A New Approach to Stochastic State Selections in Quantum Spin Systems

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We propose a new type of Monte Carlo approach in numerical studies of quantum systems. Introducing a probability function which determines whether a state in the vector space survives or not, we can evaluate expectation values of powers of the Hamiltonian from a small portion of the full vector space. This method is free from the negative sign problem because it is not based on importance sampling techniques. In this paper we describe our method and, in order to examine how effective it is, present numerical results on the $4 \times 4$, $6 \times 6$ and $8 \times 8$ Heisenberg spin one-half model. The results indicate that we can perform useful evaluations with limited computer resources. An attempt to estimate the lowest energy eigenvalue is also stated.

KEYWORDS: quantum spin, large size, numerical calculation, Monte Carlo, eigenvalue

1. Introduction

A great many methods have been investigated so far to numerically calculate various quantities in quantum spin systems. They are classified into two categories, the exact diagonalization\(^1\) and the Monte Carlo\(^2,3\) approaches. Both of them provide us very useful ways to study quantum spin systems but, as was repeatedly reported, the former is difficult to apply to large size systems and the latter often suffers from the negative sign problem. In this paper we introduce a new method based on the power method\(^3,4\) in order to evaluate eigenvalues of these systems. Our purpose is to show that one can effectively investigate the ground state by means of a stochastic selection of states.

The method we propose here is a kind of Monte Carlo approach, where stochastic variables play an important role. It, however, differs much from the conventional quantum Monte Carlo methods which employ random walks or importance samplings.\(^3\) In our method random variables are used to reduce the number of states of the vector space which is huge for most systems of large sizes. To this end we consider a new type of the probability function to which we refer as on-off probability function in this paper. Since it “switches off” many states in the vector space we can calculate approximate expectation values of powers of the Hamiltonian from a small number of the “on” states. Repeating this process we can obtain averaged values which are very close to the exact values. Physical quantities such as the energy eigenvalue of the system would then be estimated from these expectation values with some additional assumptions. Throughout this paper we use the
two-dimensional Heisenberg spin one-half model as a concrete example in numerical calculations.

In the next section we define the on-off probability function and explain its analytical properties. We then show, in a simple instance using the exact ground state for the $4 \times 4$ Heisenberg spin system, how we make use of this probability function when we calculate a quantity concerning to the vector space. Numerical results are presented in order to demonstrate that it nicely works. Section 3 is to describe our approach in a quantum system whose Hamiltonian is $\hat{H}$. We define random choice matrices and present a way to stochastically calculate expectation values of $\langle \psi | \hat{H}^L | \psi \rangle$ with them. Two cases of $| \psi \rangle$ which draw our interest are then discussed. One is that the state is the exact eigenstate of $\hat{H}$, $| \psi \rangle = | \psi_E \rangle$, and another is an approximate of $| \psi_E \rangle$ which we denote as $| \psi_A \rangle$. In section 4 we present our numerical results on the Heisenberg spin systems. Results on a $4 \times 4$ lattice, where it is easy to obtain $| \psi_E \rangle$, are given in detail so that we can make a close inspection of the method. Then results on the $6 \times 6$ and $8 \times 8$ lattices are presented together with the description of the state $| \psi_A \rangle$ we generated. We also show several assumptions we employed to estimate the energy eigenvalues for these lattice sizes. The values we present in this section for the $6 \times 6$ and $8 \times 8$ lattices are compatible with the ones reported in the preceding studies with different approaches.\(^5\) The final section is devoted to summary and comments.

2. On-off Probability Function

Let us introduce a probability function which is given by

$$P(\eta) = \frac{1}{a} \delta(\eta - a) + (1 - \frac{1}{a}) \delta(\eta),$$

where $a$ is a constant which is greater than or equal to 1. In this paper we refer it as the on-off probability function because the variable $\eta$ takes only two values, $a$ (on) or 0 (off), with the probability $1/a$ and $1 - 1/a$, respectively. Clearly

$$\langle \langle 1 \rangle \rangle \equiv \int P(\eta) d\eta = 1,$$

$$\langle \langle \eta \rangle \rangle \equiv \int \eta P(\eta) d\eta = 1,$$

$$\langle \langle \eta^2 \rangle \rangle \equiv \int \eta^2 P(\eta) d\eta = a,$$

where $\langle \langle \rangle \rangle$ denotes the statistical average. In order to demonstrate the role of this probability function we consider, as a simple example, the sum of absolute values of all (non-zero) coefficients in a state $| \psi \rangle = \sum_i | \psi_i \rangle | c_i \rangle (c_i \neq 0)$ of the two-dimensional Heisenberg spin model,

$$S \equiv \sum_{i=1}^{n} |c_i|,$$
and try to evaluate it by summing up less number of $|c_i|$’s. For this purpose we calculate the following sum

$$S_{\{\eta\}} \equiv \sum_{i=1}^{n} |c_i| \eta_i,$$

(6)

where $\{\eta\}$ denotes a set of random variables $\{\eta_1, \eta_2, \cdots, \eta_n\}$ generated by the following on-off probability functions

$$P_i(\eta_i) = \frac{1}{a_i} \delta(\eta_i - a_i) + (1 - \frac{1}{a_i}) \delta(\eta_i),$$

(7)
a_i being $\max(1, \epsilon/|c_i|)$ for a given constant $\epsilon$. It is easy to see that

$$\langle \langle S_{\{\eta\}} \rangle \rangle = \sum_{i=1}^{n} |c_i| \langle \langle \eta_i \rangle \rangle = S.$$

The variance of $S_{\{\eta\}}$ is given by

$$\sigma^2_S \equiv \langle \langle S_{\{\eta\}}^2 \rangle \rangle - \langle \langle S_{\{\eta\}} \rangle \rangle^2 = \sum_{|c_i|<\epsilon} (\epsilon |c_i| - |c_i|^2)$$

(8)

where $\langle \langle \eta_i \eta_j \rangle \rangle = \delta_{ij} \langle \langle \eta_i^2 \rangle \rangle + (1 - \delta_{ij}) \langle \langle \eta_i \rangle \rangle \langle \langle \eta_j \rangle \rangle = \delta_{ij} a_i + (1 - \delta_{ij})$ is used.

