A Hybrid Method for Global Updates in Monte Carlo Study

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We propose a new algorithm which works effectively in global updates in Monte Carlo study. We apply it to the quantum spin chain with next-nearest-neighbor interactions. We observe that Monte Carlo results are in excellent agreement with numerically exact ones obtained by the transfer matrix method.

The Monte Carlo method has been an indispensable tool for theoretical study in physics. An essential point of the method is to generate configurations according to their Boltzmann weights. For this purpose one usually starts with an initial configuration and obtains a new configuration sequentially by some rule that guarantees the ergodicity and satisfies the condition of the detailed balance. Widely used rules are the heat bath method and the Metropolis algorithm. The heat bath method is useful for systems which have a small number of candidates for updating because one has to calculate weights for all candidates to determine which one should make the new configuration. The Metropolis algorithm is suitable for complicated systems since in this algorithm it is enough to know the weight just for one candidate to decide whether one should accept or reject that candidate for updating. The problem in the latter is that the efficiency of updating would be bad if the selection of the candidate is not appropriate.

In the previous papers\(^1\),\(^2\) for quantum Monte Carlo study using the Suzuki-Trotter formula we proposed re-structuring method to improve the negative sign problem and applied it to one dimensional spin-1/2 system with next-nearest-neighbor interactions. The Hamiltonian of this system is

$$\hat{H} = \frac{1}{2} \sum_{i=1}^{N} (\sigma_i \sigma_{i+1} + \sigma_i \sigma_{i+2}) ,$$

where \(N\) is the number of sites on the chain and \(\sigma_{N+1} = \sigma_1\). It turned out that this method is very useful for this model. We found however that it was difficult to make Monte Carlo simulations with large values of the Trotter number for technical reasons on the so-called global updates, which are necessary in the quantum Monte Carlo method in addition to the usual local updates. In the global updates one needs to change spin states on all sites along some lines connecting these sites, which usually depend on the size of the system, while in the local updates limited part of the system irrelevant to whole size of the system should be updated. In the conventional approach to the model, where the state on each site is represented spin up or spin down, conservation property of the quantum number \(J_z\) (\(z\)-component of the total spin \(J\)) is helpful to carry out global updates for large sizes of the system. In the re-structuring approach, on the contrary, we employ eigenstates of \(\sigma_{2i-1} \sigma_{2i}\), that is 1, \(\Theta\),
or $-1$, instead of eigenstates of $\sigma_z^i$, where $\sigma_z^i$ denotes $z$-component of the Pauli matrix on site $i$. They are eigenstates of $\sigma_z^{i-1} + \sigma_z^i$ with eigenvalues $2, 0, 0, -2$, namely triplet states and a singlet state obtained from two spin-$1/2$-states. Because of two $J_z=0$ states we need to consider $\sim 2^n$ candidates for a global update in the Trotter direction with the Trotter number $n$, which causes shortage of computer memory when $n$ becomes large. Even for small values of $n$ we found the Metropolis algorithm gives too poor efficiency to obtain results. In previous Monte Carlo work we therefore simulated systems with the Trotter number $n \leq 4$ only by employing the heat bath method with an approximation to discard $\Delta J_z = 2$ candidates. The agreement between Monte Carlo data and numerically exact calculations are satisfactory, but small discrepancy remains. In this paper we propose hybrid use of the heat bath method and the Metropolis algorithm which is applicable for large values of the Trotter number. We will see the discrepancy mentioned above is completely resolved.

Now let us describe the hybrid method. In this method we choose a candidate state applying the heat bath method repeatedly and use the Metropolis algorithm to determine whether we accept it or not. For concrete description we consider the quantum spin-$1/2$ system on an $N$-sited chain with next-nearest-neighbor

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**Fig. 1.** (a) A schema of a part of the two-dimensional lattice with the Trotter number $n=4$ to show how the candidate states are chosen for the $n$-direction global update in the hybrid method. The horizontal (vertical) arrow denotes the space (the Trotter) direction. (b) States of the sites around the plaquettes $Q_1$ and $Q_2$. States $\alpha_i(\beta_i)$ denote the old (the candidate) states on sites $(i, j)$. The arrows are the same as in (a). (c) A plaquette with sites $a$, $b$, $c$ and $d$. The arrows are the same as in (a).
interactions.\textsuperscript{1,2)} After the re-structuring the system reduces to an effective quantum spin system sitting on an $N/2$-sited chain which has nearest-neighbor interactions only. Along the Trotter direction we have $2n$ sites with the Trotter number $n$. Each site $(i, j)$ on such two-dimensional lattice, where $i(j)$ denotes the location in the space (Trotter) direction, is characterized by a spin state $S_{i(j)}$ with $S=\mp 1$, $\Theta$, $\ominus$ or $-1$. For one $n$-direction global updates with a fixed $i$ we have to find a set of $S_{i(j)}$ ($j=1, 2, \cdots, 2n$), as a candidate. Let us denote $S_{i(j)}$ in the old configuration as $a_j$ and its candidate as $\beta_j$ hereafter. First we consider the plaquette $Q_1$ in Fig. 1 (a) only, where it is easy to pick up $\beta_1$ and $\beta_2$ according to the probability $P^{(1)}$,

