Re-Structuring Method for the Negative Sign Problem
in Quantum Spin Systems

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We present detailed discussion 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-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.

§ 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 the Monte Carlo approach using the Suzuki-Trotter formula.2) Studies through this method have 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 paper4) we showed that a new approach (re-structuring (RS) method) is useful in obtaining Monte Carlo results for one-dimensional quantum spin-1/2 system with next-nearest-neighbor interactions, which suffers from the NS problem in the antiferromagnetic case. An essential point of the RS method is to choose a set of states for the path integral which is appropriate to numerical calculation. The conventional choice of the set, whose states consist of eigenstates of the z-component of the Pauli matrices on each lattice site, is the simplest one but the NS problem turns out to be serious for this set. Since any other choice is possible as long as the set is complete, we employ a set made of eigenstates of the 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, inspire us with confidence that the 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 analyze 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
the RS method to the conventional one. In § 2 the model and the conventional approach, which is necessary in our analyses for comparison, are scanned. Section 3 is for detailed descriptions of the RS formulation. Results from our analyses are given in § 4 and the final section will be devoted to a summary and discussion.

§ 2. Model and conventional approach

The system we study is the quantum spin-1/2 system with next-nearest-neighbor interactions on a one-dimensional chain, the simplest one among those where a serious NS problem appears. 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 $\sigma_{N+i} = \sigma_i$ (periodic boundary condition). The partition function $Z$ is given by $Z = \text{tr}(e^{-\beta \hat{H}})$ with the inverse temperature $\beta$.

Let us describe the conventional approach. States on each site are represented in terms of the $z$-component of the spin, namely up and down, or $+$ and $-$. In this representation states of the system are given by

$$| \alpha \rangle = | s_1, s_2, s_3, \ldots, s_N \rangle,$$

where $s_i = +$ or $-$. The identity operator is then

$$\hat{I} = \sum_{\{s_i\}} | s_1, s_2, \ldots, s_N \rangle \langle s_1, s_2, \ldots, s_N |.$$

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

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$^*$ For technical reasons the number of sites in this case should be restricted to be multiples of four.
the expression
\[ Z = \lim_{n \to \infty} \text{tr}\left( (e^{-\beta \tilde{H}_n} e^{-\beta \tilde{H}_n} e^{-\beta \tilde{H}_n} e^{-\beta \tilde{H}_n})^n \right), \] (2)

where
\[ \tilde{H}_1 = \frac{1}{2} \sum_{i=1}^{N/2} \sigma_{2i-1} \sigma_{2i}, \]
\[ \tilde{H}_2 = \frac{1}{2} \sum_{i=1}^{N/2} \sigma_{2i} \sigma_{2i+1}, \]
\[ \tilde{H}_3 = \frac{1}{2} \sum_{i=1}^{N/4} (\sigma_{4i-3} \sigma_{4i-1} + \sigma_{4i-2} \sigma_{4i}), \]
\[ \tilde{H}_4 = \frac{1}{2} \sum_{i=1}^{N/4} (\sigma_{4i-1} \sigma_{4i+1} + \sigma_{4i} \sigma_{4i+2}). \]

With the above complete set and the partial Hamiltonians we obtain the partition function \( Z_c^{(n)} \) used in Monte Carlo calculations,
\[ Z_c^{(n)} = \sum_{\{a_j, a'_j, a''_j, a'''_j\}} w(\{a_j, a'_j, a''_j, a'''_j\}), \] (3)

where
\[ w(\{a_j, a'_j, a''_j, a'''_j\}) = \prod_{j=1}^{n} \langle a_j | e^{-\beta \tilde{H}_1} | a'_j \rangle \langle a'_j | e^{-\beta \tilde{H}_2} | a''_j \rangle \]
\[ \times \langle a''_j | e^{-\beta \tilde{H}_3} | a'''_j \rangle \langle a'''_j | e^{-\beta \tilde{H}_4} | a_{j+1} \rangle, \]
the suffix \( j \) numbering sites along the Trotter axis and \( a_{n+1} \equiv a_n \).

