extend the study at finite temperatures, a quantum Monte Carlo calculation was used by invoking the generalized Trotter formula (Suzuki-Trotter formula), and gave informations on the magnetic properties of this model [16]. However there exists a serious negative sign problem there and also lattice sizes used there were small one. Therefore it is desirable to invoke a quantum Monte Carlo method which is free from the negative sign problem and also is able to extend a lattice size with ease. The Decoupled Cell method (DCM) and the modified Decoupled Cell method (mDCM), which were proposed in 1984 and 1993, and used extensively since then, is the one which is free from these difficulties [17-19].

It is the purpose of the paper to study the thermodynamic properties of the quantum $J_1 - J_2$ model on the square lattice by applying mDCM and show the results obtained. In the next section we give a detailed account of DCM and mDCM. In the section 3 we show the results obtained by applying mDCM to $J_1 - J_2$ model. The last section is devoted to discussion. The preliminary report of this work was published in ref.[23].

2. The Decoupled and the modified Decoupled Cell method

To explain the basic idea of DCM let us consider a quantum spin system ($s = 1/2$) whose Hamiltonian is given by H. The state of the i-th site can be specified by a variable $s = \pm 1/2$, and the state of the total system by an N-dimensional state vector $|S>= |s_1, s_2, ..., s_N>$ whose i-site state is s_i. The probability of the state S in the canonical distribution is given by

$$P(S) =< S|\exp(-\beta H)|S > /Z, \tag{1}$$

where $\beta = (1/kT)$ and Z stands for the partition function of a system. As in the classical Metroplis method, the condition of irreducibility and recurrency of the Markov chain is satisfied by assigning positive transition probabilities between states that are different from each other only at one site $i(i = 1, 2, ..., N)$. The problem in the quantum mechanical case is how to obtain adequate transition probabilities consistent with the condition of the detailed balance at equilibrium

$$P(S)W(S \to S') = P(S')W(S' \to S) \tag{2}$$

where $W(S \to S')$ is the transition probability from a spin configuration S to S'.

Let $L_i(\nu)$ be a set of sites whose distance from the i-th site does not exceed a certain integer ν and $\overline{L}_i$ be a set of all sites not belonging to $L_i(\nu)$. We call such $L_i(\nu)$ the decoupled cell (DC) of radius ν with its center at the i-site. Let S_i denote the state of $L_i(\nu)$ excepting the i-site and $\overline{S}_i$ denote the state $\overline{L}_i$. The state of the total system can then be written as $S = (s_i, S_i, \overline{S}_i)$. The transition probability between $S = (s_i, S_i, \overline{S}_i)$ and $S' = (-s_i, S_i, \overline{S}_i)$ can be obtained from Eq.(1) if one knows the value of

$$q(S) = \frac{P(S)}{P(S')} = \frac{< S|\exp(-\beta H)|S >}{< S'|\exp(-\beta H)|S' >}. \tag{3}$$

Let $H(\nu, i)$ be the Hamiltonian of a DC which is obtained from H by deleting all the terms containing operators of $\overline{L}_i$. The basic ingredient of DCM is to approximate Eq.(3) by

$$q^{(\nu)}(S_i) = \frac{< s_i, S_i | \exp(-\beta H(\nu, i)) | s_i, S_i >}{< -s_i, S_i | \exp(-\beta H(\nu, i)) | - s_i, S_i >}. \tag{4}$$

This approximation is based on the presumption:

The dependence of q on $\overline{S}_i$ gradually decreases by increasing ν.

The right hand side of Eq.(4) can be obtained readily by solving the eigenvalue problem of $H(\nu, i)$ by computer. Let $(E_n, \phi_n; n = 1, 2, .., f =$ a number of spin states of DC) be eigenvalues and eigenfunctions of $H(\nu, i)$. With their use Eq.(4), $q^{(\nu)}(S_i)$ can be rewritten as

$$q^{(\nu)}(S_i) = \frac{\sum_n | < s_i, S_i | \phi_n > |^2 \exp(-\beta E_n)}{\sum_n | < -s_i, S_i | \phi_n > |^2 \exp(-\beta E_n)}. \tag{5}$$

