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Cluster Monte Carlo Algorithm for the Study of Quantum X-Y Model

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A Monte Carlo study for the one-dimensional quantum X-Y model by cluster algorithm is presented. For chains of $L = 32$, 64 and 128 at $\beta J = 1.0$-10.0 temperature region, the dynamic properties are analyzed carefully and the corresponding thermodynamic quantities are computed. This method many be developed to apply to the lattice fermions systems.

Key words: cluster Monte Carlo method, quantum X-Y model, integrated autocorrelation time, lattice field theory.

1. INTRODUCTION

The quantum X-Y model was first proposed in 1956 for the study of lattice quantum fluids [1]. Later, the model was interesting because it related to the progress, both in the experimental and theoretical aspects, of low-dimensional magnetic systems. For the one-dimensional (1D) X-Y system, among the more general Heisenberg ferro- and antiferromagnets, the studies have been carried out by the Monte Carlo (M-C) simulations and analytical calculations. The results obtained by the simulations are commonly used to develop new methods or algorithms for the study of the systems in the 2D or higher-dimension to compare with the experimental observations, as well as to make a helpful check for the analytical results.

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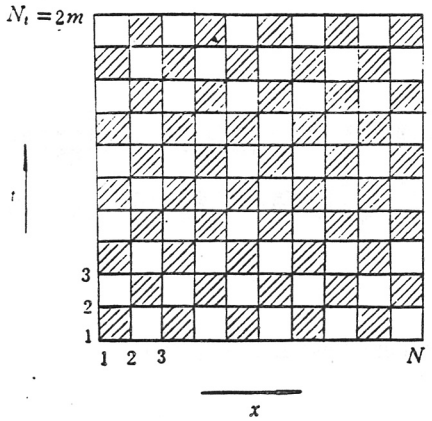

Fig. 1
The 2D induced classical spin system with the four-spin couplings depicted by the shaded plaquettes.

Up to now a few papers were devoted to the simulations for the quantum X-Y model. Cullen and Landau [2] in 1983 have made a systematical M-C study for the 1D X-Y model for $s = 1/2$ by the Suzuki-Trotter transformation to an induced classical spin system with the small Trotter number m. However there arise some problems in their simulations. Because many configurations are forbidden for the induced classical system, the local M-C updating is of very low efficiency at the low temperature region, which causes a different results to the exact calculations. Some other researchers [5,6] concerned on the 2D X-Y model to have a deep insight on its important characters, which was encouraged by the corresponding study for the classical (planar) X-Y model. The latter had the remarkable theory of Kosterlitz and Thouless (KT) [4], which provided a clear physical picture and correctly predicted a KT transition at $kT_c/J = 0.898$. In this paper a loop-cluster M-C algorithm is presented, which avoids the appearance of the forbidden configurations. Then it is applied to the study both at the low temperature region and with the large m. The calculations show evidences that it overcomes the slowing down effects, caused by other local updating methods. This advantage was also shown in our early works for the study of the Heisenberg ferro- and antiferromagnets [7].

The system defined on a chain with the periodic boundary conditions is described by the following Hamiltonian:

$$H = J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \equiv J \sum_{i=1}^{N} H_i , \tag{1}$$

with positive constant $J = 1.0$. Where i denotes the lattice site and N the number of sites on the chain. $S_i = (S^x, S^y)$ is the spin operator defined on each lattice site and can be presented by the Pauli matrix,

$$S^x = \frac{1}{2}\sigma^x, \quad S^y = \frac{1}{2}\sigma^y. \tag{2}$$

The periodic boundary condition gives $S_{N+1} = S_1$.

