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A modified Decoupled Cell Method (mDCM) for quantum Monte Carlo simulation is proposed to remove the difficulty in the Decoupled Cell Method (DCM), which causes a negative specific heat and an unexpected sudden increase of a susceptibility in a low temperature region. In one-dimensional XY-model ($s=1/2$), the results obtained by mDCM were shown not to have any negative specific heat and for the susceptibility along z-axis, gave fairly good agreement with the exact one.

Recently a number of studies have been reported on the Monte Carlo methods for quantum many-body systems.[1)~3)] Many years ago the decoupled cell Monte Carlo method (DCM) was proposed as a new method of Monte Carlo calculations for quantum systems as a direct extension of the Metropolis method for classical systems[4)] and was used to low-dimensional quantum spin systems.[5)~12)] In one-dimensional XY-model ($s=1/2$), for which the exact solution were known,[13)] results obtained by DCM were found to give a good approximation for the internal energy and the zero-field susceptibility by increasing the size of the decoupled cell (DC).[5)] However at low temperatures the result of the internal energy is not appropriately estimated, for it gives a negative value of the specific heat. The reason for this flaw may be attributed to a breakdown of the detailed balance of the Monte Carlo update due to the noncommutativity between the local interaction operators at low temperatures. In order to remove this difficulty there are two possibilities. The one is to enlarge the size of DC, but it is limited by the capability of computer power. The remaining is to improve DCM to recover the detailed balance, extending the basic concept of DCM for a certain size of DC.

It is the purpose of this paper to look for the second possibility to improve DCM, which could be useful even in the low temperature region. First we explain the basic ingredient of DCM taking quantum spin systems ($s=1/2$) as an example. In the Metropolis method a required canonical distribution is generated as the limit distribution of a Markov chain. This Markov chain can be any one so long as (i) the transition probability $W(S\to S')$ from a spin state S to a state S' satisfies the condition of detailed balance:

$$P(S)W(S\to S')=P(S')W(S'\to S) \tag{1}$$

and (ii) the Markov chain is irreducible and recurrent. Here $P(S)$ is the probability

of a spin state S. In the quantum spin systems ($s=1/2$) 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 $S=|s_1, s_2, \cdots, s_N\rangle$ whose i-th component is s_i. The probability of S in the canonical distribution is now given by

$$P(S)=\langle S|\exp(-\beta H)|S\rangle/Z\,, \tag{2}$$

where $\beta=(1/kT)$ and Z stands for the partition function of a system. As in the classical Metropolis method the condition (ii) is satisfied by giving positive transition probabilities between states that are different from each other only at one site $i(i=1, 2, \cdots, N)$. The problem in quantum case is how to obtain adequate transition probabilities consistent with (i). Let $L_i(\nu)$ be a set of sites whose distance from the i-site does not exceed a certain integer ν and $\bar{L}_i$ 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, and its center is i-site. Let S_i denote the state of $L_i(\nu)$ except i-site and let $\bar{S}_i$ denote the state of $\bar{L}_i$. The state of the total system can then be written as $S=(s_i, S_i, \bar{S}_i)$. The transition probability between $S=(s_i, S_i, \bar{S}_i)$ and $S'=(-s_i, S_i, \bar{S}_i)$ can be obtained through (1) if one knows the value of

$$\begin{aligned} q(S)&=P(S)/P(S') \\ &=\langle S|\exp(-\beta H)|S\rangle/\langle S'|\exp(-\beta H)|S'\rangle\,. \end{aligned} \tag{3}$$

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

$$q^{(\nu)}(S_i)=\langle s_i, S_i|\exp(-\beta H(\nu, i))|s_i, S_i\rangle/\langle -s_i, S_i|\exp(-\beta H(\nu, i))|-s_i, S_i\rangle\,. \tag{4}$$

Then the transition probability W_{DC} defined in terms of DC is given by

$$W_{\mathrm{DC}}(-s_i\to s_i)=\max(1, q^{(\nu)}(S_i))\,. \tag{5}$$

The physical meaning of replacing (3) by the approximation (4) was fully discussed by Matsuda et al.[8] If we use (5) as the transition probability from the state $S'=(-s_i, S_i, \bar{S}_i)$ to the state $S=(s_i, S_i, \bar{S}_i)$ in Monte Carlo calculation, we are able to get a Markov chain of a quantum system by using the Metropolis algorism. Thus DCM gives natural extension of the classical Monte Carlo method to quantum systems. However it should be noted that the transition probability (5) does not satisfy the detailed balance. The probability $W_{\mathrm{DC}}(s_i\to -s_i)$ is a function of the neighbouring spins in the cell, which includes finite spins. However when we calculate the transition probability of some other spin in the cell, we introduce W_{DC} with the form of (5) independently. If $H(\nu, i)$ commutes with each other, the detailed balance is satisfied automatically as far as it is satisfied locally. Thus (5) gives correct transition probabilities for classical systems. But in quantum systems where $H(\nu, i)$ does not commute with each other, the transition probability defined at each 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 the one for $W_{\mathrm{DC}}(s_i\to -s_i)$. 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 i-site in it. Here we reformulate the DCM taking into account the above considerations.