The transition probability W_{DC} defined in DCM is given by

$$W_{DC}(-s_i \rightarrow s_i) = max[1, q^{(\nu)}(S_i)]. \tag{6}$$

The physical meaning of replacing Eq.(3) by Eq.(4) was fully discussed by Matsuda et al. [20]. If we use Eq.(6) as the transition probability from the state $S' = (-s_i, S_i, \overline{S}_i)$ to the state $S = (s_i, S_i, \overline{S}_i)$ in Monte Carlo calculation, we are able to obtain the Markov chain of the given quantum mechanical system using the Metroplis algorithm. Thus DCM gives a natural extension of the classical Monte Carlo method to quantum systems. The detailed computational procedure of DCM is given in references [17,21] . We applied DCM to one-dimensional XY model and compared the results with the exact one [22] which is derived analytically and found that by increasing the size of DC the obtained results gradually approach the exact one except for very low temperature region, where the calculated value of an internal energy gives a negative specific heat and the perpendicular susceptibility increases abruptly contrary to the fact that the exact analytical solution is finite at absolute zero of temperature [17,21].

These difficulties in the low temperature region might be attributed to the breakdown of the detailed balance originating from the finiteness of a DC used there. In order to remove this difficulty there are two possibilities. The first is to enlarge the size of DC, but it is limited by the capability of computer power. The second is to improve DCM to recover the detailed balance, extending the basic concept of DCM for a certain size of DC. As we pointed out previously, DCM could be regarded as a natural extension of the classical Monte Carlo method to quantum systems. However, it should be noted that the transition probability defined by Eq.(6) does not satisfy the detailed balance. The probability $W_{DC}(s_i \rightarrow -s_i)$ is a function of the neighbouring spins in the cell, which includes a finite number of spins. However, when we calculate the transition probability of some other spin in the same cell, we introduce W_{DC} in the form of Eq.(6) independently. If the cell Hamiltonians $H(\nu, i)$ commute with each other, the detailed balance is satisfied automatically as far as it is satisfied locally. Thus Eq.(6) gives correct transition probabilities for classical systems. But in quantum systems where $H(\nu, i)$ do not commute with each other, the transition probability defined at each lattice site independently does not satisfy the detailed balance. The flip of a spin s_k causes a change of all the transition probabilities for which $H(\nu, i)$ includes s_k. Thus the changes cannot be reduced to that of $W_{DC}(s_i \rightarrow -s_i)$. From this point of view, in determining the transition probability it is important to include not only the DC whose central site is i, but all the DC which include the i-site. Here we reformulate DCM taking into account the above considerations.

First we decompose a system into identical cells (decoupled cell; DC), whose shape and size are given. The way of a decomposition is not unique. It depends on the size and shape of DC. With a decomposition, labeled by j and a k-th cell, we associate the cell Hamiltonian $H_n(j,k)$, where n is the number of lattice sites included in each cell (DC). Then the Hamiltonian of a system is written as a sum of $H_n(j,k)$ as

$$H = \frac{1}{r(n)} \sum_j (\sum_k H_n(j,k)), \tag{7}$$

where the sum over k means the sum over all cells on a lattice and that over j means the sum over all different decompositions. The symbol $r(n)$ denotes the number of different decompositions.

Using Eq.(7) the probability of a certain spin configuration $|S, s_i>$ is given by

$$P(S,s_i) = \frac{1}{Z} < S,s_i| \exp(-(\frac{\beta}{r(n)} \sum_j (\sum_k H_n(j,k)))|S,s_i>, \tag{8}$$

where Z is the partition function of a system. The ket (bra)$|S,s_i>$ ($<S,s_i|$) represents a spin configuration of a system, in which the i-th spin is s_i, with $s_i = \pm(1/2)$. We approximate Eq.(8), invoking the basic concept discussed above, as

$$P(S,s_i) = \frac{1}{Z} \Pi_j \Pi_k < \sigma(j,k)| \exp(-(\frac{\beta}{r(n)} H_n(j,k)))|\sigma(j,k)>, \tag{9}$$

where $|\sigma(j,k)>$ represents a spin state of a cell (DC) labeled by (j,k).