By the checkerboard decompositions, H can be decomposed into two parts, $H = H_I + H_{II}$:

$$H_I = J \sum_{i=\text{odd}} H_i , \qquad H_{II} = J \sum_{i=\text{even}} H_i . \tag{3}$$

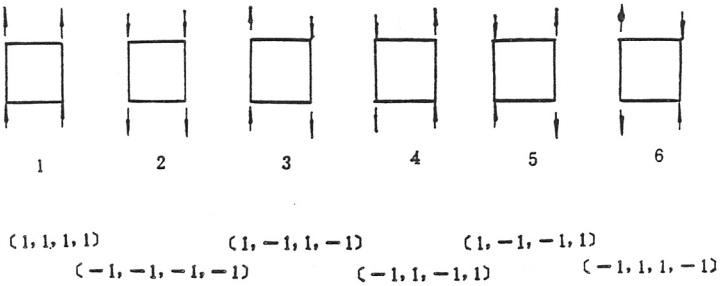

Fig. 2
Six allowed configurations for each interaction plaquette, the spin $s(x,t)$ is located at each corner of the plaquette.

Then, following the Suzuki-Trotter formula [2], we write the corresponding partition function of H as

$$Z = \mathrm{Tr}[\exp(-\beta H)] = \lim_{m\to\infty} \mathrm{Tr}[\exp(-\varepsilon H_{\mathrm{I}})\exp(-\varepsilon H_{\mathrm{II}})]^m, \tag{4}$$

where $\beta = 1/T$ is the inverse temperature and $\varepsilon = \beta/m$ determines the lattice spacing in the Euclidean "time" direction (Trotter direction). After inserting complete sets of eigenstates $|+1\rangle$ and $|-1\rangle$ of σ^z between the factors of $\exp(-\varepsilon H_i)$, we map the 1D quantum system to a 2D induced classical system of Ising-like variables $s(x,t) = \pm 1$. The partition function (4) is written approximately by

$$Z^{(m)} = \prod_{(x,t)} \sum_{s(x,t)=\pm 1} \exp(-S\{s(x,t)\}), \tag{5}$$

Here $S\{s(x,t)\}$ denotes the four-spin interactions associated with the time-like plaquettes (shaded plaquettes in Fig. 1), only the six configurations are allowed in Fig. 2. Their elements reduced from the transfer matrix are given by,

$$\begin{aligned} T(1) &= T(2) = 1 \\ T(3) &= T(4) = \mathrm{ch}(\varepsilon\beta J/2) \\ T(5) &= T(6) = \mathrm{sh}(\varepsilon\beta J/2), \end{aligned} \tag{6}$$

The algorithm constructs loops by first selecting a starting point (x,t) at random and put bond within the shaded plaquette in the x-direction, the t-direction or the diagonal-direction (next-nearest-neighbor) according to the normalized probabilities given in Table 1. Here P_1, P_2, and P_3 are determined such that the detailed balance condition is satisfied,

$$\begin{aligned} P_1 &= [1 + \exp(-\varepsilon\beta J/2)]/2 \\ P_2 &= [1 + \exp(-\varepsilon\beta J/2)]/[\exp(\varepsilon\beta J/2) + \exp(-\varepsilon\beta J/2)] \\ P_3 &= [\exp(\varepsilon\beta J/2) - 1]/[\exp(\varepsilon\beta J/2) + \exp(-\varepsilon\beta J/2)]. \end{aligned} \tag{7}$$

Then a new state is obtained by flipping the two spins at the bond.

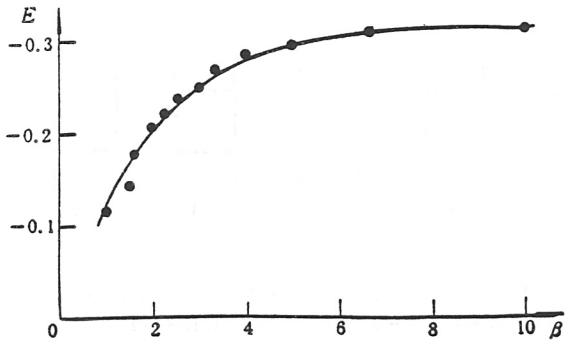

Fig. 3
M-C results of the energy versus the β on the $L = 64$ chain, where the line indicates the exact result [9].

