The Stochastic State Selection Method
for Energy Eigenvalues in the Shastry-Sutherland Model

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We apply a recently developed stochastic method to the Shastry-Sutherland model on $4 \times 4$ and $8 \times 8$ lattices. This method, which we call the Stochastic State Selection Method here, enables us to evaluate expectation values of powers of the Hamiltonian with very limited number of states. In this paper we first apply it to the $4 \times 4$ Shastry-Sutherland system, where one can easily obtain the exact ground state, in order to demonstrate that the method works well for this frustrated system. We numerically show that errors of the evaluations depend much on representations of the states and that the restructured representation is better than the normal one for this model. Then we study the $8 \times 8$ system to estimate energy eigenvalues of the lowest $S = 1$ state as well as of the lowest excited $S = 0$ state, where $S$ denotes the total spin of the system. The results, which are in good accordance with our previous data obtained by the Operator Variational method, support that an intermediate spin-gap phase exists between the singlet dimer phase and the magnetically ordered phase. Estimates of the critical coupling and of the spin gap for the transition from the dimer phase to the intermediate phase are also presented.

KEYWORDS: quantum spin, large size, numerical calculation, Monte Carlo, Shastry-Sutherland

1. Introduction

Considerable effort has been exerted to develop effective methods to calculate various quantities in quantum spin systems.\textsuperscript{1–3)} A new method we have proposed in a previous paper\textsuperscript{4)} is a kind of Monte Carlo approach, where stochastic variables play an important role. It is completely different from the conventional quantum Monte Carlo methods which employ random walks or importance samplings.\textsuperscript{3)} In our method, which we call the Stochastic State Selection (SSS) method hereafter, random variables are used to reduce the number of states in the vector space which is huge for most systems of large sizes. To generate these random variables we introduce a probability function named on-off probability function, which \textit{“switches off”} a number of states in the vector space so that we can calculate approximate expectation values of powers of the Hamiltonian from a small number of the \textit{“on”} states. Repeating this process with a new set of random variables we can obtain averaged expectation values which are very close to the exact ones.

The fundamental idea in the SSS method is deeply connected with the variational approach to quantum spin systems, where one searches for an effective basis, a set of states which can be treated within the limit of computer facilities. In the variational approach there are two essential
steps: increasing the number of states in the wave function under current investigation, and then reducing it. In the former step one usually operates the Hamiltonian to the wave function, which is a mathematically established procedure. How to formulate the latter step, on the other hand, is quite controversial. In early works states with small coefficients are dropped, but the resultant wave functions are not satisfactory. Sampling the states using the Monte Carlo techniques has also been suggested in recent works. In the SSS method one can reduce the number of states based on a mathematically justified way. It is this remarkable property that makes us to believe the method is worth investigating.

In the previous paper we described the SSS method and applied it to the two-dimensional spin one-half Heisenberg model. In this paper we demonstrate that it can be applied to the system suffering from the negative sign problem, too. A concrete example is the Shastry-Sutherland (SS) model on a $4 \times 4$ lattice, whose results reproduce the exact values in good precision. Next we try to obtain physical quantities, the energy eigenvalues with fixed values of total spin, for the $8 \times 8$ lattice changing the coupling ratio across the critical region.

In the next section we briefly explain the SSS method. After defining the on-off probability function and the random choice matrix, we describe how we calculate expectation values of $\hat{H}^L$, $\hat{H}$ being the Hamiltonian of the system under study. Section 3 is a short description of the SS model, where we explain the Hamiltonian and several properties of this model. In section 4 numerical results on a $4 \times 4$ lattice near the critical point are presented for two representations, normal and restructured. Deviations of the data here indicate that the restructured representation is more effective for the coupling ratio we study in this section, which supports the picture that the orthogonal dimers dominate here. Based on these discussions we try in section 5 to obtain physical quantities on a $8 \times 8$ lattice, the energy eigenvalues with the total spin $S = 0$ and $S = 1$, in the intermediate region of the coupling ratio. As noted previously, there are two model-dependent problems to be solved. One of them is how we generate a good approximate state $|\psi_A\rangle$. Another is how we extract eigenvalues from the expectation values $\langle \psi_A | \hat{H}^L | \psi_A \rangle$. In addition to the calculations of expectation values for the restructured representation, extensive discussions on these subjects are given in this section. We will show that we successfully obtain the results on the energy eigenvalues which indicate a phase transition from the singlet dimer phase to an intermediate spin-gap phase. Finally, the last section is devoted to summary and discussions.