The transition probability $W(s_i \rightarrow -s_i)$ is defined by

$$W(s_i \rightarrow -s_i) = max[1, \frac{P(S,-s_i)}{P(S,s_i)}], \tag{10}$$

where $P(S,\pm s_i)$ is defined by Eq.(8). We approximate Eq.(8) , by substituting Eq.(9) into $P(S,\pm s_i)$ in Eq.(10) , to obtain W_{DC} in the modified Decoupled Cell Method (mDCM) as

$$\begin{aligned} & W_{DC}(s_i \rightarrow -s_i) \\ = \; & max[1, \frac{\Pi_j \Pi_k < \sigma(j,k), -s_i| \exp(-\frac{\beta}{r(n)} H_n(j,k))|\sigma(j,k), -s_i>}{\Pi_j \Pi_k < \sigma(j,k), s_i| \exp(-\frac{\beta}{r(n)} H_n(j,k))|\sigma(j,k), s_i>}]. \end{aligned} \tag{11}$$

The product over k in Eq.(11) must be over all cells which include the i-site; the total number of such cells is equal to the number of spins in a cell, that is n. Here it must be noted that in DCM only the cell whose center is i-site is taken into account in Eq.(11) . If the Hamiltonian H of a system consists of only a nearest neighbour coupling, Eqs.(10) and (11) coincide with those of classical ones in the classical limit. However it should be noted that in one-dimensional lattice when the Hamiltonian H includes the second-neighbour interaction beside the nearest neighbour interaction, each second-neighbour interaction is included in Eq.(9) by a factor $\frac{n-2}{n-1}$, whereas the nearest neighbour interaction is included in Eq.(9) by $\frac{n-1}{n-1} = 1$. Thus Eq.(11) does not give a correct expression in the classical limit in this case (in one-dimensional lattice with a second-neighbour interaction). In two-dimensional lattice proper size and shape of a cell (DC) depend on the type of lattice and the range of interactions. For the detailed account of the possible decompositions

of a certain two-dimensional lattice with nearest- and second-neighbour interactions, into DC of the given shape and size , the reader is referred to ref.[18]. Thus we complete the modification of DCM and have a modified Decoupled Cell method (mDCM) .

3. $J_1 - J_2$ model

The Hamiltonian of the quantum $J_1 - J_2$ model is defined as

$$H = 2J_1 \sum_{i,j}^{nn} \mathbf{S}_i \cdot \mathbf{S}_j + 2J_2 \sum_{i,j}^{nnn} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{12}$$

Here J_1 and J_2 are the nearest-neighbor and next-nearest-neighbor interactions, both of which are antiferromagnetic ($J_1, J_2 > 0$) on a square lattice. $\mathbf{S}_i$ is a quantum spin operator ($S = 1/2$) of the i-th lattice site. The Hamiltonian is isotropic, so that we take the z-axis as the axis of a diagonal representation. The thermodynamic quantities we calculate here are an internal energy, specific heat, total magnetization, susceptibility of a total system and also spin configurations at various temperatures for the 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 in here is depicted in Fig.1, where the interaction on each edge is $\frac{J_1}{2}$ instead of J_1. This is because coupling constants on the edge of DC are split equally into two neighboring DC in the cell decomposition of the Hamiltonian. The number n of lattice sites included in DC in Fig.1 is 9. The total number N of lattice sites in the system used in the present Monte Carlo calculations are 32×32 with a periodic boundary condition.

Calculations were performed using the Metropolis Monte Carlo procedure. The run was taken at $k_B T = 2.0 J_1$, starting from a random configuration. The first 1000 Monte Carlo steps (MCS) were used to make 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 $k_B T = 0.1 J_1$. At each temperature the initial configuration was taken from that of the final one of the previous temperature and first 1000 MCS were used to get the thermal equilibrium.

