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# The stochastic state selection method combined with the Lanczos approach to eigenvalues in quantum spin systems

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## Abstract

We describe a further development of the stochastic state selection method, a new Monte Carlo method we have proposed recently to make numerical calculations in large quantum spin systems. Making recursive use of the stochastic state selection technique in the Lanczos approach, we estimate the ground state energy of the spin-1/2 quantum Heisenberg antiferromagnet on a 48-site triangular lattice. Our result for the upper bound of the ground state energy is  $-0.1833 \pm 0.0003$  per bond. This value, being compatible with values from other work, indicates that our method is efficient in calculating energy eigenvalues of frustrated quantum spin systems on large lattices.

## 1. Introduction

One widely used approach in numerical studies of quantum spin systems is the quantum Monte Carlo method. This method has helped us greatly to understand many properties of non-frustrated quantum spin systems, especially of the spin-1/2 quantum Heisenberg antiferromagnet on bipartite lattices [1–4]. Nevertheless, the method is ineffective for frustrated systems owing to the so-called sign problem. It is quite difficult, therefore, to draw any definite conclusion from numerical calculations of two-dimensional large systems of fermions or frustrated spins. However, there are active studies of numerical methods to investigate these systems. One of these is the path-integral renormalization group method for fermion systems developed by Kashima and Imada [5]. Using the Slater determinant as the basis state they improve the exact diagonalization method with the truncation of the Hilbert space. Another method is proposed by Sorella [6], who extends the fixed node method making full use of insights into the physics of the target system. One should also note the work of Henelius and Maeshima *et al* [7, 8] in extending the density matrix renormalization group method introduced by White [9, 10].

Recently we have developed another Monte Carlo method, which we call the *stochastic state selection* (SSS) method, to calculate eigenvalues in large quantum systems [11–14]. The SSS method has little in common with the ordinary Monte Carlo methods because it is not based on importance samplings. A new type of stochastic algorithm in this method enables us to select a relatively small number of elements from a vast vector space in a mathematically justified manner. Using those selected elements we calculate inner products. It is guaranteed that we can obtain correct values of these inner products through the statistical averaging process.

So far we have used the SSS method in combination with the power method, since it is a simple and straightforward way of applying the SSS method to the numerical study of energy eigenvalues. In this paper we employ the Lanczos approach instead of the power method. The Lanczos method gives us reliable results on small lattices for which we can keep every state in the vector space; for larger lattices we need to make some truncations because the vector space becomes huge. The use of truncated states in the Lanczos method, however, has been unsuccessful in either theoretically justifying its methodology or in obtaining better numerical eigenvalues [15]. Our purpose in this work is to show that for a large frustrated system we can evaluate the coefficients necessary in the Lanczos approach by means of the SSS method.

As a concrete example, we calculate an energy eigenvalue on a  $N_s$ -site triangular lattice for the ground state energy of the spin-1/2 quantum Heisenberg antiferromagnet. The Hamiltonian of the system is

$$\hat{H} = \frac{J}{4} \sum_{(i,j)} \sigma_i \sigma_j, \quad (1)$$

where  $\sigma_i$  denotes Pauli spin matrices on the  $i$ th site of a triangular lattice with  $N_s$  sites and the sum runs over all  $N_b (=3N_s)$  bonds of the lattice. The coupling  $J$  is set to 1 throughout this paper. The reason why we study this system here is that, as is well known, it is one of the systems that is strongly frustrated in two dimensions [4, 16–23]. As far as we know, reported results on the model by means of the exact diagonalization method are only for lattices smaller than or equal to 36 sites [16]. The largest lattice size is also 36 in our previous work [13], where the recursive SSS method and the power method are employed. In the present study, with an improved approach, we first calculate the lowest energy eigenvalue of the  $N_s = 27$ ,  $S_z = 1/2$  system in order to confirm that our new approach works well. For this system we mimic conditions of a virtual small computer so that we can conclude that the results obtained in reduced vector space are reliable (table 1). We then proceed to the  $N_s = 48$ ,  $S_z = 0$  system (table 2), for which our result is  $E/JN_b = -0.1833 \pm 0.0003$ . A happy combination of the recursive SSS method with the Lanczos approach in this paper enables us to estimate the ground state energy of the 48-site system.