In this system \( w(\{a_j, a'_j, a''_j, a'''_j\}) \), the total product of the expectation values for 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,
\[ \langle A \rangle = \frac{A_+ - A_-}{Z_+ - Z_-}, \] (4)

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

§ 3. RS method

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

We start from rewriting (1) in the following form:
\[ \tilde{H} = \frac{1}{2} \sum_{i=1}^{N/2} (\sigma_{a,i} \sigma_{a,i+1} + \sigma_{b,i} \sigma_{b,i+1} + \sigma_{a,i} \sigma_{b,i} + \sigma_{b,i} \sigma_{a,i+1}), \]
where we denote odd and even sites with suffix \( a \) and \( b \), respectively,
We employ the complete set for which the operator products $\sigma_{a,i}\sigma_{b,i}$ are diagonalized. Explicitly, we use

$$|a\rangle = |S_1, S_2, \ldots, S_{N/2}\rangle,$$

where $S_i = 1, \Theta_i$, or $-1$ with

$$|1\rangle = |a, i, +b, i\rangle,$$

$$|\Theta_i\rangle = \frac{1}{\sqrt{2}}(|a, i, -b, i\rangle + |a, i, +b, i\rangle),$$

$$|-1\rangle = |a, i, -b, i\rangle.$$

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

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

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

$$\hat{H}_o = \frac{1}{2} \sum_{i=1}^{2N \bar{h}_{o}\sigma_{a,2i-1}\sigma_{a,2i} + \sigma_{b,2i-1}\sigma_{b,2i} + \sigma_{b,2i-1}\sigma_{b,2i} + \sigma_{a,2i-1}\sigma_{a,2i} + \frac{1}{2} \sigma_{a,2i-1}\sigma_{b,2i-1} + \frac{1}{2} \sigma_{a,2i}\sigma_{b,2i},$$

$$\hat{H}_e = \frac{1}{2} \sum_{i=1}^{2N \bar{h}_{e}\sigma_{a,2i}\sigma_{a,2i+1} + \sigma_{b,2i}\sigma_{b,2i+1} + \sigma_{b,2i}\sigma_{a,2i+1} + \sigma_{a,2i}\sigma_{b,2i} + \frac{1}{2} \sigma_{a,2i+1}\sigma_{b,2i+1} + \frac{1}{2} \sigma_{a,2i}\sigma_{b,2i+1}.$$  

The expression of the partition function with these partial Hamiltonians is

$$Z = \lim_{n \to \infty} \text{tr} \left( e^{-\beta \bar{h}_o/n} e^{-\beta \bar{h}_e/n} \right).$$

Inserting identity operators made of the $\sigma_i$'s in (5) between the exponents we obtain the partition function in the RS method,

$$Z_{RS} = \sum_{\sigma_0, \ldots, \sigma_{N-1}} \prod_{j=1}^{N} \langle \sigma_j | e^{-\beta \bar{h}_o/n} | \sigma_j \rangle \langle \sigma_j | e^{-\beta \bar{h}_e/n} | \sigma_{j+1} \rangle.$$  

In order to obtain the Boltzman weights to be used in Monte Carlo simulations, we need to construct $\langle S_{2i-1}, S_{2i} | \exp(-\beta/2n) \bar{h}_{o}\rangle | S_{2i-1}, S_{2i} \rangle$ from the local matrix elements $\langle S_{2i-1}, S_{2i} | \bar{h}_{o}\rangle | S_{2i-1}, S_{2i} \rangle$ as well as $\langle S_{2i-1}, S_{2i+1} | \exp(-\beta/2n) \bar{h}_{e}\rangle | S_{2i}, S_{2i+1} \rangle$ from the local matrix elements $\langle S_{2i}, S_{2i+1} | \bar{h}_{e}\rangle | S_{2i}, S_{2i+1} \rangle$. Since these matrix elements are independent of $i$ and since