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

$$\epsilon = \frac{1}{Nr(n)} \sum_{j=1}^{r(n)} (\sum_{k} < H_n(j,k) >), \tag{13}$$

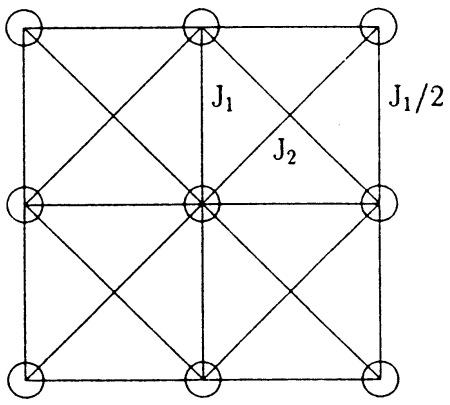


Fig.1 A size of a decoupled cell (DC).

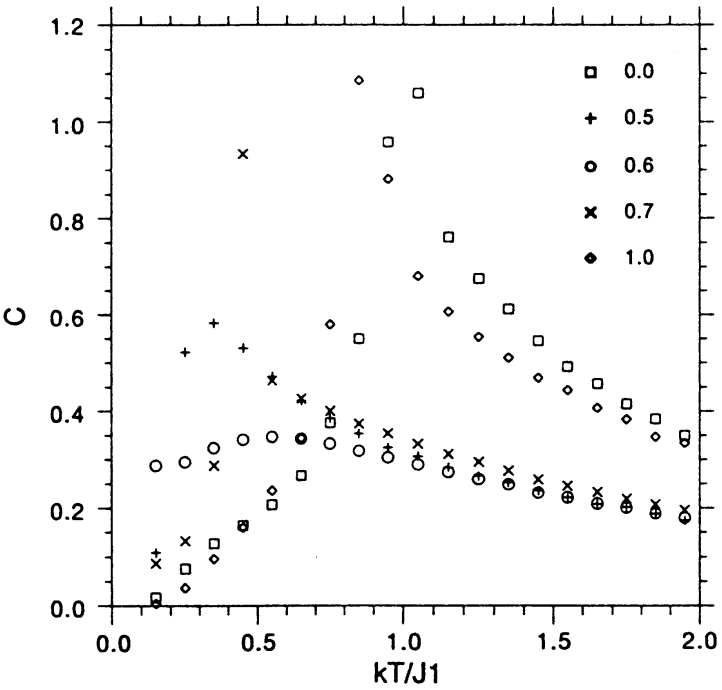


Fig.2 Specific heat of the quantum $J_1 - J_2$ model ($J_1 - J_2$ model), where numbers in the figure represent the numerical value of α.

where $<\ >$ denotes the 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 the sum of cells over a whole lattice and the sum over all the different decompositions. For the DC depicted in Fig.1 $r(n=9)$ is 4 . The specific heat c is calculated as

$$c = \frac{\Delta\epsilon}{\Delta T} \tag{14}$$

where $\Delta\epsilon$ and ΔT are energy and temperature differences, respectively. The total magnetization M_z along z-axis is

$$M_z = < \sum_i S_i^z > \tag{15}$$

Here $<\ \Omega\ >$ denotes the canonical average of Ω . The mean square magnetization of a system, which is written as $m_z(2)$, is defined as

$$m_z(2) = \frac{1}{N} < (\sum_i S_i^z)^2 > \tag{16}$$

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

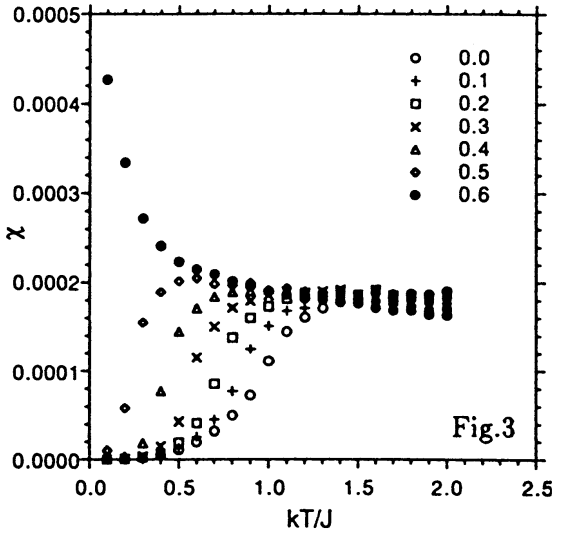
$$\chi = \frac{1}{Nk_BT} < (\sum_i S_i^z)^2 > = \frac{m_z(2)}{k_BT}. \tag{17}$$

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

$$C^z(r) = < S_i^z S_{i+r}^z > \tag{18}$$

was calculated along x- and y-axis.