Let $N_i = 1(0)$ if $\eta_i \neq 0(=0)$ and $N = \sum N_i$. Then we know by $\langle \langle N \rangle \rangle$ how many non-zero $\eta_i$’s appear in (6). Since

$$P_{N_i}(N_i) = \frac{1}{a_i} \delta(N_i - 1) + (1 - \frac{1}{a_i}) \delta(N_i),$$

$$\langle \langle N_i \rangle \rangle = \int_0^\infty N_i P_{N_i}(N_i) dN_i = \frac{1}{a_i},$$

we obtain

$$\langle \langle N \rangle \rangle = \sum_{i=1}^{n} N_i = \sum_{|c_i|\geq\epsilon} 1 + \sum_{|c_i|<\epsilon} \frac{|c_i|}{\epsilon}.$$

(9)

In numerical work we substitute the average over $n_{\text{smpl}}$ randomly generated $\{\eta\}$’s for the statistical average $\langle \langle \cdots \rangle \rangle$, namely we measure

$$\langle \langle S_{\{\eta\}} \rangle \rangle_{\text{smpl}} \equiv \frac{1}{n_{\text{smpl}}} \sum_{k=1}^{n_{\text{smpl}}} S_{\{\eta\}_k},$$

(10)

where $\{\eta\}_k$ denotes the $k$-th set of the generated random variables $\{\eta\} = \{\eta_1, \eta_2, \cdots, \eta_n\}$. The variance is then given by

$$\rho^2_S \equiv \langle \langle S_{\{\eta\}}^2 \rangle \rangle_{\text{smpl}} - \langle \langle S_{\{\eta\}} \rangle \rangle_{\text{smpl}}^2.$$

(11)

As the statistical error we employ

$$Er \equiv 2 \sqrt{\frac{\rho^2_S}{n_{\text{smpl}}}}.$$

(12)
Note that, according to the Chebyshev inequality in statistics,

$$\langle \langle S_\{\eta\} \rangle \rangle_{\text{smpl}} - Er \leq \langle \langle S_\{\eta\} \rangle \rangle \leq \langle \langle S_\{\eta\} \rangle \rangle_{\text{smpl}} + Er$$

in 75% confidence level provided that $\sigma^2_S$ can be replaced by $\rho^2_S$. 6)

The results for the exact ground state of the $4 \times 4$ Heisenberg spin model, which has 12870 non-zero coefficients, are shown in Table I. In this case it is straightforward to calculate $S(= \langle \langle S_\{\eta\} \rangle \rangle)$, $\sigma^2_S$ and $\langle \langle N \rangle \rangle$ from (5), (8) and (9) since we know all $c_i$ of the state. In Table I we see that $\langle \langle S_\{\eta\} \rangle \rangle_{\text{smpl}}$, $\rho^2_S$ and $\langle \langle N \rangle \rangle_{\text{smpl}}$ calculated with $n_{\text{smpl}} = 10^4$ are in good agreement with them. We also see that $\epsilon = 0.2$ is enough to estimate $S$ in the precision of 0.1%. In other words we can estimate $S$ in the precision of 0.1% from only 367 of 12870 non-zero coefficients of the state.

3. Powers of Hamiltonian

In this section we discuss on the expectation values of the $L$-th power of the Hamiltonian $\hat{H}$. First we make a brief comment on the power method to evaluate the maximum eigenvalue of $\hat{H}$. Suppose the eigenstates of $\hat{H}$ are $|\psi_i\rangle$, $\hat{H}|\psi_i\rangle = |\psi_i\rangle E_i$ ($i = 0, \cdots, N_V - 1$) where $N_V$ is the size of the full vector space, and $|E_0\rangle > |E_i\rangle$ for $i > 0$. In the power method one repeatedly operates $\hat{H}$ to a trial state $|\psi\rangle$, which is expressed as

$$|\psi\rangle = \sum_{i=0}^{N_V-1} |\psi_i\rangle b_i,$$

so that one obtains for sufficiently large $L$

$$\hat{H}^L |\psi\rangle = \sum_{i=0}^{N_V-1} |\psi_i\rangle b_i E_i^L \sim |\psi_0\rangle b_0 E_0^L$$

and

$$\langle \psi | \hat{H}^L | \psi \rangle \sim b_0^2 E_0^L.$$ (15)

Note that from the expectation values $\langle \psi | \hat{H}^L | \psi \rangle$ one can acquire information relative to the energy eigenvalue. For large size systems, however, it soon becomes impracticable to calculate $\hat{H}^L |\psi\rangle$ or $\langle \psi | \hat{H}^L | \psi \rangle$ because one can not keep the huge number of coefficients for $\hat{H}^L |\psi\rangle$ in the full vector space. One therefore has to do with truncated vector spaces.

Now we describe our formulation. Let us start with a state

$$|\psi\rangle = \sum_{i=1}^{N_V} |i\rangle c_i,$$ (16)

where $\{|i\rangle\}$ denotes an arbitrary basis of the full vector space. In our method we stochastically find a limited vector space where we can calculate the expectation values $E(L) \equiv \langle \psi | \hat{H}^L | \psi \rangle$ for
large $L$. For this purpose we introduce an $N_V \times N_V$ diagonal matrix $M_{\{\eta\}}$, which we call random choice matrix hereafter,

$$M_{\{\eta\}} = \begin{pmatrix}
\eta_1 & 0 & \cdots & 0 \\
0 & \eta_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \eta_{N_V}
\end{pmatrix}, \quad (17)$$

with random variables $\eta_i$ determined according to (7). When $c_i = 0$ we employ $\epsilon/\delta$ as $a_i$ in (7), where the parameter $\delta(< \epsilon)$ is a positive constant independent of $i$.