$$\langle S_{2i-1}, S_{2i} | \bar{h}_{o}\rangle | S_{2i-1}, S_{2i} \rangle = \langle S_{2i}, S_{2i+1} | \bar{h}_{e}\rangle | S_{2i}, S_{2i+1} \rangle.$$
we only need to know the values of
\[ \langle S_1', S_2' | \sigma_{a,1} \sigma_{a,2} | S_1, S_2 \rangle \]
\[ = \langle S_1', S_2' | \sigma_{b,1} \sigma_{a,2} | S_1, S_2 \rangle \]
\[ + \langle S_1', S_2' | \sigma_{b,1} \sigma_{a,2} | S_1, S_2 \rangle \]
\[ + \frac{1}{2} \langle S_1', S_2' | \sigma_{a,1} \sigma_{b,1} | S_1, S_2 \rangle \]
\[ + \frac{1}{2} \langle S_1', S_2' | \sigma_{a,2} \sigma_{b,2} | S_1, S_2 \rangle . \]
\[ (11) \]

It is an easy task to calculate each matrix element in (11). For example,
\[ \langle -1_1, 1_2 | \sigma_{a,1} \sigma_{a,2} | \Theta_1, \Theta_2 \rangle \]
\[ = \langle -a_1, -b_1 | \sigma_{a,2} + a_2 + b_2 | \]
\[ \times (2 \sigma_{a,1} \sigma_{a,2} + 2 \sigma_{a,1} \sigma_{a,2} + \sigma_{a,1} \sigma_{a,2}) \]
\[ \times \sqrt{2} (\langle +a_1, -b_1 \rangle + \langle -a_1, +b_1 \rangle) \]
\[ \times \frac{1}{\sqrt{2}} (\langle +a_2, -b_2 \rangle + \langle -a_2, +b_2 \rangle) \]
\[ = \langle -1_1, 1_2 | \]
\[ \times (\langle 1_1, -1_2 \rangle + \langle -1_1, 1_2 \rangle + 1_1, 1_2 \rangle \]
\[ = -1 , \]
where
\[ \sigma^z = \frac{1}{2} (\sigma^x + i \sigma^y) . \]

The values of \[ \langle S_1', S_2' | \sigma_{a,1} | S_1, S_2 \rangle \] are summarized in Table I.

Table I. The values of the matrix elements
\[ \langle S_1', S_2' | \sigma_{a,1} | S_1, S_2 \rangle \] described in § 3. The rows and the columns denote the states \[ \langle S_1', S_2' \rangle \] and \[ \langle S_1, S_2 \rangle \], respectively, all the other matrix elements are zero.

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\section*{§ 4. Transfer matrix and exact diagonalization}

In this section we present results from analyses with the RS partition function (10) on the \( N=8 \) chain by the transfer matrix method and the exact diagonalization. Results from the conventional partition function (3) are also provided for comparison. Purposes of these analyses are twofold. One is to confirm the RS algorithm and the previous Monte Carlo results. Another is to study how systems with \( Z_{e}(n) \) and \( Z_{b}(n) \) depend on the Trotter number \( n \).
First, let us show results for the ratio of negatively weighted configurations to all configurations, \( P = Z_-/(Z_++Z_-) \), calculated by the transfer matrix method. We use the 'real-space' transfer matrix\(^6\) to realize the same boundary condition as those in other methods. In the conventional approach we calculate the product of the matrix \( T_n \), whose matrix element \((T_n)_{\alpha'\alpha} \) corresponds to \( \langle \alpha' | \exp(-\beta \hat{H}_n/n) | \alpha \rangle \). Therefore

\[
Z_n^{(n)} = \text{tr}((T_1 T_2 T_3 T_4)^n).
\]

Similarly, with \((T_{0(e)})_{\alpha'\alpha} = \langle \alpha' | \exp(-\beta \hat{H}_{0(e)}/n) | \alpha \rangle\),

\[
Z_{0(e)}^{(n)} = \text{tr}((T_e T_0)^n).
\]

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

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 (1) to the partition function \( Z' \) calculated from the modified Hamiltonian that gives absolute weights.\(^3\) The modified Hamiltonian consists of the modified partial Hamiltonians whose matrix elements are obtained by changing signatures of all positive off-diagonal elements in partial Hamiltonians \( \hat{H}_1, \hat{H}_2, \hat{H}_3 \) and \( \hat{H}_e \) (\( \hat{H}_0 \) and \( \hat{H}_e \)) in the conventional (the RS) case.