In Fig.2 we show the result of the specific heat for various values of α. There are two things to be noticed. The peak in the specific heat is sharp in the extreme cases



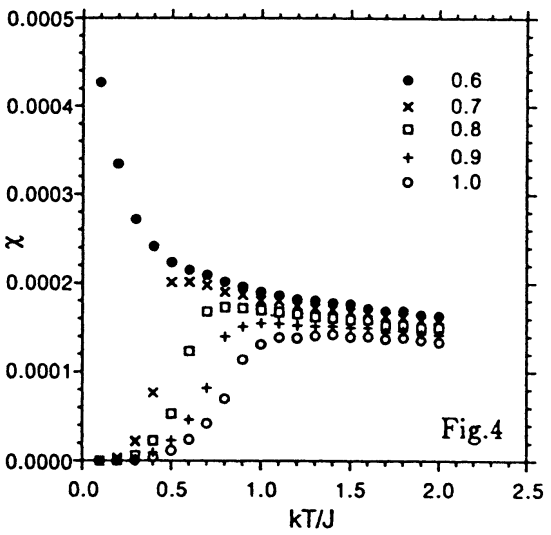
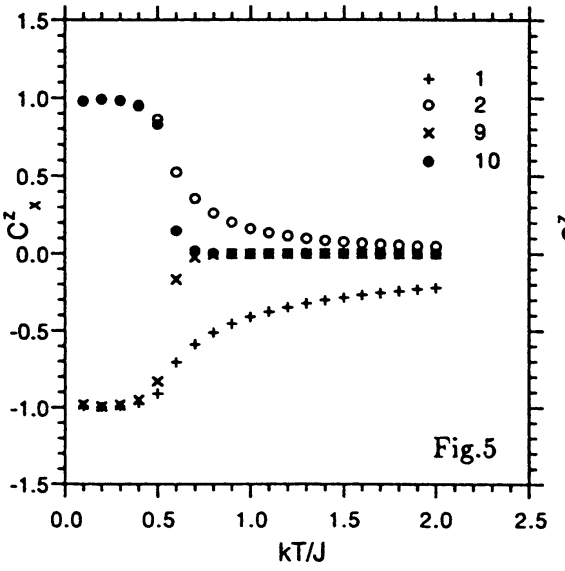


Fig.3 The magnetic susceptibility χ of $J_1 - J_2$ model for $\alpha < 0.6$, where numbers in the figure represents α.

Fig.4 The magnetic susceptibility χ of $J_1 - J_2$ model for $\alpha > 0.6$, where numbers in the figure represents α.



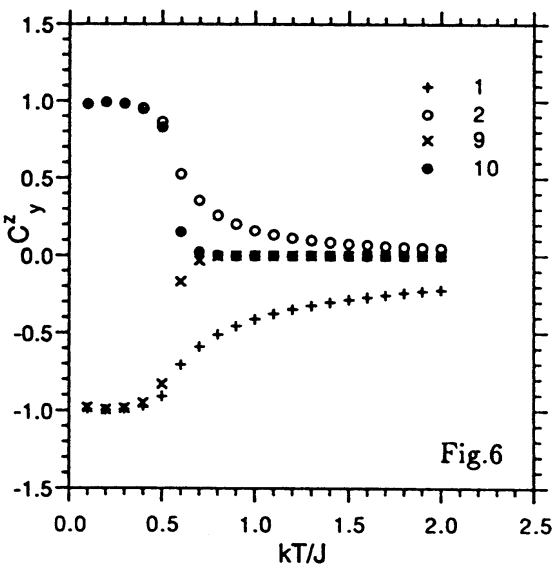


Fig.5 The spin correlation function $C^z(r)$ along x-axis, where numbers in the figure mean distance in unit of lattice constant. ($\alpha = 0.3$)