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

$$H=(1/r(n))\sum_{j=1}^{r(n)}(\sum_k H_n(j, k)) , \tag{6}$$

where the sum over k means the sum of cells over a whole lattice and that over j does the sum over all different decompositions. $r(n)$ is the number of different decompositions.

Using (6) the probability of a certain spin configuration $|S, s_i\rangle$ is given by

$$P(S, s_i)=(1/Z)\langle S, s_i|\exp(-(\beta/r(n))\sum_{j=1}^{r(n)}(\sum_k H_n(j, k)))|S, s_i\rangle , \tag{7}$$

where Z is the partition function of a system. The ket (bra) $|S, s_i\rangle$ ($\langle S, s_i|$) represents the spin configuration of a system, in which i-th spin is s_i, with $s_i=\pm(1/2)$. We approximate (7), by invoking the basic concept discussed above, as

$$P(S, s_i)\fallingdotseq(1/Z)\prod_j\prod_k\langle\sigma(j, k)|\exp(-(\beta/r(n))H_n(j, k))|\sigma(j, k)\rangle , \tag{8}$$

where $|\sigma(j, k)\rangle$ represents a spin state of a cell (DC) labeled by (j, k). The transition probability $W(s_i\rightarrow -s_i)$ is defined by

$$W(s_i\rightarrow -s_i)=\max[1, P(S, -s_i)/P(S, s_i)] , \tag{9}$$

where $P(S, \pm s_i)$ is defined by (7). We approximate (9) by substituting (8) into $P(S, \pm s_i)$ in (9) to get W_{DC} in modified decoupled cell method (mDCM) as

$$W_{\mathrm{DC}}(s_i\rightarrow -s_i)$$

$$=\max\left[1, \frac{\prod_j\prod_k\langle\sigma(j, k), -s_i|\exp(-(\beta/r(n))H_n(j, k))|\sigma(j, k), -s_i\rangle}{\prod_j\prod_k\langle\sigma(j, k), s_i|\exp(-(\beta/r(n))H_n(j, k))|\sigma(j, k), s_i\rangle}\right] . \tag{10}$$

The product over k in (10) must be done 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 the i-site is taken into account in (10). If the Hamiltonian H of a system consists of only a nearest neighbor coupling, (9) and (10) coincide with those of classical ones in the classical limit. However it should be noted that in one-dimensional case when the Hamiltonian H includes in it the next nearest coupling constants beside the nearest neighbor coupling, each of the next nearest neighbor coupling is included in (8) by a factor $(n-2)/(n-1)$, whereas a nearest neighbor coupling is included in (8) by $1=(n-1)/(n-1)$; see Table I(a).

Table I.

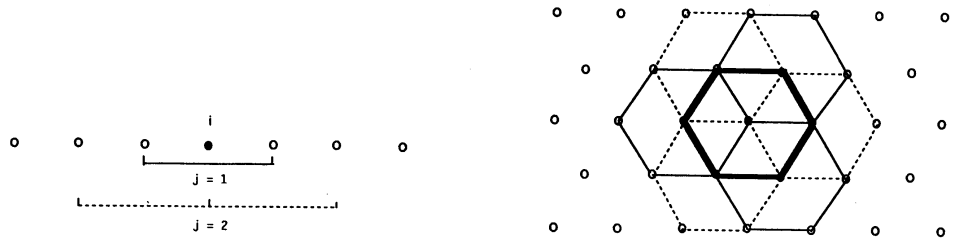
(a) One dimension.

1D lattice	spins/cell	decompositions =overlaps of nearest neighbors[a)]	overlaps of next neighbors[b)]
	n	$n-1$	$n-2$

(b) Two dimensional lattice.

2D lattice	cell shape	spins/cell	decompositions =overlaps of nearest neighbors[a)]	overlaps of next neighbors[b)]	
square	lozenge	5	2	1	
		13	8	6	
square	square	9	4	4	
trigonal	hexagonal	7	3	0	2
		19	12	10	10
trigonal	parallelogram	9	4	4	2

[a)] The number of decompositions is equal to the number of overlaps of a nearest neighbor coupling included in the sum of cell hamiltonians H_n over all decompositions in Eq. (6); couplings on the edge of a cell are split into two neighboring cells in the cell decomposition of hamiltonian. [b)] The number of overlaps in the next nearest couplings.