\(^*\) Small discrepancy in low temperature region might suggest that additional improvements in global flips, which are related to the ergodicity,\(^7\) are necessary.
For the $N=8$ chain it is not difficult to calculate all the energy eigenvalues $E_i$ ($i=1, \cdots, 2^n$) by the exact diagonalization. We therefore can obtain the value of the exact partition function at any temperatures by the equation

$$Z = \sum_{i=1}^{2^n} \exp(-\beta E_i).$$

The same is true for the denominator in (12),

$$Z' = \sum_{i=1}^{2^n} \exp(-\beta E'_i)$$

with the energy eigenvalues $E'_i$ for the modified Hamiltonian. We refer to the ratio $R$ calculated from (13) and (14) as $R_{bc}$. It should be noted that the value of $R_{bc}$ 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 the ground state energy of each Hamiltonian. As discussed in Ref. 3), at very low temperatures where contribution from the lowest energy eigenvalue 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 the energy of the ground state of the Hamiltonian (of the modified Hamiltonian). Existence of the severe NS problem implies $E_0 > E'_0$.

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

For the second purpose we also calculate $R$ by the transfer matrix method with several values of the Trotter number $n$. All numerical results on $R$ are summarized in Fig. 2(b). Here we would like to point out two features. One is that, as is expected, the $R_{bc}$ is much larger in the RS method than in the conventional method, especially at low temperatures. Another feature is rather unexpected one. In the RS method it turned out that the $R$'s for finite Trotter numbers, which should coincide with $R_{bc}$ in the $n \to \infty$ limit, are always larger than $R_{bc}$. In the conventional method, on the contrary, all the values of $R$ calculated by the transfer matrix method lie below $R_{bc}$. This encourages us to promote the RS method in the 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 Fig. 3, the exact values obtained by the exact diagonalization,

$$\langle E \rangle = \frac{\sum_{i=1}^{2^n} E_i \cdot e^{-\beta E_i}}{\sum_{i=1}^{2^n} e^{-\beta E_i}},$$

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

§ 5. Discussion

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

Let us comment on possible applications of the RS method to other quantum spin systems. Qualitatively the RS method will be effective for any frustrated systems where the NS problem appears. But its power to bring quantitative improvement in numerical calculations does strongly depend on system's interactions and spatial construction of clusters.

One interesting application would be to investigate quantum spin-1/2 \( XY \) chain with next-nearest-neighbor interactions. For qualitative discussion we calculate energy eigenvalues of the system on the \( N=8 \) chain by 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 the RS (the conventional) method. These results suggest that the RS method works more powerfully in 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 \( J \) chain by Nakamura and Saika. They reported that the RS method is quite useful for this system.\(^8\)

We would like to point out a very lucky case where the NS problem is completely solved, although it might be less interesting from the physical point of view. This is one-dimensional antiferromagnetic quantum spin-1/2 system with third-nearest-neighbor interactions in addition to next-nearest-neighbor one, where all couplings have the same strength.\(^*1\) A severe NS problem appears for this system in the conventional approach. When one chooses eigenstates of the nearest interaction for the nearest two spins, matrix elements of the effective Hamiltonian become quite

\(^*1\) The number of sites of this system also should be multiples of four for technical reasons.
simple so that negatively weighted configurations do not appear at all.

In two-dimensional cases systems on the triangular lattice will be the most important in application. If we employ the eigenstates for the cluster of two neighboring spins as we did in the 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 to cluster three spins, 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 the complete set which improves the NS problem will help us to gain deep insight into the ground state of the system under investigation.

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