The plan of this paper is as follows. In the next section we explain our method. Section 3 is devoted to a detailed account of the trial state on triangular lattices. Calculations with stochastic state selections are described in section 4. The final section gives a summary and discussion.

## 2. Method

In this section we present brief descriptions of the SSS method and our Lanczos approach.

### 2.1. The SSS method

Stochastic state selection is realized by a number of random variables. Let us expand a state  $|\phi\rangle$  by some basis  $\{|i\rangle\}$ ,  $|\phi\rangle = \sum_{i=1}^N c_i |i\rangle$ . Then we generate a random variable  $\eta_i$  following

**Table 1.** Estimated values of  $\alpha$ s and  $\beta$ s in the Lanczos approach for the  $N_s = 27$  system, for which we know that  $E_{\text{exact}} = -15.125972$  [16]. For this lattice we simply collect all  $S_z = 1/2$  states to form a basis. The size of the full Hilbert space is therefore  ${}_{27}C_{13} = 20058300$ . We start from a trial state with 1072935 basis states obtained after the procedures in section 3, for which  $\alpha_1 = -14.5680$ . The last three rows in the table present exact values which are calculated in the full Hilbert space without any stochastic selection. When we calculate  $\alpha$ s and  $\beta$ s inside a limited partial Hilbert space, we set the maximum size of the space to be 4500000.

$L$	2	3	4
$\beta_{L-1}$	$1.5405 \pm 0.0015$	$6.14 \pm 0.18$	$6.09 \pm 0.55$
$\alpha_L$	$-4.999 \pm 0.014$	$-3.53 \pm 0.39$	$-1.8 \pm 1.5$
$\tilde{\alpha}_L$	$-14.8099 \pm 0.0023$	$-14.927 \pm 0.010$	$-14.990 \pm 0.030$
$\beta_{L-1}^{\text{exact}}$	1.540 10	6.230 49	6.063 25
$\alpha_L^{\text{exact}}$	-5.015 80	-3.728 43	-1.859 16
$\tilde{\alpha}_L^{\text{exact}}$	-14.8101	-14.9354	-15.0061

**Table 2.** Estimated values of  $\alpha$ s and  $\beta$ s in the Lanczos approach for the  $N_s = 48$  system. The maximum number of basis states is limited to  $1.1 \times 10^8$ . As is described in section 3 we first calculate a trial state with 75746657 basis states, for which  $\alpha_1$  is  $-25.950$ . Then, following equations (11) and (12) in section 4, we estimate  $\beta_1$  and  $\alpha_2$ . Thirdly we calculate  $\tilde{\alpha}_2$  and  $u_1^{(2)}, u_2^{(2)}$  by an exact diagonalization. In a similar way to that stated in section 4 in detail, we evaluate quantities for  $L = 3$  and 4.

$L$	2	3	4
$\beta_{L-1}$	$1.7082 \pm 0.0021$	$12.63 \pm 0.16$	$13.2 \pm 2.0$
$\alpha_L$	$-12.007 \pm 0.066$	$-1.43 \pm 0.45$	$12.1 \pm 6.6$
$\tilde{\alpha}_L$	$-26.1559 \pm 0.0011$	$-26.3189 \pm 0.0096$	$-26.393 \pm 0.049$
$u_1^{(L)}$	$+0.99279 \pm 0.00007$	$+0.9719 \pm 0.0016$	$+0.955 \pm 0.013$
$u_2^{(L)}$	$-0.11986 \pm 0.00056$	$-0.2101 \pm 0.0051$	$-0.248 \pm 0.024$
$u_3^{(L)}$	—	$+0.1066 \pm 0.0048$	$+0.153 \pm 0.030$
$u_4^{(L)}$	—	—	$-0.052 \pm 0.024$

the on-off probability function

$$P_i(\eta) \equiv \frac{1}{a_i} \delta(\eta - a_i) + \left(1 - \frac{1}{a_i}\right) \delta(\eta) \quad \frac{1}{a_i} \equiv \min\left(1, \frac{|c_i|}{\epsilon}\right). \quad (2)$$

A positive parameter  $\epsilon$  common to all  $P_i(\eta)$  ( $i = 1, 2, \dots, N$ ) controls the reduction rate. Note that  $\eta_i = a_i$  or  $\eta_i = 0$  and statistical averages are  $\langle\langle \eta_i \rangle\rangle = 1$  and  $\langle\langle \eta_i^2 \rangle\rangle = a_i$ . A random choice operator  $\hat{M}_{\{\eta\}}$  is defined by

$$\hat{M}_{\{\eta\}} \equiv \sum_{j=1}^N |j\rangle \eta_j \langle j|. \quad (3)$$