(a) (b)

Fig. 1. (a) The cell decomposition of one-dimensional lattice by DC, which includes three lattice sites in it. Cells enclosed by the same type of line are included in the same decomposition.
(b) The decomposition of triangular lattice by hexagon, which is the DC. Cells enclosed by the same type of line are included in the same decomposition. The number of possible decompositions is three.

Therefore (10) does not give a correct expression in the classical limit in this case (in one-dimensional lattice). In two-dimensional lattice proper size and shape of a cell (DC) depend on the type of lattice and also the range of couplings. For each lattice and DC we show in Table I(b), the number of lattice sites in DC, the feasible number $r(n)$ of decomposition of a lattice into an array of DC, which is equal to the number of overlaps of a nearest neighbour coupling included in the sum of H_n over all decompositions in (6), and also the number of overlap of the next nearest neighbor coupling. The shape of DC is restricted, for a whole lattice must be split completely into a two-dimensional array of DC. Couplings on the edge of DC are split equally

into two neighboring DC in the cell(DC) decomposition of the Hamiltonian. If a next nearest neighbor coupling exists, the shape of DC for which the number of overlaps of nearest neighbor coupling is the same as that of the next neighbor couplings will be appropriate, because they give the correct classical limit. In Figs. 1(a) and (b) we show DC including i-site in each case of one-dimensional lattice and a hexagonal cell decomposition of a triangular lattice. Thus we complete the modification of DCM (mDCM). In calculating the internal energy of a system we have used the following expression,

$$\varepsilon \equiv \langle H \rangle / N$$

$$= (1/r(n)) \sum_{j=1}^{r(n)} (\sum_{k} \langle H_n(j, k) \rangle) / N \,, \tag{11}$$

where $\langle\ \rangle$ denotes the average with respect to the cell Hamiltonian $H_n(j, k)$.

We have applied mDCM thus formulated, to 1-D quantum XY-model ($s=1/2$) and calculated the internal energy ε and the perpendicular susceptibility $\chi_\perp$ by increasing the size of DC from 3 to 11. Simulations were performed using the Metropolis Monte Carlo procedure.[4] The number of lattice points used here is 128. The run was taken at $T=1.5J$, where J is an exchange interaction, 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 MSC were used to calculate the thermodynamic quantities. The system is then cooled in steps down to $0.05\,J$. 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. We show in Fig. 2 the result of the internal energy ε with the exact solution of Katsura. For comparison we show ε calculated by DCM in Fig. 3. We see from these figures that in mDCM we do not have negative specific heat in low temperature region and that by increasing the size of DC the result gradually approaches the exact one. However we have to

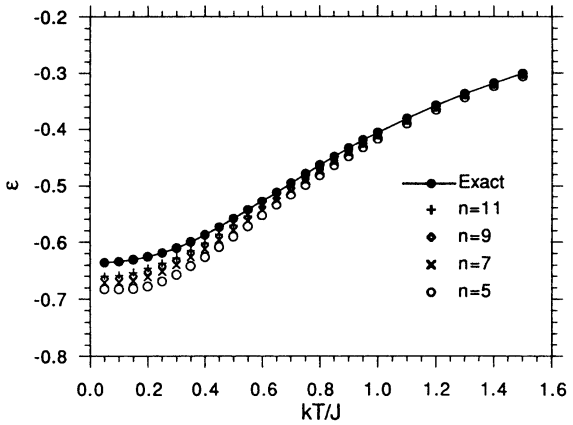


Fig. 2. The internal energy ε per lattice site for 1D XY model ($s=1/2$) in zero external field. The solid line is the exact result by Katsura.[13] The numbers in the figure represent the number of lattice sites in DC.

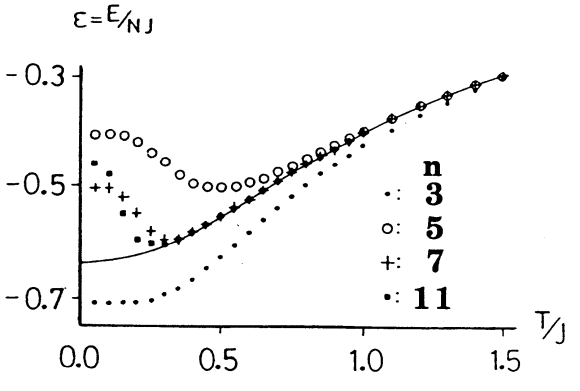


Fig. 3. The internal energy ε per lattice site for 1D XY model ($s=1/2$) in zero external field obtained by DCM. The solid line is the exact result by Katsura.[13] The numbers in the figure represent the number of lattice sites in DC.