\[ P^{(1)} = \frac{W(\gamma_1, \beta_1, \gamma_2, \beta_2)}{\sum_{\xi_1} \sum_{\xi_2} W(\gamma_1, \xi_1, \gamma_2, \xi_2)} \]

with $\gamma_j$ being the state of the nearest-neighbor site of the site $(i, j)$ (see Fig. 1 (b)) and $W(\xi_a, \xi_b, \xi_c, \xi_d)$ being the Boltzmann weight for a plaquette depicted in Fig. 1 (c).\textsuperscript{*)} Next we choose $\beta_3$ in the plaquette $Q_2$ according to the probability $P^{(2)}$,

\[ P^{(2)} = \frac{W(\beta_2, \gamma_2, \beta_3, \gamma_3)}{\sum_{\xi_3} W(\beta_2, \gamma_2, \xi_3, \gamma_3)} \]

with $\gamma_2$ and $\gamma_3$ in Fig. 1 (b). Similarly we choose $\beta_{j+1}(j=3, 4, \cdots, 2n-1)$ sequentially.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{The $R$ ratio, the ratio between $(Z_+-Z_-)$ and $(Z_++Z_-)$ of the re-structured quantum spin system calculated by the Monte Carlo simulations with the hybrid method (mc) and by the transfer matrix method (tm) on an $N=8$ chain. Here $Z_+(Z_-)$ denotes number of positively (negatively) weighted configurations generated in the simulation. Exact values of $R$ are also plotted for comparison. Monte Carlo results in the figure with the Trotter number $n=2, 4, 8$ ($n=16$) is an average of a dozen of data calculated from 10000 (100000) configurations after 2000 (20000) sweeps for thermalization. The errors are statistical ones only.}
\end{figure}

\textsuperscript{*)} We have $4^4=256$ values of $W$ in this model. Actually, only 62 of them are non-zero.
according to the probability $P^{(j)}$ which is, for odd $j$,

$$P^{(j)} = W(\gamma_j, \beta_j, \gamma_{j+1}, \beta_{j+1}) / \sum_{\zeta_{j+1}} W(\gamma_j, \beta_j, \gamma_{j+1}, \zeta_{j+1})$$

or, for even $j$,

$$P^{(j)} = W(\beta_j, \gamma_j, \beta_{j+1}, \gamma_{j+1}) / \sum_{\zeta_{j+1}} W(\beta_j, \gamma_j, \zeta_{j+1}, \gamma_{j+1})$$

Finally we compare the probability $P_{\text{new}}$ and $P_{\text{old}}$

$$P_{\text{new}} = W(\beta_{2n}, \gamma_{2n}, \beta_1, \gamma_1)$$

$$\times \prod_{k=1, n-1, 2(n-1)} W(\beta_{2k}, \gamma_{2k}, \zeta_{2k+1}, \gamma_{2k+1}) \sum_{\zeta_{2k+2}} W(\gamma_{2k+1}, \beta_{2k+1}, \gamma_{2k+2}, \zeta_{2k+2}),$$

$$P_{\text{old}} = W(\alpha_{2n}, \gamma_{2n}, \alpha_1, \gamma_1)$$

$$\times \prod_{k=1, n-1, 2(n-1)} W(\alpha_{2k}, \gamma_{2k}, \zeta_{2k+1}, \gamma_{2k+1}) \sum_{\zeta_{2k+2}} W(\gamma_{2k+1}, \alpha_{2k+1}, \gamma_{2k+2}, \zeta_{2k+2}),$$

and decide, following the Metropolis algorithm, whether we replace $\alpha_1, \alpha_2, \ldots, \alpha_{2n}$ by $\beta_1, \beta_2, \ldots, \beta_{2n}$ or not. It is easy to see that this method satisfies the condition of the detailed balance. In Fig. 2 we plot Monte Carlo results on the $R$ ratio obtained by this method, together with numerical exact calculations by the transfer matrix method. We perform simulations on an $N=8$ chain with the Trotter number up to 16. We observe that the Monte Carlo data and the results from the transfer matrix method almost coincide for every value of $n$. It should be also noted that the agreement is remarkable even for large values of the inverse temperature $\Gamma$ because of much better efficiency of the updating than the efficiency in the previous heat bath method.

To summarize we propose a hybrid method for global updates in the Monte Carlo algorithm. Through numerical work for a quantum spin system we show the method is quite powerful. Since the procedure in this method is quite general we expect it is applicable to many systems in the quantum Monte Carlo studies. We also expect the method is helpful in the classical statistical mechanics with the cluster algorithm, where the global updates become important especially when the correlation length is large. We would like to emphasize that the hybrid method enables us to choose appropriate candidates for the update at only a little cost of the computer time and the memory.

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