The fundamental idea of updating process is originated from the algorithm of Wolff-Swendsen-Wang [8]. First, given any site (x,t), the plaquette configuration is described by the spin orientations at the four corners of the plaquette and there are two plaquettes for the $s(x,t)$. If $s(x,t) = 1$ we select one of the spins on the plaquette at later time slice to put a bond according the probabilities Pi; otherwise the spin on the other plaquette at the early time slice is chosen to put a bond similarly. Once this next point on the loop is determined, as shown above, the process is repeated until the loop is closed, i.e., the final bond meets the first bond. Second, all the spins on the loop are flipped collectively, $\{s'(x,t) = s(x,t),(x,t) \in \text{Loop}\}$. A Monte Carlo sweep is defined by constructing the loop and flipping all the spins on the loop collectively.

It is of convince to write the partition function in the form

$$Z^{(m)} = \sum_j \exp(-\beta E_j^{(m)}), \tag{8}$$

where $E_j^{(m)}$ is the energy of the j-th state as obtained from the induced classical spin system (5) with the Trotter number m. The m-th approximation of the energy is then gotten as

$$E^{(m)} = -\frac{\partial}{\partial\beta} \ln Z^{(m)} = \frac{1}{Z^{(m)}} \sum_j E_j^{(m)} \exp(-\beta E_j^{(m)}) = \langle F^{(m)} \rangle, \tag{9}$$

where $\langle \cdots \rangle$ means the M-C average.

$$F_j^{(m)} = \frac{\partial}{\partial\beta} (\beta E_j^{(m)}). \tag{10}$$

For the calculation of the specific heat $C^{(m)}$, one finds that

$$c^{(m)} = -\beta^2 \frac{\partial E^{(m)}}{\partial\beta} = \beta^2 [\langle F^{(m)2} - G^{(m)} \rangle - \langle F^{(m)} \rangle^2]; \tag{11}$$

$$G_j^{(m)} = \frac{\partial}{\partial\beta} F_j^{(m)}. \tag{12}$$

Table 1
The directions of generating a bond and the corresponding probabilities as a function of the plaquette configurations.

Initial state		Direction of generating a band	Flipped state	Probability
Label	Configuration			
1	[1,1,1,1]	t-direction diagonal x-direction	[−1,1,−1,1] [−1,1,1,−1] [−1,−1,1,1]	P_1 $1-P_1$ 0
2	[−1,−1,−1,−1]	t-direction diagonal x-direction	[1,−1,1,−1] [1,−1,−1,1] [1,1,−1,−1]	P_1 $1-P_1$ 0
3	[1,−1,1,−1]	t-direction diagonal x-direction	[−1,−1,−1,−1] [−1,−1,1,1] [−1,1,1,−1]	P_2 $1-P_2$ 0
4	[−1,1,−1,1]	t-direction diagonal x-direction	[1,1,1,1] [1,1,−1,−1] [1,−1,−1,1]	P_2 $1-P_2$ 0
5	[1,−1,−1,1]	t-direction diagonal x-direction	[−1,−1,1,1] [−1,−1,−1,−1] [−1,1,−1,1]	P_3 $1-P_3$ 0
6	[−1,1,1,−1]	t-direction diagonal x-direction	[1,1,−1,−1] [1,1,1,1] [1,−1,1,−1]	P_3 $1-P_3$ 0

The expression for the uniform and staggered susceptibilities, χ_u and χ_s, is,

$$\chi^{(m)} = \beta[\langle M^{(m)2}\rangle - \langle M^{(m)}\rangle^2], \tag{13}$$

The corresponding magnetic moments for χ_u and χ_s in the j-th state are given by

$$M_j^{(m)} = \frac{1}{2m}\left[\sum_t \sum_x s(x,t)\right]_j \tag{14}$$

$$[M_s^{(m)}]_j = \frac{1}{2m}\left[\sum_t \sum_x (-1)^{t+x} s(x,t)\right]_j \tag{15}$$