Using this  $\hat{M}_{\{\eta\}}$  we obtain a state  $\hat{M}_{\{\eta\}}|\phi\rangle = \sum c_i \eta_i |i\rangle$ , which has fewer non-zero elements than  $|\phi\rangle$ . An expectation value  $\langle\phi|\hat{O}|\phi\rangle$  with an operator  $\hat{O}$  is exactly equal to the statistical average  $\langle\langle \phi|\hat{O}\hat{M}_{\{\eta\}}|\phi\rangle\rangle$ . When we want to emphasize that different random choice operators are used, we will denote them by  $\hat{M}_{\{\eta^{(k)}\}}$  ( $k = 1, 2, \dots$ ).

## 2.2. The Lanczos approach

In the Lanczos approach we start from a state  $|\psi^{(1)}\rangle$  and calculate, for some  $L$ , orthogonal states  $|\psi^{(m)}\rangle$  ( $m = 2, 3, \dots, L$ ) together with  $\alpha_m$  ( $m = 1, 2, \dots, L$ ) and  $\beta_m$  ( $m = 1, 2, \dots, L - 1$ ),

$$|\psi^{(m)}\rangle \equiv \frac{1}{\beta_{m-1}} \{ \hat{Q}(\alpha_{m-1}) |\psi^{(m-1)}\rangle - \beta_{m-2} |\psi^{(m-2)}\rangle \}, \quad (4)$$

$$\alpha_m \equiv \langle \psi^{(m)} | \hat{Q}(0) | \psi^{(m)} \rangle, \quad (5)$$

$$\beta_m \equiv \sqrt{\langle \psi^{(m)} | \hat{Q}(\alpha_m)^2 | \psi^{(m)} \rangle - \beta_{m-1}^2}, \quad (6)$$

where we define  $\beta_0 \equiv 0$  and  $\hat{Q}(\alpha) \equiv \hat{H} - \alpha$  with the Hamiltonian  $\hat{H}$ , so that we obtain the tridiagonal matrix

$$\mathcal{A}_L \equiv \begin{bmatrix} \alpha_1 & \beta_1 & 0 & 0 & \cdots & 0 & 0 \\ \beta_1 & \alpha_2 & \beta_2 & 0 & \cdots & 0 & 0 \\ 0 & \beta_2 & \alpha_3 & \ddots & \cdots & 0 & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & \ddots & \ddots & \beta_{L-1} \\ 0 & 0 & 0 & \cdots & 0 & \beta_{L-1} & \alpha_L \end{bmatrix}. \quad (7)$$

The  $L$ th approximate eigenvalue for the ground state is given by the lowest eigenvalue of  $\mathcal{A}_L$ . Let us denote the lowest eigenvalue of  $\mathcal{A}_L$  by  $\tilde{\alpha}_L$  and its eigenvector by  $\mathbf{u}^{(L)} \equiv [u_1^{(L)}, u_2^{(L)}, \dots, u_L^{(L)}]^T$  hereafter. Once we know  $\mathcal{A}_L$ ,  $\tilde{\alpha}_L$  and  $\mathbf{u}^{(L)}$  for some  $L$ , we can in principle evaluate  $\beta_L$  and  $\alpha_{L+1}$  from the relations

$$\langle \tilde{\psi}^{(L)} | \hat{Q}(\tilde{\alpha}_L)^2 | \tilde{\psi}^{(L)} \rangle = \{u_L^{(L)}\}^2 \beta_L^2, \quad (8)$$

$$\langle \tilde{\psi}^{(L)} | \hat{Q}(\tilde{\alpha}_L) \hat{Q}(0) \hat{Q}(\tilde{\alpha}_L) | \tilde{\psi}^{(L)} \rangle = \{u_L^{(L)}\}^2 \beta_L^2 \alpha_{L+1}, \quad (9)$$

with a state

$$|\tilde{\psi}^{(L)}\rangle \equiv \sum_{m=1}^L u_m^{(L)} |\psi^{(m)}\rangle. \quad (10)$$

This would lead us to a larger matrix  $\mathcal{A}_{L+1}$  and its lowest eigenvalue  $\tilde{\alpha}_{L+1}$  would give us a better estimate of the ground state energy.

