Abstract

We present detailed discussions on a new approach we proposed in a previous paper to numerically study quantum spin systems. This method, which we will call re-structuring method hereafter, is based on rearrangement of intermediate states in the path integral formulation. We observed our approach brings remarkable improvement in the negative sign problem when applied to one-dimensional quantum spin 1/2 system with next-to-nearest neighbor interactions. In this paper we add some descriptions on our method and show results from analyses by the exact diagonalization and by the transfer matrix method of the system on a small chain. These results also indicate that our method works quite effectively.
Section 1 Introduction

Recent development in experiments on condensed matter has shown us very interesting systems where strong quantum effects should be realized. One of them is the quantum spin system in low dimensions. Much theoretical work has been done to obtain quantitative as well as qualitative properties of these quantum effects [1].

One powerful tool to numerically investigate quantum spin systems is Monte Carlo approach using the Suzuki-Trotter formula [2]. Study through this method has brought us very intriguing results on the ferromagnetic system. It is widely known, however, if one applies this method to frustrated systems one often encounters the so-called negative sign (NS) problem [3]. The NS problem, which becomes more serious on larger lattices, makes it very difficult to get statistically meaningful results in numerical calculations.

In a previous paper [4] we showed that a new approach (re-structuring (RS) method) is useful to obtain Monte Carlo results for one-dimensional quantum spin 1/2 system with next-to-nearest neighbor interactions, which suffers from the NS problem in the antiferromagnetic case. Essential point of RS method is to choose a set of states for the path integral which is appropriate to numerical calculation. Conventional choice of the set, whose states consist of eigenstates of z-component of the Pauli matrix on each lattice site, is the simplest one but the NS problem turns out to be serious with this set. Since any other choice is possible as long as the set is complete, we employ a set made of eigenstates of local Hamiltonian for every two neighboring sites. Although a complete solution for the NS problem could not be obtained, our results, which show much improvement in numerical calculations, inspires us with confidence that quantum Monte Carlo method effectively works if a set of states for the path integral is appropriately chosen.

In this paper we add descriptions on our method in some detail. We then analyse the same system by the exact diagonalization and by the transfer matrix method on a small chain. We will see these analyses are also helpful to confirm superiority of RS method to the conventional one. In section 2 the model and the conventional approach, which is necessary in our analyses for comparison, are scanned. Section 3 is for detailed descriptions of RS formulation. Results from our analyses are given
in section 4 and final section will be devoted to summary and discussions.

Section 2 Model and Conventional approach

The system we study is the quantum spin 1/2 system with next-to-nearest neighbor interactions on a one-dimensional chain, the simplest one among those suffering from serious NS problem. The Hamiltonian of this system is

\[ \hat{H} = \frac{1}{2} \sum_{i=1}^{N} (\vec{\sigma}_i \vec{\sigma}_{i+1} + \vec{\sigma}_i \vec{\sigma}_{i+2}), \]  

(1)

where \( N \) is number of sites on the chain and \( \vec{\sigma}_{N+i} \equiv \vec{\sigma}_i \) (periodic boundary condition). The partition function \( Z \) is given by \( Z = tr(e^{-\beta \hat{H}}) \) with inverse temperature \( \beta \).

Let us describe the conventional approach. State on each site is represented by \( z \)-component of the spin, namely up and down, or + and −. In this representation states of the system are given by

\[ | \alpha \rangle = | s_1, s_2, s_3, ..., s_N \rangle, \]

where \( s_i = + \) or −. The identity operator is then

\[ \hat{1} = \sum_{\{s_i\}} | s_1, s_2, ..., s_N \rangle \langle s_1, s_2, ..., s_N |. \]

To use this identity operator in the Suzuki-Trotter formula, we divide the Hamiltonian into four parts\(^1\) as schematically shown in Fig. 1(a). Thus we come to an expression

\[ Z = \lim_{n \to \infty} tr\{ (e^{-\beta \hat{H}_1/n} e^{-\beta \hat{H}_2/n} e^{-\beta \hat{H}_3/n} e^{-\beta \hat{H}_4/n})^n \}, \]