Using independent random choice matrices $M_{\{\eta(m)\}} = \text{diag.}\{\eta_1^{(m)}, \eta_2^{(m)}, \ldots, \eta_{N_V}^{(m)}\}$ ($m = 1, 2, \cdots, L + 1$) we define

$$E_{\{\eta\}}(L) = \langle \psi | M_{\{\eta(L+1)\}} \hat{H} M_{\{\eta(L)\}} \hat{H} M_{\{\eta(L-1)\}} \cdots \hat{H} M_{\{\eta(1)\}} | \psi \rangle. \quad (18)$$

Here we use the coefficient $c_i$ of the initial wave function $| \psi \rangle$ in the on-off probability function (7) for any $m$. In order to explain the essential point of the method in numerical studies, let $n_b(m)$ and $n_a(m)$ the number of non-zero components of the state $\hat{H} M_{\{\eta(m-1)\}} \cdots \hat{H} M_{\{\eta(1)\}} | \psi \rangle$ and $M_{\{\eta(m)\}} \hat{H} M_{\{\eta(m-1)\}} \cdots \hat{H} M_{\{\eta(1)\}} | \psi \rangle$, respectively. We first keep $n_b(1)$ non-zero components of $| \psi \rangle$. Then we operate $M_{\{\eta(1)\}}$ to $| \psi \rangle$. Since many of the random variables $\eta_i^{(1)}$ ($i = 1, 2, \cdots, N_V$) are zero, the state $M_{\{\eta(1)\}} | \psi \rangle$ has much less non-zero components (i.e. $n_a(1) \ll n_b(1)$). The number of non-zero components increases when we next operate $\hat{H}$ to $M_{\{\eta(1)\}} | \psi \rangle$ ($n_b(2) > n_a(1)$), but it drastically decreases after operating $M_{\{\eta(2)\}}$ to the state ($n_a(2) \ll n_b(2)$). Choosing the parameter $\epsilon$ in the on-off probability functions we can repeat the operation up to $L$ within the range of our computer facilities.

From (18) we are led to, with $h_{ij} = \langle i | \hat{H} | j \rangle$,

$$\langle E_{\{\eta\}}(L) \rangle = \sum_i \sum_j \cdots \sum_k \sum_l c_i \eta_i^{(1)} h_{ij}^{(2)} \cdots h_{kl}^{(L)} \eta_k \eta_l^{(L+1)} c_l = \sum_i \sum_j \cdots \sum_k \sum_l c_i h_{ij} \cdots h_{kl} c_l \langle \eta_i^{(1)} \eta_j^{(2)} \cdots \eta_k^{(L)} \eta_l^{(L+1)} \rangle \quad (19)$$

because $\langle \eta_i^{(1)} \eta_j^{(2)} \cdots \eta_k^{(L)} \eta_l^{(L+1)} \rangle = \langle \eta_i^{(1)} \rangle \langle \eta_j^{(2)} \rangle \cdots \langle \eta_k^{(L)} \rangle \langle \eta_l^{(L+1)} \rangle = 1$, which is guaranteed by the fact that $\eta_i^{(m)}$ and $\eta_j^{(m')} \neq m'$. Henceforth we abbreviate $\langle \eta_i^{(m)} \rangle$ and $\langle [\eta_i^{(m)}]^2 \rangle$ as $\langle \eta_i \rangle$ and $\langle \eta_i^2 \rangle$ because they do not depend on $m$. It should be noted that the variances of $\eta_i^{(m)}$ are the same for all $m$.

The variance of $E_{\{\eta\}}(L)$ is
\[
\sigma_{\eta}(L)^2 \equiv \langle \langle E_{\eta}(L)^2 \rangle \rangle - \langle \langle E_{\eta}(L) \rangle \rangle^2
\]
\[
= \sum_{i,j,j'} \sum_{k,k'} \sum_{l,l'} c_i h_{ij} \cdots h_{k,l} c_l \cdot c_{i'} h_{i'j'} \cdots h_{k',l'} c_{l'}
\times \langle \langle \eta_i^{(1)} \eta_i^{(2)} \rangle \rangle \cdots \langle \langle \eta_k^{(1)} \eta_k^{(2)} \rangle \rangle \cdots \langle \langle \eta_k^{(L)} \eta_k^{(L)} \rangle \rangle - E(L)^2
\]
\[
= \sum_{i,j,j'} \sum_{k,k'} \sum_{l,l'} c_i h_{ij} \cdots h_{k,l} c_l \cdot \{1 + \delta_{ii'}( \langle \langle \eta_i^{2} \rangle \rangle - 1)\}
\times \{1 + \delta_{jj'}( \langle \langle \eta_j^{2} \rangle \rangle - 1)\}
\times \{1 + \delta_{kk'}( \langle \langle \eta_k^{2} \rangle \rangle - 1)\}
\times \{1 + \delta_{ll'}( \langle \langle \eta_l^{2} \rangle \rangle - 1)\}
\]
\[
- E(L)^2, \tag{20}
\]

where we use \( \langle \langle \eta_i^{(m)} \eta_i^{(m)} \rangle \rangle = (1 - \delta_{ii'}) \langle \langle \eta_i \rangle \rangle \langle \langle \eta_i \rangle \rangle + \delta_{ii'} \langle \langle \eta_i^{2} \rangle \rangle = 1 + \delta_{ii'}( \langle \langle \eta_i^{2} \rangle \rangle - 1) \).

Let us add a few expressions which are useful to check our numerical values presented in the next section. They are obtained from (19) and (20) when the state \( | \psi \rangle \) is an exact eigenstate \( | \psi_E \rangle = \sum | \psi_i \rangle f_i (f_i \neq 0) \) of \( \hat{H} \), namely when \( \hat{H}| \psi_E \rangle = | \psi_E \rangle E \) or \( \sum_j h_{ij} f_j = E f_i \).