In order to perform a successful numerical evaluation with a small value of  $L$ , it is necessary to make  $|\psi^{(1)}\rangle$  as good as possible. Remember that it is difficult to directly calculate  $\alpha_m$  and  $\beta_m$  for large systems with such a  $|\psi^{(1)}\rangle$ , because our available computer memory resources would not be enough to keep whole elements of  $\hat{H}|\psi^{(1)}\rangle$ . We therefore truncate each state by operating on it with  $\hat{M}_{[\eta]}$ . Details of our stochastic selection will be mentioned in section 4.

## 3. Trial state

Before describing the stochastic selection in our calculation, it will be necessary to explain how we prepare the trial state  $|\psi^{(1)}\rangle$  to start with. In this section and the next we concentrate our attention on the  $N_s = 48$  case, which involves more technical issues than the  $N_s = 27$  case does.

First let us comment on our basis by which we describe the states  $|\psi^{(m)}\rangle$ . The representation we use is the conventional one where a state is represented by  $z$ -components

of all spins of the system. Here we add an assumption about symmetries. On a triangular lattice with 48 spins there are 48 translation operators as well as six rotation and two inversion ones that commute with the Hamiltonian (1). Since we expect that the ground state is invariant under these operations [16], we construct a basis  $\{|\Phi_i\rangle\}$  which ensures all of these invariances. Note that each basis state  $|\Phi_i\rangle$  therefore contains a maximum of 576 ( $= 48 \times 6 \times 2$ ) degenerate spin configurations in it. The total number of  $|\Phi_i\rangle$  with  $S_z = 0$  therefore is about  $6 \times 10^{10}$ .

Now we come to the starting point of our numerical work, which is to calculate coefficients of  $|\psi^{(1)}\rangle$  with the basis stated above. We do this in the same way that we did in our previous work [13], where we obtained an approximate ground state  $|\psi_A\rangle$  for the spin system on a 36-site triangular lattice. The only difference is that we include as many degenerate Ising-like configurations as possible in the initial trial state this time. The basic idea for this improvement comes from Wannier's rigorous proof [24] that a classical antiferromagnetic Ising system on a triangular lattice is heavily degenerated in its minimum energy, namely its energy at zero temperature, which is  $-N_s/4$  for the  $N_s$ -site system.

Using the conventional Monte Carlo method at low temperature ( $T = 0.5$ ), where the classical energy is used as the Boltzmann weight, we pick up states with the classical minimum energy, which is  $-12$  for the  $N_s = 48$ -site system. We find 13 087  $|\Phi_i\rangle$ s that fulfil conditions  $\langle \Phi_i | \hat{H} | \Phi_i \rangle = -12.0$  and  $S_z = 0$ . We then form an initial trial state  $|\Psi_0\rangle$  by linearly combining all of them with the equal weight  $1/\sqrt{13\,087}$ . Within this partial Hilbert space with 13 087 basis states we next pursue the state  $|\Psi_t\rangle$  which has the lowest energy in the conventional exact diagonalization. We observe that  $\langle \Psi_t | \hat{H} | \Psi_t \rangle = -20.1$ .

The final stage in calculating a trial state  $|\psi^{(1)}\rangle$  is to repeat following procedures until the obtained value does not change within five decimal digits.

- (i) Extend the partial Hilbert space  $\{|\Phi_i\rangle; \langle \Phi_i | \hat{H} | \Phi_i \rangle = -12.0, S_z = 0\}$  by operating on  $\hat{H}$  a few times with  $|\Psi_t\rangle$  until the available computer memory is exhausted. The maximum number of basis states we can permit is  $\sim 1 \times 10^8$ .
- (ii) Within the Hilbert space determined in (i), pursue the state  $|\Psi'_t\rangle$  with which  $\langle \Psi'_t | \hat{H} | \Psi'_t \rangle$  is as low as possible.
- (iii) Form a state  $|\Psi''_t\rangle$  by dropping small coefficients of  $|\Psi'_t\rangle$ . We usually request that the size of the reduced Hilbert space, which is spanned by basis states included in  $|\Psi''_t\rangle$ , should be a few per cent of the one obtained in (i).
- (iv) Replace  $|\Psi_t\rangle$  by  $|\Psi''_t\rangle$ .