(2)

where

\[ \hat{H}_1 = \frac{1}{2} \sum_{i=1}^{N/2} \vec{\sigma}_{2i-1} \vec{\sigma}_{2i}, \]

\[ \hat{H}_2 = \frac{1}{2} \sum_{i=1}^{N/2} \vec{\sigma}_{2i} \vec{\sigma}_{2i+1}, \]

\(^1\)For technical reasons number of sites in this case should be restricted to be multiple of four.
\[
\hat{H}_3 = \frac{1}{2} \sum_{i=1}^{N/4} (\vec{\sigma}_{4i-3} \vec{\sigma}_{4i-1} + \vec{\sigma}_{4i-2} \vec{\sigma}_{4i}), \\
\hat{H}_4 = \frac{1}{2} \sum_{i=1}^{N/4} (\vec{\sigma}_{4i-1} \vec{\sigma}_{4i+1} + \vec{\sigma}_{4i} \vec{\sigma}_{4i+2}).
\]

With above complete set and partial Hamiltonians we obtain the partition function \(Z_C^{(n)}\) used in Monte Carlo calculations,

\[
Z_C^{(n)} = \sum_{\{\alpha_j, \alpha'_j, \alpha''_j, \alpha'''_j\}} w(\{\alpha_j, \alpha'_j, \alpha''_j, \alpha'''_j\}), \tag{3}
\]

where

\[
w(\{\alpha_j, \alpha'_j, \alpha''_j, \alpha'''_j\}) = \prod_{j=1}^{n} < \alpha_j | e^{-\beta \hat{H}_1/n} | \alpha'_j > < \alpha'_j | e^{-\beta \hat{H}_2/n} | \alpha''_j > \\
	imes < \alpha''_j | e^{-\beta \hat{H}_3/n} | \alpha'''_j > < \alpha'''_j | e^{-\beta \hat{H}_4/n} | \alpha_{j+1} >,
\]

suffix \(j\) numbering sites along the Trotter axis and \(\alpha_{n+1} \equiv \alpha_1\).

In this system \(w(\{\alpha_j, \alpha'_j, \alpha''_j, \alpha'''_j\})\), total product of expectation values over one configuration, can be negative. Appearance of this negative weight brings the NS problem. In order to numerically calculate some physical quantity \(\langle A \rangle\) one then should subtract contributions of negatively signed configurations, \(A_-\), from those of positively signed ones, \(A_+\). Namely,

\[
\langle A \rangle = \frac{A_+ - A_-}{Z_+ - Z_-}, \tag{4}
\]

where \(Z_+(Z_-)\) is number of configurations with positive (negative) weight. The result would suffer from serious cancellation when \(Z_- \approx Z_+\).

### Section 3 RS Method

Formulations of RS method is outlined in our previous paper [4]. Here we briefly repeat them and add detailed information on its effective Hamiltonian.

We start from rewriting (1) in the following form

\[
\hat{H} = \frac{1}{2} \sum_{i=1}^{N/2} (\vec{\sigma}_{a,i} \vec{\sigma}_{a,i+1} + \vec{\sigma}_{b,i} \vec{\sigma}_{b,i+1} + \vec{\sigma}_{a,i} \vec{\sigma}_{b,i} + \vec{\sigma}_{b,i} \vec{\sigma}_{a,i+1}),
\]
where we denote odd and even sites with suffix $a$ and $b$, respectively,

$$
\sigma_{a,i} \equiv \sigma_{2i-1}, \quad \sigma_{b,i} \equiv \sigma_{2i}.
$$

We employ the complete set for which the operator products $\sigma_{a,i}\sigma_{b,i}$ are diagonalized. Explicitly, we use