Monte Carlo simulation is performed on the $L = 32$, 64 and 128 chains. The number of slices in the t-direction, $N_t = 2m$, is chosen such that $\varepsilon = \beta/m \leq 0.1$, which controls the systematic error being less than 1.0%. On the temperature region of $1.0 \leq \beta \leq 10.0$, our calculations are carried out. For the $L = 32$ and 64 chains, 12 points of β are taken to do the simulations. For the longest chain, $L = 128$, 5 points of β, where the peak of the specific heat is located, are taken. In the simulation, the random configurations are always taken as initial ones followed by 10,000 sweeps for thermalization and 40,000 sweeps for M-C average using the loop-cluster algorithm described.

Table 2
The numerical results of autocorrelation times.

T	$2m$	τ_e		τ_{χ_s}	
		$L = 32$	$L = 64$	$L = 32$	$L = 64$
0.10	256	2.00(10)	2.18(10)	0.34(3)	0.35(3)
0.15	192	2.05(10)	1.84(09)	0.30(2)	0.29(2)
0.20	128	2.14(10)	2.14(10)	0.32(2)	0.30(2)
0.25	128	2.24(11)	1.74(09)	0.27(2)	0.32(2)
0.30	128	2.19(10)	1.62(09)	0.26(2)	0.27(2)
0.35	96	1.82(09)	1.55(08)	0.28(2)	0.32(2)
0.40	64	1.87(09)	1.62(09)	0.25(2)	0.29(2)
0.45	64	2.01(10)	1.72(09)	0.26(2)	0.30(2)
0.50	64	2.00(10)	1.67(09)	0.27(2)	0.28(2)
0.60	64	1.62(08)	1.66(09)	0.25(2)	0.25(2)
0.80	64	1.74(09)	1.72(09)	0.24(2)	0.26(2)
1.00	64	1.57(08)	1.54(08)	0.26(2)	0.25(2)

The results of the estimations for the thermal observable show that they are almost invariant under the condition $\varepsilon < 0.1$ with the different the L and N_t. In Figs. 3-5, the results of the internal energy, the specific heat and the uniform susceptibility are shown for the chain $L = 64$ respectively. To compare with the exact results obtained by Katsura [9], we include the corresponding curves in our figures and find that, especially on the low temperature region, they are consistent with each other.

Another interesting problem is to demonstrate the efficiency of the loop-cluster algorithm. For the purpose we measure the autocorrelation functions $C_0(t)$, which is defined

$$C_0(t) = \langle O(t_0) \cdot O(t_0 + t) \rangle, \tag{16}$$

where O denotes the observable, the internal energy E and the staggered susceptibility χ_s. And then carefully analyze the $C_0(t)$ to obtain the integrated autocorrelation times τ_0^L by

$$\exp(-1/\tau_0^L) = \sum_{t=1}^{\infty} C_0(t) \Big/ \sum_{t=0}^{\infty} C_0(t). \tag{17}$$

Using the data obtained and noticing that the size of the closed loop is the variable with the M-C sweeps, we re-scale the exponential autocorrelation times τ_0 by

$$\tau_0 = \tau_0^L \times \text{size of the closed loop}/(L \times 2m), \tag{18}$$

where τ_0^L is the measured data for the autocorrelation times by 1-hit loop-cluster updating simulation. Some numerical results are listed in the Table 2, which are collected to calculate the dynamical exponent Z_0 defined by $\tau_0 \propto 1/\varepsilon^{Z_0}$. In the limit of $\varepsilon \to 0$, we find, as shown in Fig. 6,

$$Z_e = 0.2(1), \quad Z_{\chi_s} = 0.0(1). \tag{19}$$

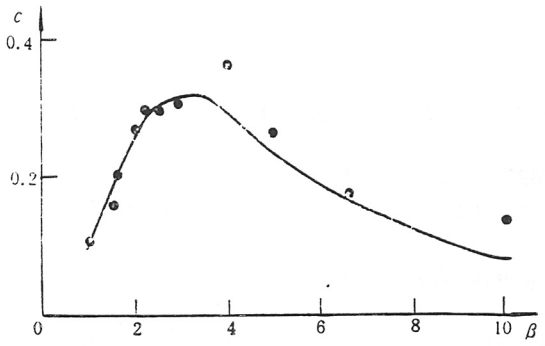

Fig. 4
M-C results of the specific heat, where the line indicates the exact result.