Fig.6 The spin correlation function $C^z(r)$ along y-axis , where numbers in the figure mean distance in unit of lattice constant. ($\alpha = 0.3$)

of $\alpha = 0$ and 1, and appears in the high temperature region. This sharpening of the peaks might be interpreted as the gradual ordering of the system into the Neel state and the collinear state, respectively. Second, the height and the position of peaks in the intermediate values of α become low and move to the low temperature region. Thus, the

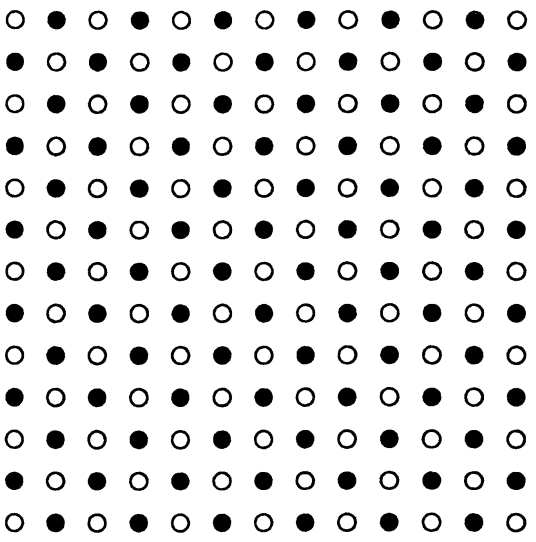


Fig.7 The spin configuration of $J_1 - J_2$ model for $\alpha = 0.3$ at $k_B T = 0.1 J_1$.

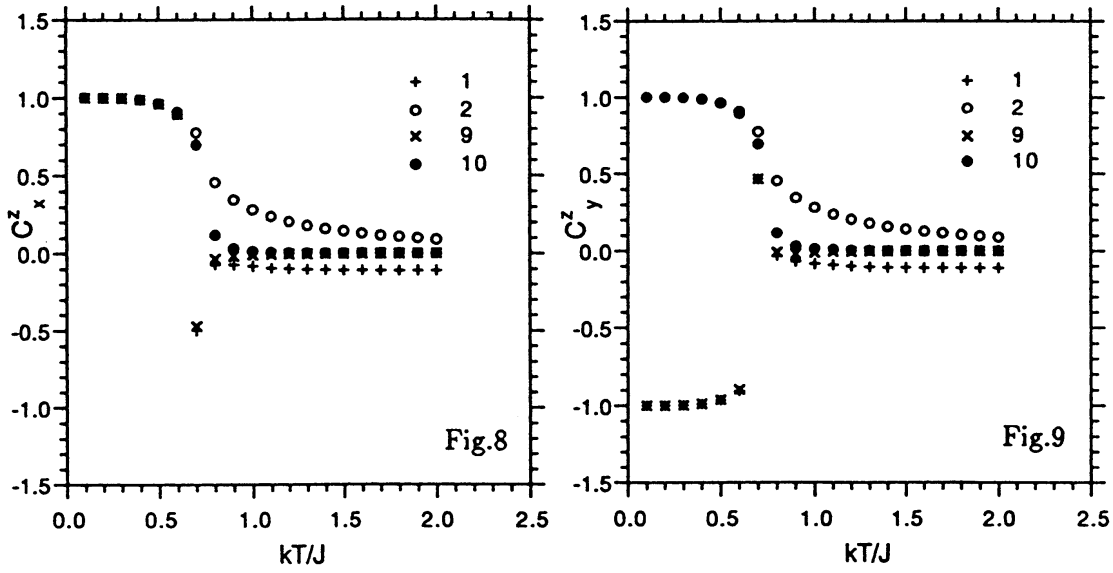


Fig.8 The spin correlation function $C^z(r)$ along x-axis, where numbers in the figure mean distance in unit of lattice constant. ($\alpha = 0.9$)