$$
| \alpha > = | S_1, S_2, ..., S_{N/2} >, \tag{5}
$$

where $S_i = 1_i, \oplus_i, \ominus_i$ or $-1_i$ with

$$
| 1_i > = | a_i, +b_i >,
$$

$$
| \oplus_i > = \frac{1}{\sqrt{2}}(| a_i, -b_i > + | -a_i, +b_i >),
$$

$$
| \ominus_i > = \frac{1}{\sqrt{2}}(| a_i, -b_i > - | -a_i, +b_i >),
$$

$$
| -1_i > = | -a_i, -b_i >.
$$

Hamiltonian (1) is accordingly divided into “odd” and “even” parts

$$
\hat{H} = \hat{H}_o + \hat{H}_e, \tag{6}
$$

where, as shown in Fig. 1(b),

$$
\hat{H}_o = \frac{1}{2} \sum_{i=1}^{N/4} \hat{h}_{oi}
$$

$$
\hat{h}_{oi} = (\sigma_{a,2i-1}\sigma_{a,2i} + \sigma_{b,2i-1}\sigma_{b,2i} + \sigma_{b,2i-1}\sigma_{a,2i} + \frac{1}{2}\sigma_{a,2i-1}\sigma_{b,2i-1} + \frac{1}{2}\sigma_{a,2i}\sigma_{b,2i}),
$$

$$
\hat{H}_e = \frac{1}{2} \sum_{i=1}^{N/4} \hat{h}_{ei}, \tag{7}
$$

$$
\hat{h}_{ei} = (\sigma_{a,2i}\sigma_{a,2i+1} + \sigma_{b,2i}\sigma_{b,2i+1} + \sigma_{b,2i}\sigma_{a,2i+1} + \frac{1}{2}\sigma_{a,2i-1}\sigma_{b,2i-1} + \frac{1}{2}\sigma_{a,2i}\sigma_{b,2i}).
$$

Expression of the partition function with these partial Hamiltonians is

$$
Z = \lim_{n \to \infty} tr\{(e^{-\beta\hat{H}_o/n}e^{-\beta\hat{H}_e/n})^n\}. \tag{9}
$$
Inserting identity operators made of \( \alpha \)'s in (3) between the exponents we obtain partition function in RS method,

\[
Z^{(n)}_{RS} = \sum_{\{\alpha_j, \alpha'_j\}} \prod_{j=1}^n < \alpha_j | e^{-\beta \hat{H}_o/n} | \alpha'_j > < \alpha'_j | e^{-\beta \hat{H}_e/n} | \alpha_{j+1} > .
\]  

(10)

In order to obtain Boltzman weights to be used in Monte Carlo simulations, we need to construct\( < S'_{2i-1}, S'_{2i} | \hat{h}_{oi} | S_{2i-1}, S_{2i} > \) from local matrix elements\( < S'_{2i-1}, S'_{2i} | \hat{h}_{ei} | S_{2i-1}, S_{2i} > \) as well as\( < S'_{2i}, S'_{2i+1} | \exp(-\beta \hat{h}_{ei}) | S_{2i}, S_{2i+1} > \) from local matrix elements\( < S'_{2i}, S'_{2i+1} | \hat{h}_{ei} | S_{2i}, S_{2i+1} > \). Since these matrix elements are \( i \)-independent and

\[
< S'_{2i-1}, S'_{2i} | \hat{h}_{oi} | S_{2i-1}, S_{2i} >= < S'_{2i}, S'_{2i+1} | \hat{h}_{ei} | S_{2i}, S_{2i+1} > ,
\]

we only need to know values of

\[
< S'_1, S'_2 | \hat{h}_{oi} | S_1, S_2 >= < S'_1, S'_2 | \hat{a}_{a,1} \hat{a}_{a,2} | S_1, S_2 >
\]

\[+ < S'_1, S'_2 | \hat{b}_{b,1} \hat{b}_{b,2} | S_1, S_2 > + < S'_1, S'_2 | \hat{a}_{b,1} \hat{a}_{a,2} | S_1, S_2 >
\]

\[+ \frac{1}{2} < S'_1, S'_2 | \hat{a}_{a,1} \hat{b}_{b,1} | S_1, S_2 > + \frac{1}{2} < S'_1, S'_2 | \hat{a}_{b,2} \hat{b}_{b,2} | S_1, S_2 > .
\]  

(11)