\[
\langle \langle E_{\eta}(L) \rangle \rangle = E_E(L) = E_L, \tag{21}
\]
\[
\sigma_{E_{\eta}}(1) = 2E^2 \sum_i f_i^4 (\langle \langle \eta_i^{2} \rangle \rangle - 1)
\]
\[
+ \sum_{i,j} f_i^2 f_j^2 (h_{ij})^2 (\langle \langle \eta_i^{2} \rangle \rangle - 1)(\langle \langle \eta_j^{2} \rangle \rangle - 1), \tag{22}
\]
\[
\sigma_{E_{\eta}}(2) = 3E^4 \sum_i f_i^4 (\langle \langle \eta_i^{2} \rangle \rangle - 1)
\]
\[
+ 2E^2 \sum_{i,j} f_i^2 f_j^2 (h_{ij})^2 (\langle \langle \eta_i^{2} \rangle \rangle - 1)(\langle \langle \eta_j^{2} \rangle \rangle - 1)
\]
\[
+ \sum_{i,k} f_i^2 f_k^2 (h_{ik})^2 (\langle \langle \eta_i^{2} \rangle \rangle - 1)(\langle \langle \eta_k^{2} \rangle \rangle - 1)
\]
\[
+ \sum_{i,j,k} f_i^2 f_k^2 (h_{ij})(h_{jk})^2 (\langle \langle \eta_i^{2} \rangle \rangle - 1)(\langle \langle \eta_j^{2} \rangle \rangle - 1)(\langle \langle \eta_k^{2} \rangle \rangle - 1), \tag{23}
\]

where we added the suffix \( E \) to clearly show that the quantities are for an exact eigenstate. Note that we can analytically evaluate them using \( \langle \langle \eta_i^{2} \rangle \rangle = a_i = \epsilon / | f_i | \).

In numerical study we first consider the case \( | \psi \rangle = | \psi_E \rangle \) on a small lattice, and then proceed to the case that the state is an approximate one denoted by \( | \psi_A \rangle \). In both cases we measure \( \langle \langle E_{\eta}(L) \rangle \rangle_{\text{smpl}} \) and \( \rho^2_{\eta}(L) \) from \( n_{\text{smpl}} \) samples in the same manner as (10) and (11) in the previous section, namely,

\[
\langle \langle E_{\eta}(L) \rangle \rangle_{\text{smpl}} \equiv \frac{1}{n_{\text{smpl}}} \sum_{k=1}^{n_{\text{smpl}}} E_{\eta,k}(L), \tag{24}
\]
\[
\rho^2_{\eta}(L) \equiv \langle \langle [E_{\eta}(L)]^2 \rangle \rangle_{\text{smpl}} - \langle \langle E_{\eta}(L) \rangle \rangle^2_{\text{smpl}}. \tag{25}
\]
The error of $E_{(\eta)}(L)$ is evaluated by

$$Er(L) = 2\sqrt{\frac{\rho_{(\eta)}^2(L)}{n_{\text{smpl}}}}.$$ (26)

4. Numerical Results

In this section we report our results for the two-dimensional Heisenberg spin model. The state on each site is represented by a $z$ component of the spin. Let us first concentrate on the case of $4 \times 4$ lattice. This lattice size is suitable for making a careful examination of the method because we can start with the exact ground eigenstate $|\psi_E\rangle$ and its eigenvalue $E$. Table II (III) shows the $L = 1$ ($L = 2$) results on $\langle E_{(\eta)}(L) \rangle_{\text{smpl}}$ obtained with $10^4$ samples for various values of $\epsilon$. Values of $\sigma_{E_{(\eta)}}^2(L)$ calculated from (22) or (23) are also presented in the table. We see that $\sigma_{E_{(\eta)}}^2(L)$ and $\rho_{E_{(\eta)}}^2(L)$ are in good agreement. We also see that the exact value $E = -11.2285$ lies in the range $\langle E_{(\eta)}(L) \rangle_{\text{smpl}} \pm Er(1)$ except for $\epsilon = 0.05$, while $\langle E_{(\eta)}(L) \rangle_{\text{smpl}} - E^2 | < Er(2)$ for all values of $\epsilon$. In Table IV we present $\langle E_{(\eta)}(L) \rangle_{\text{smpl}}$ up to $L = 10$ fixing $\epsilon = 0.1$ or $\epsilon = 0.01$. We observe that the error increases as $L$ does, but its dependence on $L$ is weak. The relative error for $\epsilon = 0.1$ ranges from $0.11\% (L = 1)$ to $0.48\% (L = 10)$ while for $\epsilon = 0.01$ it is between $0.006\% (L = 1)$ and $0.015\% (L = 10)$. Note that $Er(L)$ decreases for smaller values of $\epsilon$, which however costs more computer resources. Figure 1 plots distributions of $E_{E_{(\eta)}k}(L)$ ($L = 1, 2, 3, 5, 10$), which shows the deviation from the exact $\delta$ function. The abscissa is 50 times of the ratio of each $E_{E_{(\eta)}k}(L)$ ($k = 1, 2, \cdots, n_{\text{smpl}}$) to $E_E(L)$. For small values of $L$ we see that the distribution is symmetric about the exact value $E^L$ and the peak is high. For large $L$, on the other hand, the peak becomes lower and the asymmetry grows; the data localize in the region where $E_{E_{(\eta)}k}(L) < E^L$ and the distribution has a long tail toward large value of $E_{E_{(\eta)}k}(L)$. These features should be taken into account in the process of the error estimation.

How about the number of states that appear in the calculation? We measure $\langle N \rangle_{\text{smpl}}$ before and after we operate $M_{(\eta)\{L\}}$ to the state $\hat{H}M_{\{\eta\}(L-1)} \cdots \hat{H}M_{\{\eta\}(1)} |\psi_E\rangle$, which we denote $\langle N^E_{b}(L) \rangle_{\text{smpl}}$ and $\langle N^E_{a}(L) \rangle_{\text{smpl}}$, respectively. Table V shows the results up to $L = 10$. For $\epsilon = 0.1$, we observe that $\langle N^E_{a}(L) \rangle_{\text{smpl}} \ll \langle N^E_{b}(L) \rangle_{\text{smpl}}$ for each $L$ and $\langle N^E_{a}(L) \rangle_{\text{smpl}}$ shrinks to almost a half of the whole vector space. This observation proves the merit of using the random choice matrices. When we set $\epsilon = 0.01$, however, the results are not so appealing because we have to deal with almost all states of the vector space every time we operate $\hat{H}$. We also see in the table that, as $L$ grows, $\langle N^E_{a}(L) \rangle_{\text{smpl}}$ converges to a constant which depends on the value of $\epsilon$.