After this calculation we obtain the trial state  $|\psi^{(1)}\rangle$  from the last  $|\Psi''_t\rangle$ . We observe that  $|\psi^{(1)}\rangle$  comprises 75 746 657 basis states. Then we obtain  $\alpha_1 = \langle \psi^{(1)} | \hat{H} | \psi^{(1)} \rangle = -25.950$ . It should be noted that we can calculate this inner product exactly because we do not need to keep the 'outer' part of  $\hat{H} |\psi^{(1)}\rangle$  which is orthogonal to the vector space attached to  $|\psi^{(1)}\rangle$ .

#### 4. Calculations

With the Hamiltonian (1) and the trial state  $|\psi^{(1)}\rangle$  described in the previous section, we calculate the matrix elements in  $\mathcal{A}_L$  up to  $L = 4$ . This section is to show in detail how we carry out the calculations with stochastic selections. Note that all the values and the conditions stated below in this section are those for the  $N_s = 48$  lattice. Comments on the results summarized in tables 1 and 2 will be presented in the next section.

The first step here is to estimate  $\beta_1$  and  $\alpha_2$  so that we can solve the eigenvalue problem with  $\mathcal{A}_2$ . Using the recursive SSS [13], we calculate the most probable value of  $\beta_1^2 = \langle \psi^{(1)} | \hat{Q}(\alpha_1)^2 | \psi^{(1)} \rangle$  from the statistical average of

$$\langle \psi^{(1)} | \cdot \hat{Q}(\alpha_1) \hat{M}_{\{\eta^{(2)}\}} \hat{Q}(\alpha_1) \hat{M}_{\{\eta^{(1)}\}} | \psi^{(1)} \rangle. \quad (11)$$

Here we insert a symbol  $\cdot$  after  $\langle \psi^{(1)} |$  in order to represent that we calculate the inner product between  $|\psi^{(1)}\rangle$  and  $\hat{Q}(\alpha_1)\hat{M}_{\{\eta^{(2)}}\}\hat{Q}(\alpha_1)\hat{M}_{\{\eta^{(1)}}\}|\psi^{(1)}\rangle$ . Note that each random choice operator in the recursive SSS method depends on the preceding intermediate state. We generate each  $\hat{M}_{\{\eta\}}$  adjusting the value of  $\epsilon$  to be as small as possible for a Pentium IV machine equipped with 2 GB memory. Our result from 22 samples is  $\beta_1 = 1.7082 \pm 0.0021$ , where the error is estimated by the standard deviation of the data. When we evaluate  $\alpha_2$ , we approximate  $|\psi^{(2)}\rangle = \hat{Q}(\alpha_1)|\psi^{(1)}\rangle/\beta_1$  by  $\hat{Q}(\alpha_1)\hat{M}_{\{\eta\}}|\psi^{(1)}\rangle/\beta_1$ . Namely we calculate

$$\langle \psi^{(1)} | \cdot \hat{Q}(\alpha_1)\hat{M}_{\{\eta^{(3)}}\}\hat{Q}(0)\hat{M}_{\{\eta^{(2)}}\}\hat{Q}(\alpha_1)\hat{M}_{\{\eta^{(1)}}\}|\psi^{(1)}\rangle \tag{12}$$

to obtain  $\beta_1^2\alpha_2$ . The statistical average from 40 samples gives us  $\alpha_2 = -12.007 \pm 0.066$ . Here we take account of both the statistical error for (12) and the error from  $\beta_1$ . It is easy to find that  $\tilde{\alpha}_2 = -26.1559$ ,  $u_1^{(2)} = 0.99279$  and  $u_2^{(2)} = -0.11986$  with the above values of  $\alpha_1$ ,  $\beta_1$  and  $\alpha_2$ . Error estimations on these quantities are carried out as follows. Let  $f$  be  $\tilde{\alpha}_2$ ,  $u_1^{(2)}$  or  $u_2^{(2)}$ . We assume, with errors  $\Delta\beta_1$  and  $\Delta\alpha_2$ ,