Fig.9 The spin correlation function $C^z(r)$ along y-axis , where numbers in the figure mean distance in unit of lattice constant. ($\alpha = 0.9$)

peak there indicates that one can not expect any finite temperature transition. For the total magnetization M_z we always have observed zero as it should be. In Figs.3 and 4 we show the result of the susceptibility χ. From this figure we see that in the case of $\alpha = 0.6$, χ increases in the low temperature region , whereas above and below $\alpha = 0.6$, χ decreases to zero, showing that there exists ordered states of a spin configuration for those values of α. In order to obtain the spin configurations we have calculated the spin pair correlation functions defined by Eq.(18) along the x- and y-axis. In Figs.5 and 6 we show $C^z(r)$ for $\alpha = 0.3$ along x- and y-axis. The numbers in each figure indicates r. From them we obtain the spin configuration, which is depicted in Fig.7 at $\frac{kT}{J_1} = 0.1$. Thus we have Neel State for $\alpha = 0.3$. We have observed similar behaviour for $\alpha = 0.0$, 0.1,0.2, 0.4 and 0.5. In Figs.8 and 9 we show $C^z(r)$ for $\alpha = 0.9$. From them we have a collinear spin

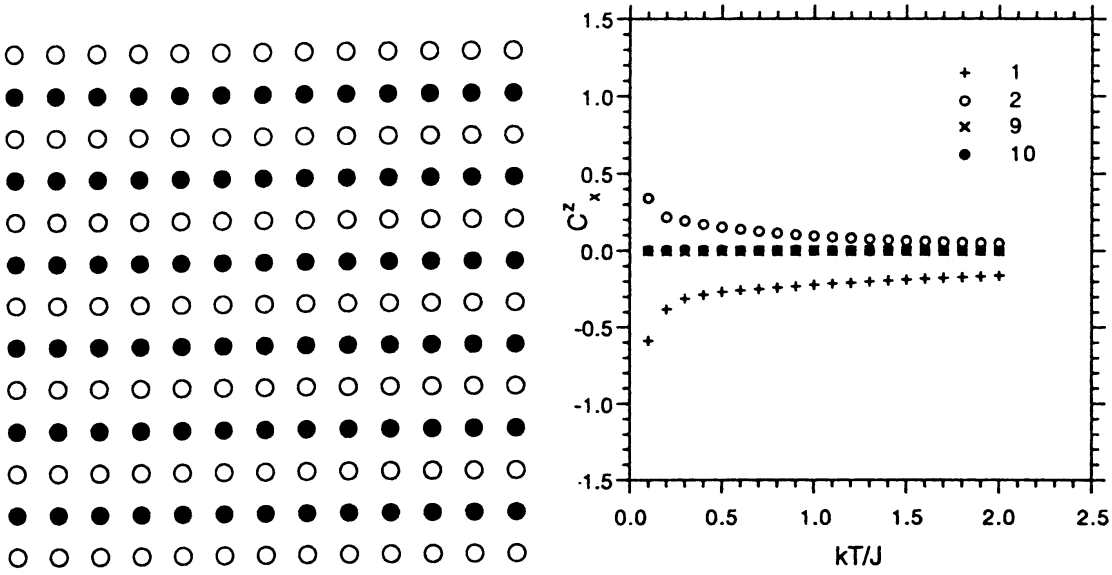


Fig.10 The spin configuration of $J_1 - J_2$ model for $\alpha = 0.9$ at $k_BT = 0.1J_1$.

Fig.11 The spin correlation function $C^z(r)$ along x-axis, where numbers in the figure mean distance in unit of lattice constant. ($\alpha = 0.6$)

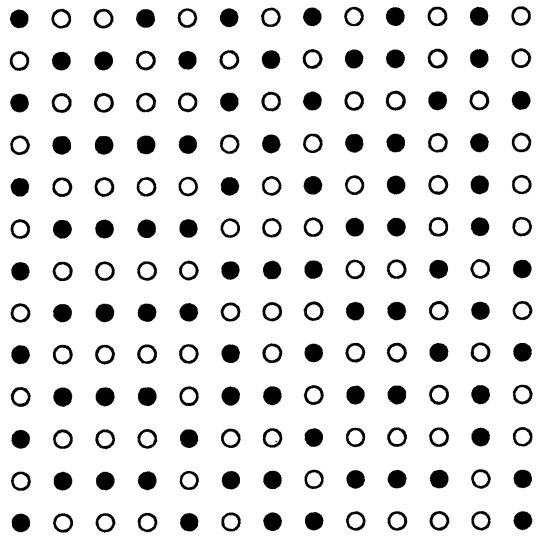


Fig.12 The spin configuration of $J_1 - J_2$ model for $\alpha = 0.6$ at $k_BT = 0.1J_1$.

configuration for this value of α. This is shown in Fig.10. For $\alpha > 0.6$ we have obtained a collinear spin configuration. From these observations we conclude that the ground state spin configuration of $J_1 - J_2$ model is Neel state for $\alpha < 0.6$ and a collinear state for $\alpha > 0.6$. At $\alpha = 0.6$ we show in Fig.11 $C^z(r)$ along x-axis. ($C^z(r)$ along y-axis is the same as that of x-axis.)