Let us show the results on the approximate state then. Here we employ $|\psi_A\rangle = C_N \sum_{|f_i| \geq c} |i\rangle f_i$ for a small constant $c$, where $C_N$ is the normalization factor. In other words we abandon the coefficient $f_i$ of the exact eigenstate $|\psi_E\rangle$ if $|f_i| < c$. For $c = 5 \times 10^{-3}$ the number of non-zero component of $|\psi_A\rangle$ is 5382 and we obtain $\langle \psi_A | \hat{H} | \psi_A \rangle = -10.7445$, which should be compared to
\[ \langle \psi_E | \hat{H} | \psi_E \rangle = -11.2285. \] Using this \(| \psi_A \rangle\) we measure \( \langle E_{A(\eta)}(L) \rangle_{\text{smpl}}, \rho_{A(\eta)}^2(L), \langle N^A_{b}(L) \rangle_{\text{smpl}} \) and \( \langle N^A_{a}(L) \rangle_{\text{smpl}} \) up to \( L = 10 \) with \( n_{\text{smpl}} = 10^4 \) and compare them to exactly calculated \( \langle \psi_A | \hat{H}^L | \psi_A \rangle \). Errors of \( E_{A(\eta)}(L) \)'s are evaluated by \( 2\sqrt{\rho_{A(\eta)}^2(L)/n_{\text{smpl}}} \). Table VI and Fig. 2 show the results with \( \delta = 0.01 \). In Table VI we see a good agreement between \( \langle E_{A(\eta)}(L) \rangle_{\text{smpl}} \) and \( \langle \psi_A | \hat{H}^L | \psi_A \rangle \) for all \( L \). We also see in Fig. 2 that for each \( L \) the shape of the distribution of \( E_{A(\eta)}(L) \) is similar to that of \( E_{E(\eta)}(L) \) in Fig. 1 although the peak is slightly lower and the asymmetry is more outstanding. It should be noted that, as is expected, for larger \( L \) we obtain better evaluation for the true value \( E_0 \). In Table VI for example, we see \( E_A(1) = -10.7445 > -\sqrt{\langle E_A(10) \rangle_{\text{smpl}}} = -11.1505 > E_0 = -11.2285. \)

Finally we report our results on lattices larger than \( 4 \times 4 \). Here we use

\[ E_{(\eta)}(L) = \langle \psi | \hat{H} M_{(\eta)^{1}\ldots(\tau)} \ldots \hat{H} M_{(\eta)^{(1)}} | \psi \rangle. \] (27)

instead of (18) in order to decrease the statistical errors.

In order to apply our method to large systems we have to obtain \(| \psi_A \rangle\) without knowing what the exact eigenstate \(| \psi_E \rangle\) is. Among several attempts we made, we took the following procedure which is based on the Suzuki-Trotter formula.

(a) Choose one trial state \(| \psi_{\text{tr}} \rangle\).
(b) Operate \( \exp(-\Delta \hat{H}_1) \cdot \exp(-\Delta \hat{H}_2) \) to \(| \psi_{\text{tr}} \rangle\), where \( \hat{H}_1 + \hat{H}_2 = \hat{H} \) and \( \Delta = 0.4 \).
(c) Abandon the small coefficients in \( \exp(-\Delta \hat{H}_1) \cdot \exp(-\Delta \hat{H}_2) | \psi_{\text{tr}} \rangle \) if necessary so that the number of non-zero components of the state is within the limit of our computers.

For the \( 6 \times 6 \) square lattice the number of non-zero components of the \(| \psi_A \rangle\) thus obtained is \( O(10^6) \) with the minimum absolute value of the non-zero coefficients \(| c_{\text{min}} | = 1.14 \times 10^{-4} \).

Then we apply the on-off probability method setting \( \epsilon = 0.0057 \) and \( \delta = | c_{\text{min}} | \). Table VII shows values of \( \langle E_{A(\eta)}(L) \rangle_{\text{smpl}}, \langle N^A_{b}(L) \rangle_{\text{smpl}} \) and \( \langle N^A_{a}(L) \rangle_{\text{smpl}} \) up to \( L = 5 \) with \( 5.5 \times 10^3 \) samples. The memory we need here is 356 MBytes including the hash table and the CPU time consumed to one sample is 1100 seconds by a Pentium III machine.

Now we have obtained reliable estimations of \( E_A(L) = \langle \psi_A | \hat{H}^L | \psi_A \rangle \) \((L = 1, 2, \ldots, 5)\). How can we estimate physical quantities, \( E_0 \) for instance, using them? We see that \( \sqrt{\langle E_{A(\eta)}(5) \rangle_{\text{smpl}}} = -23.68683 \pm 0.00083 \) is lower than \( E_A(1) = -23.56093 \). But, because \( L \) is not large enough, even \( \sqrt{\langle E_{A(\eta)}(5) \rangle_{\text{smpl}}} \) provides only a poor upper bound for the true value \( E_0 = -24.4394 \) which is obtained in ref. (5) by the exact diagonalization. One better way for the estimation would be to calculate the lowest eigenvalue \( E \) starting from the basis \(| | \psi_A \rangle, \hat{H} | \psi_A \rangle, \hat{H}^2 | \psi_A \rangle \). It is easy to obtain the orthonormalized basis \(| | \psi_0 \rangle, | \psi_1 \rangle, | \psi_2 \rangle \) from \(| | \psi_A \rangle, \hat{H} | \psi_A \rangle, \hat{H}^2 | \psi_A \rangle \) and to calculate the Hamiltonian matrix elements which are the functions of \( E_A(L) \) \((L \leq 5)\). It, however, turned out to be ineffective too; the obtained value is \( E = -23.88 \), which is still too far from \( E_0 \). So we need additional assumptions to make a better estimate of the eigenvalue. Here, based on the
low energy property described by the linear spin wave theory or more sophisticated models,\(^7\) we empirically assume

\[
\langle \psi_A | \hat{H}^L | \psi_A \rangle = q_0 E^L + q_1 \int_0^1 (x E)^L \cdot x^\alpha dx
\]

\[
= E^L (q_0 + \frac{q_1}{L + \alpha + 1}) \equiv F(L, E, q_0, q_1, \alpha)
\]