$$f(\alpha_1, \beta_1 \pm \Delta\beta_1, \alpha_2 \pm \Delta\alpha_2) \simeq f(\alpha_1, \beta_1, \alpha_2) \pm \sqrt{\left[\frac{\partial f}{\partial \beta_1} \Delta\beta_1\right]^2 + \left[\frac{\partial f}{\partial \alpha_2} \Delta\alpha_2\right]^2} \tag{13}$$

and numerically calculate  $\left[\frac{\partial f}{\partial \beta_1} \Delta\beta_1\right]$  and  $\left[\frac{\partial f}{\partial \alpha_2} \Delta\alpha_2\right]$  by solving eigenproblems of matrices

$$\begin{bmatrix} \alpha_1 & \beta_1 \pm \Delta\beta_1 \\ \beta_1 \pm \Delta\beta_1 & \alpha_2 \end{bmatrix}, \quad \begin{bmatrix} \alpha_1 & \beta_1 \\ \beta_1 & \alpha_2 \pm \Delta\alpha_2 \end{bmatrix}. \tag{14}$$

Then we proceed to estimate  $\beta_2$  and  $\alpha_3$  using (8) and (9) with  $L = 2$ . We approximate  $|\tilde{\psi}^{(2)}\rangle = u_1^{(2)}|\psi_1\rangle + u_2^{(2)}|\psi_2\rangle$  by  $\hat{P}_2(\hat{M}_{\{\eta\}})|\psi^{(1)}\rangle$ , where

$$\hat{P}_2(\hat{M}_{\{\eta\}}) \equiv u_1^{(2)} + \frac{u_2^{(2)}}{\beta_1} \hat{Q}(\alpha_1)\hat{M}_{\{\eta\}}. \tag{15}$$

We calculate statistical averages of

$$\langle \psi^{(1)} | \cdot \hat{P}_2(\hat{M}_{\{\eta^{(7)}}\})\hat{Q}(\tilde{\alpha}_2)\hat{M}_{\{\eta^{(6)}}\}\hat{Q}(\tilde{\alpha}_2)\hat{M}_{\{\eta^{(5)}}\}\hat{P}_2(\hat{M}_{\{\eta^{(4)}}\})|\psi^{(1)}\rangle \tag{16}$$

and

$$\langle \psi^{(1)} | \cdot \hat{P}_2(\hat{M}_{\{\eta^{(9)}}\})\hat{Q}(\tilde{\alpha}_2)\hat{M}_{\{\eta^{(8)}}\}\hat{Q}(0)\hat{M}_{\{\eta^{(6)}}\}\hat{Q}(\tilde{\alpha}_2)\hat{M}_{\{\eta^{(5)}}\}\hat{P}_2(\hat{M}_{\{\eta^{(4)}}\})|\psi^{(1)}\rangle \tag{17}$$

to evaluate  $\{u_2^{(2)}\}^2\beta_2^2$  and  $\{u_2^{(2)}\}^2\beta_2^2\alpha_3$ , respectively. From 34 and 128 samples of these quantities, we estimate  $\beta_2$  and  $\alpha_3$ . We also evaluate their errors, taking the error from  $u_2^{(2)}$  into account. Calculations for  $\tilde{\alpha}_3$  and  $u_m^{(3)}$  s are then straightforward including error estimations. For the results, see table 2.

In estimations of  $\beta_3$  and  $\alpha_4$  we calculate inner products between

$$\hat{Q}(\tilde{\alpha}_2)\hat{M}_{\{\eta^{(12)}}\}\hat{P}_3(\hat{M}_{\{\eta^{(11)}}\}, \hat{M}_{\{\eta^{(10)}}\})|\psi^{(1)}\rangle \tag{18}$$

and

$$\hat{R}(\hat{M}_{\{\eta^{(16)}}\})\hat{Q}(\tilde{\alpha}_2)\hat{M}_{\{\eta^{(15)}}\}\hat{P}_3(\hat{M}_{\{\eta^{(14)}}\}, \hat{M}_{\{\eta^{(13)}}\})|\psi^{(1)}\rangle, \tag{19}$$

where we use abbreviations

$$\hat{P}_3(\hat{M}_{\{\eta\}}, \hat{M}_{\{\eta'\}}) \equiv u_1^{(3)} - \frac{\beta_1}{\beta_2}u_3^{(3)} + \left\{ \frac{u_2^{(3)}}{\beta_1} + \frac{u_3^{(3)}}{\beta_1\beta_2} \hat{Q}(\alpha_2)\hat{M}_{\{\eta\}} \right\} \hat{Q}(\alpha_1)\hat{M}_{\{\eta'\}}, \tag{20}$$