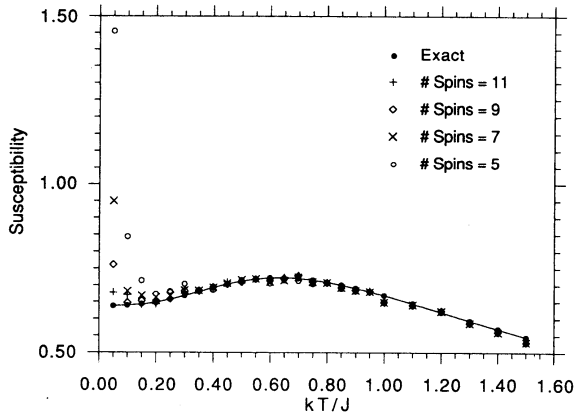


Fig. 4. The zero field susceptibility $\chi_\perp$ along z-axis per spin for 1D XY model. The solid line is the exact result by Katsura.[13] The numbers in the figure represent the number of lattice sites in DC.

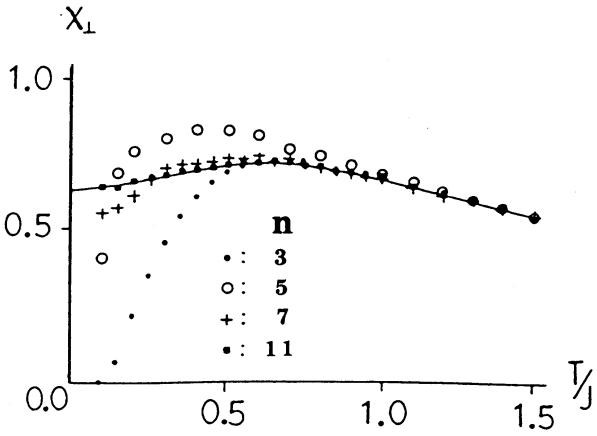


Fig. 5. The zero field susceptibility $\chi_\perp$ along z-axis per spin for 1D XY model obtained by DCM. The solid line is the exact result by Katsura.[13] The numbers in the figure represent the number of lattice sites in DC.

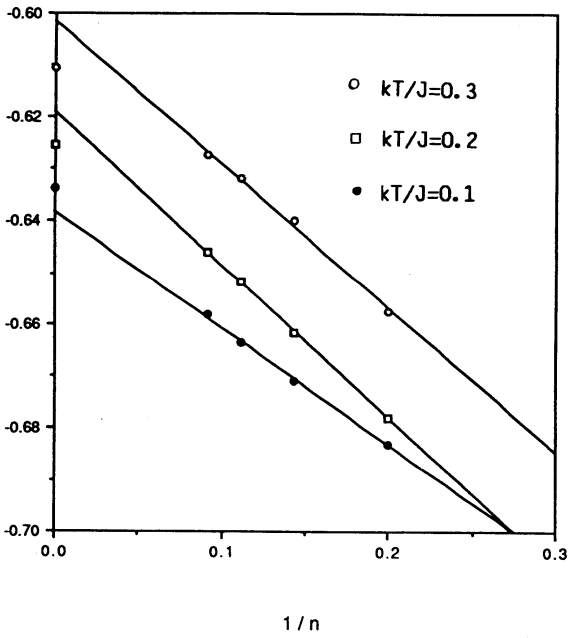


Fig. 6. The internal energy ε vs $(1/n)$ for 1D XY model at fixed temperatures. For $n\to\infty$ the exact results are indicated.

note that for the case $n=11$ the agreement to the exact result is better for DCM than mDCM above $0.35\,J$. In Figs. 4 and 5 we show the perpendicular susceptibility $\chi_\perp$ obtained by mDCM and DCM, respectively, where solid lines are the exact one. We see that the results by mDCM give better approximate values than DCM. In Fig. 6 we show the plot of ε versus 1/(size n of DC). There are no rules how to extrapolate them to the limit $n\to\infty$. Those points in Fig. 6 are best fitted arbitrarily by the straight line vs $(1/n)$ for finite n. However for $n\to\infty$ these straight lines do not give exact results. Thus we may need higher order terms of n to them.

In this paper we have proposed a modification of DCM(mDCM) as a method of Monte Carlo calculations of quantum many body systems. This mDCM might have some similarity to the cluster decomposition method proposed by Suzuki.[14] We have applied mDCM to 1D-XY model ($s=1/2$). The results do not have any of negative specific heat which was observed in DCM. We have to apply mDCM to another low-dimensional quantum spin systems in order to examine its utility. This is in progress.

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