where \(q_0, q_1\) and \(\alpha\) are free parameters which should be determined together with \(E\) by the fit. Note that \(q_0 + q_1/(\alpha + 1) = 1\) should hold due to the normalization of \(|\psi_A\rangle\). We look for the minimum of the difference \(D\) with \(L_{\text{max}} = 5\),

\[
D \equiv \sum_{L=1}^{L_{\text{max}}} \left[ 1 - \frac{\langle \langle E_A(\eta)(L) \rangle \rangle_{\text{smpl}}}{F(L, E, q_0, q_1, \alpha)} \right]^2,
\]

changing these four parameters and accept them if \(| q_0 + q_1/(\alpha + 1) - 1 | \leq 0.003\) is fulfilled and \(D\) is less than the sum of the relative errors, which amounts

\[
\sum_{L=1}^{L_{\text{max}}} \left[ \frac{\text{Er}(L)}{\langle \langle E_A(\eta)(L) \rangle \rangle_{\text{smpl}}} \right]^2 = 8.5 \times 10^{-9}.
\]

By this fit we obtain \(-24.32 \leq E \leq -24.13\), which indicates that the evaluation is useful.

It is possible to advance to \(8 \times 8\) lattice in the same manner, where the number of non-zero components of \(|\psi_A\rangle\) is \(O(10^7)\) and \(|c|_{\text{min}} = 3.28 \times 10^{-5}\). The results with \(n_{\text{smpl}} = 1.1 \times 10^3\), \(\epsilon = 0.01\) and \(\delta = |c|_{\text{min}}\) are shown in Table VIII. Note that \(\sqrt{\langle \langle E_A(\eta)(5) \rangle \rangle_{\text{smpl}}} = -41.03348 \pm 0.03817\) is lower than \(E_A(1) = -40.74998\). By the fitting using (28) we obtain an estimation \(-43.5 \leq E \leq -41.1\), which includes \(-43.103\), the value also reported in ref.(5). It is large sample errors, which would be improved by increasing \(n_{\text{smpl}}\), that cause the wide range of the evaluated \(E\) here.

5. Summary and Comments

In this paper we have suggested an alternative Monte Carlo approach which, using the stochastic variables following the on-off probability function, does not rely on random walks nor importance samplings. Our purpose is to show the way to study large size systems without keeping the full vector space. We apply this method to the two-dimensional Heisenberg spin one-half model, which was chosen as a familiar example, and carry out numerical evaluations for lattices up to \(8 \times 8\). The results show that we can obtain reliable numerical data on expectation values of the power of its Hamiltonian with reasonable computer resources.

A few remarks are in order.

One merit of this method is that it enables us to numerically evaluate expectation values in various quantum systems using relatively small portion of the whole vector space, which therefore enlarge the size of the systems we study. Another merit is that the method can be applied to
systems which have negative sign problem. Actually a work on the Shastry-Sutherland model\textsuperscript{8,9)} near the critical point as well as on the quantum spin model on a triangular lattice is in progress.\textsuperscript{10)

More studies should be necessary on two issues of the method. One of them is how one can effectively generate the approximate state $|\psi_A\rangle$. Although we can improve our estimation by increasing the number of samples $n_{\text{smpl}}$, it is desirable, in order to perform efficient estimations, to employ a good $|\psi_A\rangle$ for the following reasons. One reason is that with the better $|\psi_A\rangle$ the sample error will be smaller. Another reason is that with the better $|\psi_A\rangle$ the smaller $L$ will be enough to obtain reliable estimates. In addition to the very empirical way we adopted to obtain $|\psi_A\rangle$ in this paper, a systematic way which makes use of the Lanczos method in small vector spaces are under investigation. There we start with a trial state $|\psi_{\text{trl}}\rangle$, calculate the matrix elements of the Hamiltonian $\hat{H}$, diagonalize the matrix and define $|\psi_A\rangle$ as its lowest energy eigenstate. The basis for the matrix elements is \{ $|\psi_{\text{trl}}\rangle, \hat{H} |\psi_{\text{trl}}\rangle, \hat{H}^2 |\psi_{\text{trl}}\rangle, \cdots, \hat{H}^p |\psi_{\text{trl}}\rangle$\} with a small value of $p$, which we numerically calculate without any approximation. Another important problem is to find a sophisticated way to extract physical quantities from the expectation values. The results of several fits we tried seem to suggest there are some shortages in our simple assumptions. Both of the issues, which might be largely model-dependent, should be investigated in the future work.

The on-off probability method could be applied to any problem which is mathematically related with the Markov process. In the Markov process, which can be described by repeated operation of a probability matrix $M_p$ to an initial state $\mathbf{v}$, rapid increase of states would occur. If we can replace $(M_p)^L \mathbf{v}$ with $M_{\eta^{(L)}} M_p \cdots M_{\eta^{(1)}} M_p \mathbf{v}$ the number of states we should consider becomes much smaller. We hope our method is helpful in many fields of science.

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10) It holds for any probability function. If the probability function is Gaussian the confidence level rises to 95.4 %.
| $\epsilon$ | $\langle S_{\eta} \rangle_{\text{smpl}}$ | $\sigma_S^2$ | $\rho_S^2$ | $\langle N \rangle$ | $\langle N \rangle_{\text{smpl}}$ |
|---|---|---|---|---|---|
| 0.3 | 73.572±0.091 | 21.07 | 20.81 | 245.24 | 245.3 |
| 0.2 | 73.582±0.073 | 13.76 | 13.62 | 366.99 | 367.0 |
| 0.1 | 73.558±0.050 | 6.46 | 6.34 | 731.97 | 731.8 |
| 0.05 | 73.591±0.033 | 2.84 | 2.77 | 1451.72 | 1452.1 |