In Fig.12 we show the spin configuration at $\frac{kT}{J_1} = 0.1$, from which we see that there are seeds for the growth of Neel and collineat spin configuration, respectively.

4. Discussion

In this study we have applied mDCM, which does not have difficulties of negative sign problem, to the quantum $J_1 - J_2$ model on a square lattice and calculated the thermodynamic quantities such as an internal energy, specific heat and a magnetic susceptibility as well as spin configurations at various values of α and temperature T.

We have obtained the results that for small values of α a spin configuration is the Neel ordered state and at $\alpha = 0.5$, at which a spin configuration is degenerate in the classical case, it is still the Neel state. For $\alpha > 0.6$ we have observed that the spin configuration in the low temperature region is a collinear. At present it is not certain that at $0K$ there exits a phase transition from the Neel state to a collinear state by increasing α, or not.. In order to obtain the definite conclusion on the behavior of the system near $\alpha = 0.6$ in the low temperature region, we have to enlarge the size of DC as well as a size of a system. This will be the next problem.

References

[1] For a review, see E.Manousakis, Rev. Mod. Phys. **63** (1991) 1

[2] M.Inui, S.Doniach and M.Gabay, Phys. Rev. **B38** (1988) 6631

[3] Y.Saika and H.Nishimori, J. Phys. Soc. Jpn. **61** (1992) 3086

[4] K.Kubo and T.Kishi, J. Phys. Soc. Jpn. **60** (1990) 567

[5] J.Igarashi, J. Phys. Soc. Jpn. **62** (1993) 4449

[6] T.Aoki, J. Phys. Soc. Jpn. **63** (1994) 2356 and the references cited therein.

[7] F.Mila, D.Poilblanc and C.Bruder, Phys. Rev. **B43** (1991) 7891

[8] E.Dagotto and A.Moreo, Phys. Rev. Lett. **63** (1989) 2148

[9] K.Sano, I.Doi and K.Takano, J. Phys. Soc. Jpn. **60** (1991) 3807

[10] H.J.Schulz and T.A.L.Ziman, Europhys. Lett. **18** (1992) 355

[11] J.Richter, Phys. Rev. **B47** (1993) 5794

[12] Q.F.Zhong and S.Sorella, Europhys. Lett. **21** (1993) 629

[13] N.B.Ivanov and J.Richter, J. Phys.: Condens.Matter **6** (1994) 3785

[14] M.P.Gelfand, R.R.P.Singh and D.A.Huse, Phys. Rev. **B40** (1989) 10801

[15] I.G.Gochev, Phys. Rev. **B49** (1994) 9594

[16] T.Nakamura and N.Hatano, J. Phys. Soc. Jpn. **62** (1993) 3062

[17] S.Homma, H.Matsuda and N.Ogita, Prog. Theor. Phys. **72** (1984) 1245
75 (1986) 1058

[18] S.Miyazawa, S.Miyashita, M.S.Makivic and S.Homma,
Prog. Theor. Phys. **89** (1993) 1167

[19] S.Homma, in *Quantum Monte Carlo Methods in Condensed Matter Physics* , ed. M.Suzuki (World Scientific, Singapore, 1993) p.163

[20] H.Matsuda, K.Ishii, S.Homma and N.Ogita, Prog. Theor. Phys. **80** (1988) 583

[21] S.Homma, K.Sano, H.Matsuda and N.Ogita, Prog. Theor. Phys. **S87** (1986) 127

[22] S.Katsura, Phys. Rev. **57** (1962) 1508

[23] S.Miyazawa and S.Homma, Phys. Letters **A193** (1994) 370