$$\hat{R}(\hat{M}_{\{\eta\}}) \equiv \begin{cases} 1 & \text{to calculate } \{u_3^{(3)}\}^2\beta_3^2 \\ \hat{Q}(0)\hat{M}_{\{\eta\}} & \text{to calculate } \{u_3^{(3)}\}^2\beta_3^2\alpha_4, \end{cases} \tag{21}$$

for convenience, so that we can generate as many samples as possible within a limited CPU time. The results for  $\beta_3$  and  $\alpha_4$ , which are obtained from 6240 and 4069 samples respectively, are in table 2. The maximum number of the selected basis states amounts to  $\sim 1.1 \times 10^8$ .<sup>1</sup>

Finally, one comment would be necessary from the technical point of view. It should be noted that there are variety of ways to calculate samples using the recursive SSS method for the following two reasons:

- (i) Suppose we calculate  $\beta_1^2$ , for example. For this purpose we calculated the inner products (11). Yet, the statistical average of the inner products between  $\hat{Q}(\alpha_1)\hat{M}_{\{\eta^{(1)}\}}|\psi^{(1)}\rangle$  and  $\hat{Q}(\alpha_1)\hat{M}_{\{\eta^{(17)}\}}|\psi^{(1)}\rangle$  will also give us the same quantity.
- (ii) Locations of random choice operators are not uniquely determined. For instance, it is possible to employ

$$\hat{P}'_2(\hat{M}_{\{\eta\}}) \equiv \left[ u_1^{(2)} + \frac{u_2^{(2)}}{\beta_1} \hat{Q}(\alpha_1) \right] \hat{M}_{\{\eta\}}, \quad (22)$$

and

$$\hat{P}'_3(\hat{M}_{\{\eta\}}, \hat{M}_{\{\eta'\}}) \equiv \left[ u_1^{(3)} - \frac{\beta_1}{\beta_2} u_3^{(3)} + \left\{ \frac{u_2^{(3)}}{\beta_1} + \frac{u_3^{(3)}}{\beta_1 \beta_2} \hat{Q}(\alpha_2) \right\} \hat{M}_{\{\eta\}} \hat{Q}(\alpha_1) \right] \hat{M}_{\{\eta'\}}, \quad (23)$$

instead of  $\hat{P}_2(\hat{M}_{\{\eta\}})$  and  $\hat{P}_3(\hat{M}_{\{\eta\}}, \hat{M}_{\{\eta'\}})$ , respectively.

Although statistical averages obtained in these ways will theoretically agree with each other, their standard deviations might be different. It is not *a priori* clear what way is best for numerical calculations. In order to present an example which shows how much difference is actually observed, we calculate 300 samples of

$$\langle \psi^{(1)} | \cdot P'_3(\hat{M}_{\{\eta^{(23)}\}}, \hat{M}_{\{\eta^{(22)}\}}) \hat{Q}(\tilde{\alpha}_3) \hat{M}_{\{\eta^{(21)}\}} \hat{Q}(\tilde{\alpha}_3) \hat{M}_{\{\eta^{(20)}\}} P'_3(\hat{M}_{\{\eta^{(19)}\}}, \hat{M}_{\{\eta^{(18)}\}}) | \psi^{(1)} \rangle, \quad (24)$$

whose statistical average also should give  $\{u_3^{(3)}\}^2 \beta_3^2$ . The result is  $\beta_3 = 10.8 \pm 11.0$  with a fixed value of  $\epsilon = 0.0025$ , and we observe almost the same variance as in the measurement with  $\hat{P}_3(\hat{M}_{\{\eta\}}, \hat{M}_{\{\eta'\}})$ .

## 5. Summary and discussions

In this paper we combine our recursive SSS method with the Lanczos approach so that we can estimate the ground state energy of the spin-1/2 quantum Heisenberg antiferromagnet on a 48-site triangular lattice.

In order to examine whether the method works well, we study the 27-site system for which the ground state energy is exactly known to be  $E/JN_b = -0.1867404$ . Our results for the 27-site system in table 1 give a satisfying upper limit  $E/JN_b \leq \tilde{\alpha}_4/JN_b = -0.18506 \pm 0.00037$ . It should be noted that we obtain this upper limit within a limited partial Hilbert space.