Table I. Results on $S = \sum |c_i|$ calculated by the on-off probability method, where $c_i$ denotes the coefficient of state $|i\rangle$ for the exact ground state of the $4 \times 4$ Heisenberg quantum spin system. The number of samples, $n_{\text{smpl}}$, is $10^4$. The exact value of $S$ is 73.57224. The values of $\sigma_S^2$ and $\langle N \rangle$ calculated by (8) and (9) are also shown in the table.
| $\epsilon$ | $\langle \langle E_{E}\rangle(1) \rangle_{\text{smpl}}$ | $\sigma_{E_{E}}^{2}(1)$ | $\rho_{E_{E}}^{2}(1)$ |
|---|---|---|---|
| 0.20 | $-11.2128 \pm 0.0215$ | 1.1703 | 1.168 |
| 0.15 | $-11.2198 \pm 0.0170$ | 0.7345 | 0.738 |
| 0.10 | $-11.2285 \pm 0.0122$ | 0.3606 | 0.374 |
| 0.08 | $-11.2212 \pm 0.0095$ | 0.2283 | 0.228 |
| 0.05 | $-11.2230 \pm 0.0052$ | 0.07338 | 0.0719 |
| 0.03 | $-11.2288 \pm 0.0033$ | 0.02731 | 0.0274 |
| 0.02 | $-11.2266 \pm 0.0021$ | 0.01037 | 0.0106 |
| 0.01 | $-11.2283 \pm 0.0007$ | 0.00120 | 0.0012 |

Table II. Results on $E_{E}(1) = \langle \psi_{E} | \hat{H} | \psi_{E} \rangle$ obtained for the $4 \times 4$ Heisenberg quantum spin system by the on-off probability method with $n_{\text{smpl}} = 10^{4}$, where $| \psi_{E} \rangle$ is the exact eigenstate of the system. The exact value is $E = -11.2285$. 
| $\epsilon$ | $\langle E_{E(\eta)}(2) \rangle_{\text{smpl}}$ | $\sigma^2_{E_{E(\eta)}(2)}$ | $\nu^2_{E_{E(\eta)}(2)}$ |
|---------|---------------------------------|----------------|----------------|
| 0.20    | 126.200±0.344                   | 297.23         | 296.2          |
| 0.15    | 126.006±0.262                   | 170.68         | 171.8          |
| 0.10    | 125.988±0.175                   | 77.04          | 76.7           |
| 0.08    | 126.006±0.138                   | 47.40          | 48.2           |
| 0.05    | 126.062±0.013                   | 14.78          | 14.9           |
| 0.03    | 126.088±0.046                   | 5.332          | 5.30           |
| 0.02    | 126.079±0.028                   | 1.997          | 2.01           |
| 0.01    | 126.071±0.009                   | 0.228          | 0.23           |

Table III. Results on $E_{E}(2) = \langle \psi_{E} | \hat{H}^2 | \psi_{E} \rangle$ obtained for the $4 \times 4$ Heisenberg quantum spin system by the on-off probability method with $n_{\text{smpl}} = 10^4$. The exact value is $E^2 = 126.0788$. 
Table IV. Results on $E_E(L) = \langle \psi_E | \hat{H}_L | \psi_E \rangle$ ($L = 1, 2, \cdots, 10$) obtained for the $4 \times 4$ Heisenberg quantum spin system by the on-off probability method with $10^4$ samples. We present the data for $\epsilon = 0.1$ and $\epsilon = 0.01$ together with the exact values of $E_E(L)$.

| $L$ | $E_E(L)$ | $\epsilon = 0.1$ | $\langle E_{E(\eta)}(L) \rangle_{\text{smpl}}$ | $\epsilon = 0.01$ |
|-----|----------|------------------|-----------------------------|------------------|
| 1   | $-0.112285 \times 10^2$ | $-(0.11228 \pm 0.00012) \times 10^2$ | $-(0.112284 \pm 0.00007) \times 10^2$ |
| 2   | $0.126079 \times 10^3$ | $(0.12599 \pm 0.00017) \times 10^3$ | $(0.126078 \pm 0.00009) \times 10^3$ |
| 3   | $-0.141567 \times 10^4$ | $-(0.14163 \pm 0.00023) \times 10^4$ | $-(0.141567 \pm 0.000012) \times 10^4$ |
| 4   | $0.158959 \times 10^5$ | $(0.15900 \pm 0.00031) \times 10^5$ | $(0.158952 \pm 0.000016) \times 10^5$ |
| 5   | $-0.178486 \times 10^6$ | $-(0.17846 \pm 0.00040) \times 10^6$ | $-(0.178481 \pm 0.000020) \times 10^6$ |
| 6   | $0.200413 \times 10^7$ | $(0.20023 \pm 0.00051) \times 10^7$ | $(0.200408 \pm 0.000023) \times 10^7$ |
| 7   | $-0.225034 \times 10^8$ | $-(0.22498 \pm 0.00067) \times 10^8$ | $-(0.225029 \pm 0.000028) \times 10^8$ |
| 8   | $0.252679 \times 10^9$ | $(0.25218 \pm 0.00081) \times 10^9$ | $(0.252684 \pm 0.000034) \times 10^9$ |
| 9   | $-0.283720 \times 10^{10}$ | $-(0.2835 \pm 0.0010) \times 10^{10}$ | $-(0.283715 \pm 0.000040) \times 10^{10}$ |
| 10  | $0.318574 \times 10^{11}$ | $(0.3182 \pm 0.0015) \times 10^{11}$ | $(0.318591 \pm 0.000047) \times 10^{11}$ |
Table V. Numbers of non-zero coefficients before and after operating the random choice matrix $M_{\{\eta^{(L)}\}}$ to the state $\hat{H}M_{\{\eta^{(L-1)}\}} \cdots \hat{H}M_{\{\eta^{(1)}\}}|\psi_E\rangle$, where $\hat{H}$ and $|\psi_E\rangle$ denote the Hamiltonian and the exact ground state of the $4 \times 4$ Heisenberg quantum spin system, respectively. The number of samples is $10^4$. 