It is an easy task to calculate each matrix element in (11). For example,

\[
< -1_1, 1_2 | \hat{a}_{a,1} \hat{a}_{a,2} | \Theta_1, \Theta_2 >
\]

\[=< -a_1, -b_1 | < +a_2, +b_2 | (2\sigma_{a,1}^+ \sigma_{a,2}^- + 2\sigma_{a,1}^- \sigma_{a,2}^+ + \sigma_{a,1}^x \sigma_{a,2}^x) \frac{1}{\sqrt{2}} (| +a_1, -b_1 > + | -a_1, +b_1 >) \frac{1}{\sqrt{2}} (| +a_2, -b_2 > - | -a_2, +b_2 >)
\]

\[= < -1_1, 1_2 | ( | 1_1, -1_2 > - | -1_1, 1_2 > + | \Theta_1, \Theta_2 > ) = -1,
\]

where

\[
\sigma^\pm = \frac{1}{2}(\sigma^x \pm i \sigma^y).
\]

Values of\( < S'_1, S'_2 | \hat{h}_{oi} | S_1, S_2 > \) are summarized in Table.
Section 4 Transfer Matrix and Exact Diagonalization

In this section we present results from analyses with RS partition function (10) on an \( N = 8 \) chain by the transfer matrix method and the exact diagonalization. Results from conventional partition function (3) are also provided for comparison. Purpose of these analyses are twofold. One is to confirm RS algorithm and previous Monte Carlo results. Another is to study how systems with \( Z_{C}^{(n)} \) and \( Z_{RS}^{(n)} \) depend on Trotter number \( n \).

First let us show results for ratio of negatively weighted configurations to total configurations, \( P = Z_{-}/(Z_{+} + Z_{-}) \), calculated by the transfer matrix method. We use ‘real-space’ transfer matrix to realize the same boundary condition as those in other methods. In the conventional approach we calculate product of matrix \( T_{k} \), whose matrix element \((T_{k})_{\alpha' \alpha}\) corresponds to \( < \alpha' | \exp(-\beta \hat{H}_{k}/n) \ | \alpha > \). Therefore

\[
Z_{C}^{(n)} = tr((T_{1}T_{2}T_{3}T_{4})^{n}).
\]

Similarly, with \((T_{o(e)})_{\alpha' \alpha} = < \alpha' | \exp(-\beta \hat{H}_{o(e)}/n) \ | \alpha >\),

\[
Z_{RS}^{(n)} = tr((T_{e}T_{o})^{n}).
\]

In figure 2(a) we plot \( P \) from the transfer matrix method together with previous Monte Carlo results. We see Monte Carlo data and transfer matrix results for \( n = 2 \) agree very well. Also we observe agreement between those for larger Trotter numbers is satisfactory\(^2\). Our Monte Carlo work is thus nicely supported by an analytical calculation.

Next we calculate

\[
R = \frac{Z_{+} - Z_{-}}{Z_{+} + Z_{-}} = \frac{Z}{Z'},
\]

which equals to \( 1 - 2P \) and is the ratio of the partition function \( Z \) obtained from the Hamiltonian \((\hat{H})\) to the partition function \( Z' \) calculated from the modified Hamiltonian that gives absolute weights \(^3\).

For \( N = 8 \) chain it is not difficult to calculate all energy eigen values \( E_{i} \) \((i = 1, ..., 2^{N})\) by the exact diagonalization. We therefore can obtain value of exact par-

\(^2\)Small discrepancy in low temperature region might suggest that additional improvements in global flips, which are related to the ergodicity\(^4\), are necessary.
partition function at any temperature by equation
\[ Z = \sum_{i=1}^{2^N} \exp(-\beta E_i). \] (13)
The same is true for the denominator in (12):
\[ Z' = \sum_{i=1}^{2^N} \exp(-\beta E'_i), \] (14)
with energy eigen values \( E'_i \) for the modified Hamiltonian. We refer to the ratio \( R \) calculated from (13) and (14) as \( R_{DG} \). It should be noted that value of \( R_{DG} \) depends on method used to calculate the denominator \( Z' \). We will see RS method gives better ratio compared to the conventional method.