Now we summarize our results for the 48-site system. Starting from a state  $|\psi^{(1)}\rangle$  with  $\sim 7.6 \times 10^7$  basis states, each of which is a representative of a maximum of 576 translation-, rotation- and inversion-invariant configurations, we successfully calculate elements of the tridiagonal matrix  $\mathcal{A}_4$ , namely  $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \beta_1, \beta_2$  and  $\beta_3$  presented in table 2. Our best estimate for the upper bound of the ground state energy is given by  $\tilde{\alpha}_4$ . The result per bond is  $\tilde{\alpha}_4/JN_b = -0.1833 \pm 0.0003$ .

<sup>1</sup> Similar calculations for  $\beta_4$  and  $\alpha_5$  would be possible with a swifter computer. We estimate that the CPU time necessary to calculate these quantities with our Pentium IV machine is about 300 times as long as the CPU time we spent for  $\beta_3$  and  $\alpha_4$ .



This value should be compared with values obtained by other methods. In a figure presented by Capriotti *et al* [21], who studied the system using the Green function Monte Carlo method, we see that  $E/JN_b \simeq -0.185$  when  $N_s = 48$ . A variational Monte Carlo study [23] presents a value  $E/JN_b = -0.185 \pm 0.001$  for the 48-site system. Richter *et al* [4], on the other hand, made the finite-size extrapolation using the results for  $N_s = 24, 30$  and  $36$  obtained by the exact diagonalization method. Using the scaling formula  $e_0(\sqrt{N_s}) = A_0 + A_3/(\sqrt{N_s})^3 + \mathcal{O}(N_s^{-2})$  for the lowest energy per site  $e_0 \equiv E/JN_s = 3E/JN_b$ , they obtained  $A_0/3 = e_0(\infty)/3 = -0.1842$ .<sup>2</sup> The value for the 48-site system in this formula, which we calculate from this  $A_0$  and the value  $e_0(\sqrt{36})/3 = -0.1867912$  [16], is  $e_0(\sqrt{48})/3 = -0.1859$ . Thus we see that our result is consistent with those obtained with the Green function Monte Carlo method and the variational Monte Carlo method. This indicates that the recursive SSS method combined with the Lanczos approach proves to be one of techniques applicable to frustrated quantum systems.

A few remarks are in order.

Applications of the SSS method in study of other models, especially of frustrated ones, are in prospect. For example, we have studied the 64-site Shastry–Sutherland model combining the simple SSS method with the power method [12], where we obtained results to indicate that the intermediate phase exists. Much improved results from this model are expected with our new method presented in this paper.

The result  $\tilde{\alpha}_4/JN_b = -0.1833 \pm 0.0003$  on the 48-site triangular lattice is much more precise than our previous result  $E_{\text{fit}}/JN_b = -0.1856 \pm \begin{smallmatrix} 0.0009 \\ 0.0006 \end{smallmatrix}$  on the 36-site lattice [13]. One reason for this improvement is that, instead of the power method, we adopt a Lanczos approach with which the fitting procedure is not necessary. Another reason is that we improve the trial state noticing the existence of heavily degenerate Ising-like states that have the lowest energy in the classical Ising system on the triangular lattice. This idea, inspired by Wannier’s proof [24] on the classical Ising system, is encouraged by observations in numerical study of quantum systems on small lattices. For  $N_s = 12, 21$  and  $27$  lattices we observe that a large part of the ground state is formed by those degenerate Ising-like basis states.

We have a final remark is on the merits of the SSS method. First of all, we emphasize that this method is mathematically justified. It is guaranteed that expectation values for any operator and any state are given correctly by the statistical averages. Secondly our method is quite general in a sense that the SSS method can be substituted for the importance samplings in usual Monte Carlo methods [1, 2]. This should be compared with the variational techniques, for which one needs deep insights into properties of the system under study [20, 21]. Thirdly one can easily join the SSS technique with various methods such as the power method, the Lanczos method and the variational method. We expect this technique will be helpful in improving many methods used in numerical studies.

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<sup>2</sup> Simple extrapolation using our results on  $N_s = 36$  and  $48$  lattices yields an upper bound  $E/JN_b \leq -0.1790 \pm 0.0025$  in the  $N_s \rightarrow \infty$  limit.

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