| $L$ | $\langle N_b^E(L) \rangle_{\text{smpl}}$ | $\langle N_a^E(L) \rangle_{\text{smpl}}$ | $\langle N_b^E(L) \rangle_{\text{smpl}}$ | $\langle N_a^E(L) \rangle_{\text{smpl}}$ |
|-----|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 1   | 12870                           | 731.7                           | 12870                           | 6249.41                         |
| 2   | 7959.5                          | 564.7                           | 12797.06                        | 6242.70                         |
| 3   | 6664.4                          | 515.6                           | 12796.22                        | 6242.22                         |
| 4   | 6238.6                          | 498.5                           | 12796.22                        | 6242.85                         |
| 5   | 6083.2                          | 491.9                           | 12796.34                        | 6242.79                         |
| 6   | 6022.0                          | 488.9                           | 12796.25                        | 6243.20                         |
| 7   | 5995.0                          | 487.9                           | 12796.27                        | 6242.38                         |
| 8   | 5985.5                          | 487.3                           | 12795.97                        | 6243.45                         |
| 9   | 5981.4                          | 487.2                           | 12796.42                        | 6242.71                         |
| 10  | 5980.1                          | 487.5                           | 12796.21                        | 6243.33                         |

$\epsilon = 0.1$ and $\epsilon = 0.01$. 

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Table VI. Results on \( E_A(L) \equiv \langle \psi_A | H^L | \psi_A \rangle \) for the 4\( \times 4 \) system obtained from \( 10^4 \) samples with \( \epsilon = 0.1 \) and \( \delta = 0.01 \). We also present the exact values of \( E_A(L) \) in the second column for comparison.

| \( L \) | \( E_A(L) \) | \( \langle\langle E_{A[n]}(L)\rangle\rangle_{\text{smpl}} \) | \( \langle\langle N_{A}^L(L)\rangle\rangle_{\text{smpl}} \) | \( \langle\langle N_{A}^L(L)\rangle\rangle_{\text{smpl}} \) |
|---|---|---|---|---|
| 1 | \(-0.107445 \times 10^2\) | \(-0.10750 \pm 0.00012 \times 10^2\) | 5382.0 | 540.97 |
| 2 | \(0.119302 \times 10^3\) | \((0.11937 \pm 0.00017) \times 10^3\) | 6342.2 | 466.83 |
| 3 | \(-0.133162 \times 10^4\) | \(-0.13327 \pm 0.00025 \times 10^4\) | 5739.5 | 445.39 |
| 4 | \(0.149066 \times 10^5\) | \((0.14936 \pm 0.00038) \times 10^5\) | 5550.9 | 438.58 |
| 5 | \(-0.167056 \times 10^6\) | \(-0.16720 \pm 0.00062 \times 10^6\) | 5488.3 | 436.49 |
| 6 | \(0.187354 \times 10^7\) | \((0.1876 \pm 0.0012) \times 10^7\) | 5468.6 | 435.69 |
| 7 | \(-0.210193 \times 10^8\) | \(-0.2121 \pm 0.0028 \times 10^8\) | 5462.0 | 435.78 |
| 8 | \(0.235870 \times 10^9\) | \((0.2368 \pm 0.0034) \times 10^9\) | 5461.7 | 435.47 |
| 9 | \(-0.264725 \times 10^{10}\) | \(-0.2647 \pm 0.0033 \times 10^{10}\) | 5459.3 | 435.24 |
| 10 | \(0.297136 \times 10^{11}\) | \((0.2958 \pm 0.0049) \times 10^{11}\) | 5456.6 | 435.58 |
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Table VII. Results on $E_A(L)$ for the $6 \times 6$ system obtained from $5.5 \times 10^3$ samples with $\varepsilon = 0.0057$. The exact value of $E_A(1) = \langle \psi_A | \hat{H} | \psi_A \rangle$ is calculated to be $-23.56093$.

| $L$ | $\langle E_{A[\eta]}(L) \rangle_{\text{smpl}}$ | $\langle N^A_b(L) \rangle_{\text{smpl}}$ | $\langle N^A_a(L) \rangle_{\text{smpl}}$ |
|-----|---------------------------------|---------------------------------|---------------------------------|
| 1   | $-(0.235605 \pm 0.000005) \times 10^2$ | 1173554                        | 55121.7                         |
| 2   | $(0.557681 \pm 0.000023) \times 10^3$ | 2159459.8                      | 72578.1                         |
| 3   | $-(0.132179 \pm 0.000008) \times 10^5$ | 2952153.5                      | 88743.8                         |
| 4   | $(0.313746 \pm 0.000029) \times 10^6$ | 3677982.2                      | 103182.8                        |
| 5   | $-(0.74565 \pm 0.00013) \times 10^7$ | 4301258.0                      | 115698.3                        |

Table VIII. Results on $E_A(L)$ for the $8 \times 8$ system obtained from $1.1 \times 10^3$ samples with $\varepsilon = 0.01$. The exact value of $E_A(1)$ is $-40.74998$.

| $L$ | $\langle E_{A[\eta]}(L) \rangle_{\text{smpl}}$ | $\langle N^A_b(L) \rangle_{\text{smpl}}$ | $\langle N^A_a(L) \rangle_{\text{smpl}}$ |
|-----|---------------------------------|---------------------------------|---------------------------------|
| 1   | $-(0.407475 \pm 0.000075) \times 10^2$ | 9549922                        | 96800.9                         |
| 2   | $(0.167062 \pm 0.000054) \times 10^4$ | 9572198.2                      | 73091.7                         |
| 3   | $-(0.68731 \pm 0.00047) \times 10^5$ | 7155664.2                      | 63898.6                         |
| 4   | $(0.28338 \pm 0.00090) \times 10^7$ | 6203627.8                      | 60498.0                         |
| 5   | $-(0.11633 \pm 0.00054) \times 10^9$ | 5857166.8                      | 59281.9                         |
Fig. 1. Distributions of $E_{E\{\eta\}k}(L)$ ($k = 1, 2, \cdots, 10^4$) on the $4 \times 4$ lattice for several values of $L$. Here the ratio in the horizontal axis is defined as 50 times of $E_{E\{\eta\}k}(L)/E_E(L)$.

Fig. 2. Distributions of $E_{A\{\eta\}k}(L)$ ($k = 1, 2, \cdots, 10^4$) on the $4 \times 4$ lattice for several values of $L$. The ratio is 50 times of $E_{A\{\eta\}k}(L)/E_A(L)$.