Before going to full numerical calculations, let us comment on ground state energy of each Hamiltonian. As discussed in ref. [3], at very low temperature where contribution from the lowest energy eigen value is dominant,
\[ R \approx \exp(-\beta (E_0 - E'_0)) \]
because \( Z_+ - Z_- \approx \exp(-\beta E_0) \) and \( Z_+ + Z_- \approx \exp(-\beta E'_0) \) with \( E_0 \) (\( E'_0 \)) denoting energy of ground state for the Hamiltonian (for the modified Hamiltonian). Existence of severe NS problem implies \( E_0 > E'_0 \).

Our results are in agreement with the above discussion. Values we obtain by the exact diagonalization are \( E_0 = -8.25 \) and \( E'_0 = -10.14 \) (\(-11.32\)) for RS (conventional) method. The fact that the energy difference \( E_0 - E'_0 \) in RS method is smaller than that in the conventional method indicates improvement introduced by RS method.

For the second purpose we also calculate \( R \) by the transfer matrix method with several values of Trotter number \( n \). All numerical results on \( R \) are summarized in figure 2(b). Here we would like to point out two features. One is that, as is expected, the \( R_{DG} \) is much larger in the RS method than in the convolutional method, especially for low temperatures. Another feature is rather unexpected one. In RS method it turned out that \( R \)'s for finite Trotter numbers, which should coincide with \( R_{DG} \) in \( n \to \infty \) limit, are always larger than \( R_{DG} \). In the conventional method, on the contrary, all \( R \) values calculated by the transfer matrix method lie below \( R_{DG} \). This
encourages us to promote RS method in Suzuki-Trotter formula because it becomes possible to obtain statistically meaningful Monte Carlo results even for small values of $n$.

Finally we present results for the energy of the system. In figure 3, exact values obtained by the exact diagonalization,

$$E = \sum_{i=1}^{2N} E_i \cdot e^{-\beta E_i} / \sum_{i=1}^{2N} e^{-\beta E_i},$$

and other values calculated by the transfer matrix method are plotted. It is clear that conventional method fails to give reliable values when Trotter number is small. Even when $n = 8$, difference from exact one becomes large as temperature $T$ decreases. In the RS method, on the contrary, we get satisfactorily stable results even for $n = 2$ and all data seem to nicely converge to the exact ones when $n$ is enlarged.

Section 5 Discussions

In this paper we provide additional explanations of RS approach, which we proposed in a previous paper [4] in order to make meaningful Monte Carlo study of quantum spin systems suffering from the NS problem. From technical point of view main task is to analytically calculate matrix elements for effective Hamiltonian in (10). Descriptions on it are presented in section 3. We also present results from analyses of quantum spin 1/2 system with next-to-nearest neighbor antiferromagnetic interactions on a small chain, applying RS approach in the transfer matrix method and the exact diagonalization. In section 4 we see all results obtained through these analyses indicate that RS method is effectively works in this case.

Let us comment on possible applications of RS method to other quantum spin systems. Qualitatively the RS method will be effective for any frustrated systems suffering from the NS problem. But its power to bring how much quantitative improvement in numerical calculations does strongly depend on system’s interactions and spacial constructions of clusters.

One interesting application would be to investigate quantum spin 1/2 XY chain with next-to-nearest neighbor interactions. For qualitative discussion we calculate
energy eigen values of the system on $N = 8$ chain by the exact diagonalization. The lowest energy is $E_0 = -5.78$ for the XY Hamiltonian while $E'_0 = -7.14(-9.44)$ for the modified Hamiltonian in RS (conventional) method. These results suggest RS method works more powerfully on the XY chain in comparison with the Heisenberg chain, which should be one example of the above statement.

Another intriguing application was made to the $\Delta$ chain by Nakamura and Saika. They reported that RS method is quite useful for this system [7].

We would like to point out a very lucky case where the NS problem is completely solved, although it might be less interesting from physical point of view. This is one-dimensional antiferromagnetic quantum spin $1/2$ system with next-to-next-to-nearest neighbor interactions in addition to next-to-nearest neighbor one, where all couplings have the same strength$^3$. This system suffers from severe NS problem in the conventional approach. When one chooses eigen states of the nearest interaction for the nearest two spins, matrix elements of the effective Hamiltonian become quite simple so that negatively weighted configurations do not appear at all.