2. Stochastic State Selection Method

Here we give a brief description of the SSS method. We define the on-off probability function by

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

(1)
where $a$ is a constant which is greater than or equal to 1. It is clear by definition that
\[ \langle \langle 1 \rangle \rangle \equiv \int_{0}^{\infty} P(\eta) d\eta = 1, \]
\[ \langle \langle \eta \rangle \rangle \equiv \int_{0}^{\infty} \eta P(\eta) d\eta = 1, \]
\[ \langle \langle \eta^2 \rangle \rangle \equiv \int_{0}^{\infty} \eta^2 P(\eta) d\eta = a, \]
where $\langle \langle \rangle \rangle$ denotes the statistical average.

Let us expand a state $| \psi \rangle$ by a basis $\{ | i \rangle \}$
\[ | \psi \rangle = \sum_{i=1}^{N_V} | i \rangle c_i, \]
where $N_V$ denotes the size of the full vector space, and define the expectation values $E(L)$ ($L = 1, 2, \cdots$) as
\[ E(L) \equiv \langle \psi | \hat{H}^L | \psi \rangle. \]

We then introduce the random choice matrix, an $N_V \times N_V$ diagonal matrix,
\[ M_{\{ \eta \}} \equiv \begin{pmatrix} \eta_1 & 0 & \cdots & 0 \\ 0 & \eta_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \eta_{N_V} \end{pmatrix}. \]

Each random variable $\eta_i$ in (7) is determined by the on-off probability function
\[ P_i(\eta_i) = \frac{1}{a_i} \delta(\eta_i - a_i) + (1 - \frac{1}{a_i}) \delta(\eta_i), \]
where
\[ a_i \equiv \begin{cases} \max(1, \epsilon/|c_i|) & \text{(if } c_i \neq 0) \\ \epsilon/\delta & \text{(if } c_i = 0) \end{cases}, \]
with given constants $\epsilon$ and $\delta$ ($0 < \delta < \epsilon$). Using $(L + 1)$ independent random choice matrices $M_{\{ \eta^{(m)} \}} = \text{diag.}\{ \eta_1^{(m)}, \eta_2^{(m)}, \cdots, \eta_{N_V}^{(m)} \}$ we define
\[ E_{\{ \eta \}}(L) \equiv \langle \psi | M_{\{ \eta^{(L+1)} \}} \hat{H} M_{\{ \eta^{(L)} \}} \cdots \hat{H} M_{\{ \eta^{(1)} \}} | \psi \rangle. \]

It is easy to see that $\langle \langle E_{\{ \eta \}}(L) \rangle \rangle = E(L)$. Note that by operating $M_{\{ \eta^{(m)} \}}$ we can obtain a truncated vector space for $\hat{H} M_{\{ \eta^{(m-1)} \}} \cdots \hat{H} M_{\{ \eta^{(1)} \}} | \psi \rangle$, since $\eta_i^{(m)}$ is zero with the probability $1 - 1/a_i$. Also note that the variances of $\eta_i^{(m)}$ are the same for all $m$ because both $\langle \langle \eta_i^{(m)} \rangle \rangle$ and $\langle \langle \eta_i^{(m)} \rangle^2 \rangle$ do not depend on $m$. 

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In numerical studies we measure
\[
\langle \langle E_{\{\eta\}}(L) \rangle \rangle_{\text{smpl}} \equiv \frac{1}{n_{\text{smpl}}} \sum_{k=1}^{n_{\text{smpl}}} E_{\{\eta\}}(L),
\]

(11)
\[
\rho_{\{\eta\}}^2(L) \equiv \langle \langle [E_{\{\eta\}}(L)]^2 \rangle \rangle_{\text{smpl}} - \langle \langle E_{\{\eta\}}(L) \rangle \rangle_{\text{smpl}}^2,
\]

(12)
using \(n_{\text{smpl}}\) samples. The error of \(E_{\{\eta\}}(L)\) is evaluated by
\[
Er(L) \equiv 2\sqrt{\frac{\rho_{\{\eta\}}^2(L)}{n_{\text{smpl}}}}.
\]

(13)
The fact that the number of non-zero components much reduces by operating \(M_{\{\eta(m)\}}\) to \(\hat{H}M_{\{\eta(m-1)\}} \cdots \hat{H}M_{\{\eta(1)\}} | \psi \rangle\) is essential to numerical calculations. Let us denote by \(\langle \langle N_b(n) \rangle \rangle_{\text{smpl}}\) and \(\langle \langle N_a(n) \rangle \rangle_{\text{smpl}}\) the number of non-zero coefficients we count in the measurement before and after we operate \(M_{\{\eta(m)\}}\) to \(\hat{H}M_{\{\eta(m-1)\}} \cdots \hat{H}M_{\{\eta(1)\}} | \psi \rangle\), respectively.