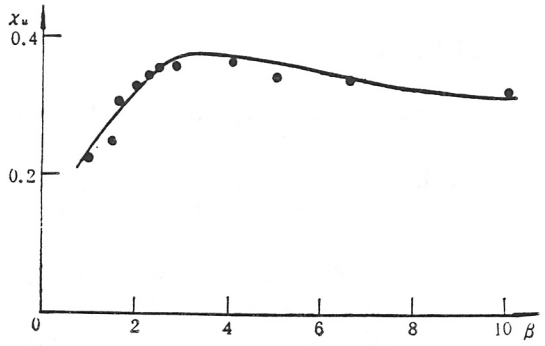

Fig. 5
M-C results of the staggered susceptibility, where the line indicates the exact result.

such that there is no indication of slowing down for $m \to \infty$ which is needed for low temperatures. Furthermore, as shown in Fig. 7, the τ_{χ_s} is fitted by

$$\tau_{\chi_s} \propto \exp(c\beta J) \tag{20}$$

with $c = 0.1(1)$ to show the character of τ when the temperature is lowered. This gives the evidence that the algorithm is still efficient at the low temperature.

To summarize, we presented a loop-cluster algorithm and performed a numerical calculations for the quantum X-Y model. In the simulations we keep m is large enough to reduce the systematic error and to get accurate estimations for several temperatures $1.0 \leq \beta J \leq 1.0$. The results for the autocorrelation times show that the algorithm can update the induced classical spin system efficiently. The algorithm can also be generalized to simulate the X-Y model in the higher dimensions directly. A work for the 2D system will be published elsewhere. At last, we hope that the loop-cluster algorithm may be play an important role in the study of the lattice fermion systems [10].

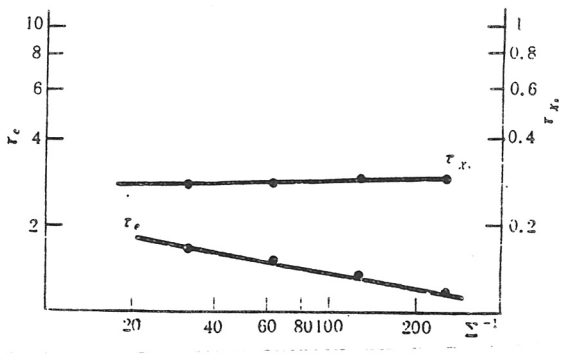

Fig. 6
A log-log plot of the autocorrelation time τ_{χ_s} versus the $1/\varepsilon$.

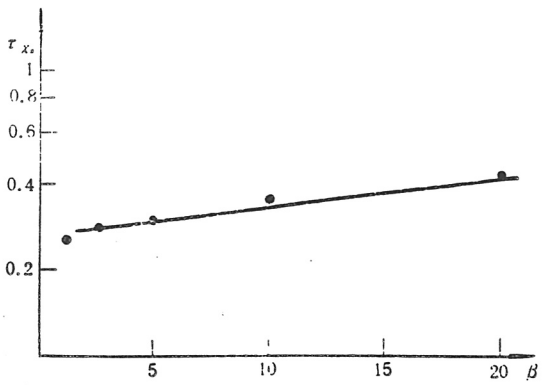

Fig. 7
A plot of τ_{χ_s} versus β on the condition of $\varepsilon = 0.078$ being a constant.

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