In two-dimensional cases systems on triangular lattice will be most important in application. If we employ eigen states for cluster of two neighboring spins as we did in one-dimensional case it is not unique which two should form a pair because more than one neighboring sites exist on the lattice. Symmetry of the lattice inspires us clustering of three spins is appropriate, for which one has to do with more complicated effective matrix elements. At present it is an open question which way gives better results.

In any case a good choice of complete set which improves the NS problem will help us to gain deep insight into the ground state of the system under investigation.

$^3$Number of sites of this system also should be multiple of four for technical reasons.
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**Table Caption**

Values of matrix elements $< S'_1, S'_2 | \hat{h}_{01} | S_1, S_2 >$ described in section 3. Rows and columns denote states $< S'_1, S'_2 |$ and $| S_1, S_2 >$, respectively. All other matrix elements are zero.

**Figure Captions**

**Figure 1**
(a) Schema to show how to divide the Hamiltonian (1) into four parts on an eight-site ($N = 8$) chain with periodic boundary condition. Sites are numbered from one to eight. Filled circles, squares, diamonds and triangles on links denote interactions to belong partial Hamiltonians $\hat{H}_1$, $\hat{H}_2$, $\hat{H}_3$ and $\hat{H}_4$ in (2), respectively.
(b) Schema to show how to re-divide the same Hamiltonian (1) into $\hat{H}_o$ and $\hat{H}_e$ in (3). Sites are renumbered from $a1$ to $b4$. Open diamonds (triangles) denote interactions to fully belong to partial Hamiltonian $\hat{H}_o$ ($\hat{H}_e$). Interactions on links with open circles should be equally shared by $\hat{H}_o$ and $\hat{H}_e$.

**Figure 2**
(a) Ratio of negative weight calculated on an $N = 8$ chain by Monte Carlo simulations (MC) and by the transfer matrix method (TM), using the RS Hamiltonian (RS) or the conventional one (conv.), with several values of Trotter number $n$.
(b) Ratio of partition functions on an $N = 8$ chain. The exact diagonalization (DG) is employed in addition to the transfer matrix method.

**Figure 3**
Energy per site calculated on an $N = 8$ chain by means of the exact diagonalization (DG) and the transfer matrix method (TM). The transfer matrix method is applied to both Hamiltonians (RS, conv.) with Trotter number $n = 2, 4$ and $8$. 
Table

|       | 1, 1 | 1, 1 | 1, ⊕ | 1, ⊖ |
|-------|------|------|------|------|
| 1, ⊕ | 1    | 1    | 3    | 1    |
| 1, ⊖ | 1    | -1   | -1   | 1    |
| 1, ⊕ | 3    | -1   | 1    | -1   |
| 1, ⊖ | 1    | 1    | -1   | -1   |

|       | -1, 1 | 1, -1 | 1, ⊕ | 1, ⊖ | 1, ⊕ | 1, ⊖ | 1, ⊕ | 1, ⊖ |
|-------|-------|-------|------|------|------|------|------|------|
| -1, 1 | -2    | 0     | 3    | 1    | 1    | -1   |       |      |
| 1, -1 | 0     | -2    | 3    | -1   | -1   | -1   |       |      |
| ⊕, ⊕  | 3     | 3     | 1    | 0    | 0    | 1    |       |      |
| ⊕, ⊖  | 1     | -1    | 0    | -1   | 1    | 0    |       |      |
| ⊕, ⊕  | 1     | -1    | 0    | 1    | -1   | 0    |       |      |
| ⊕, ⊖  | -1    | -1    | 1    | 0    | 0    | -3   |       |      |

|       | ⊕, -1 | ⊕, -1 | -1, ⊕ | -1, ⊖ |
|-------|-------|-------|-------|-------|
| ⊕, -1 | 1     | -1    | 3     | -1    |
| ⊕, -1 | -1    | -1    | 1     | 1     |
| -1, ⊕ | 3     | 1     | 1     | 1     |
| -1, ⊖ | -1    | 1     | 1     | -1    |

|       | -1, -1 | -1, -1 |
|-------|--------|--------|
| -1, -1| -1     | 4      |