3. Shastry-Sutherland Model

As is discussed in several papers,9–17) one of recent fascinating topics in two-dimensional quantum spin systems is the Shastry-Sutherland (SS) model,8) the model of orthogonal dimers with the intra-dimer coupling \(J (>0)\) and the inter-dimer coupling \(J' (>0)\).

In this model a spin is located at the sites
\[
(2n_x a + \frac{d}{2}, 2n_y a + \frac{d}{2}), \quad (2n_x a - \frac{d}{2}, 2n_y a - \frac{d}{2}),
\]
\[
((2n_x + 1)a + \frac{d}{2}, (2n_y + 1)a - \frac{d}{2}), \quad ((2n_x + 1)a - \frac{d}{2}, (2n_y + 1)a + \frac{d}{2}),
\]
on the \(2N \times 2N\) lattice in Fig. 1, where \(n_x = 0, 1, \cdots, N - 1\) and \(n_y = 0, 1, \cdots, N - 1\), \(2a\) is the unit distance between dimers and \(\sqrt{2d}\) is the distance of spins in a dimer. The Hamiltonian is given by
\[
\hat{H} = \frac{1}{4} J \sum_{n_x, n_y=0}^{N-1} \{h_a(n_x, n_y) + h_b(n_x, n_y)\}
\]
\[
+ \frac{1}{4} J' \sum_{n_x, n_y=0}^{N-1} \{h_1(n_x, n_y) + h_2(n_x, n_y) + h_3(n_x, n_y) + h_4(n_x, n_y)\},
\]
where the partial Hamiltonians are, as given in ref.17,
\[
h_a(n_x, n_y) \equiv \sigma(2n_x a + \frac{d}{2}, 2n_y a + \frac{d}{2}) \cdot \sigma(2n_x a - \frac{d}{2}, 2n_y a - \frac{d}{2}),
\]
and so on with \(\sigma(x, y)\) denoting the Pauli matrix at the location \((x, y)\).

This model provides a nontrivial system which relates an exactly solvable spin-gap model obtained in the \(J' \to 0\) limit to a square lattice model where intra-dimer interaction vanishes
It is known that the exact ground state of the SS model is the direct product of the singlet dimers when \( J' \leq J'_c \sim 0.68J \), while for sufficiently large \( J'/J \) the system is in the magnetic order phase with the Néel ground state. It is almost doubtless that another phase exists between these two phases, but the location and the properties of this phase are not definite yet. This phase is suggested to be gapless or nearly so in refs.13 and 15, while authors in refs.11, 12, 14, 16 and 17 conclude it is gapped. Numerical data for the spin-gap is presented only in refs.12 and 17.

In study of these phases a fundamental quantity to be examined is the difference between the energy of the singlet-dimer state \( E_0 \) and the lowest energy \( E \) as a function of the coupling \( J'/J \), when the momentum \( p=(0,0) \), the total spin \( S=j \) (\( j=0,1 \)) and the \( I^+ \) parity is even or odd, where the \( I^+ \) parity is the parity for the \( x-y \) reflection \( I^+\sigma(y,x)I^+=\sigma(y,x) \).

4. Numerical results on a 4×4 lattice

In this section we show the numerical results obtained on a small lattice in order to demonstrate that we can apply the SSS method to the SS model with \( J' \sim J'_c \), where the negative sign problem is serious, without any difficulty.

It is quite easy to calculate the exact ground state \( |\psi_E\rangle \) of the model on the 4×4 lattice using the Lanczos techniques. We therefore do not need to pursue any trial state here. We just measure

\[
E_{E(\eta)}(L) \equiv \langle \psi_E | M_{\{\eta(L+1)\}} \hat{H} M_{\{\eta(L)\}} \hat{H} M_{\{\eta(L-1)\}} \cdots \hat{H} M_{\{\eta(1)\}} | \psi_E \rangle
\]

\((L=1,2,\cdots)\) and compare them with \( E_E(L) = E^L \), where \( E \) denotes the eigenvalue of \( \hat{H} \), namely \( \hat{H} | \psi_E \rangle = E | \psi_E \rangle \).

In this section we fix the coupling ratio \( J'/J = 0.7 \), a value slightly above the critical point, for which \( E/J = -6.3502 \). Here we calculate \( \langle E_{E(\eta)}(L) \rangle_{\text{smpl}} \) using two representations. One of them is the normal one, where the state on each site of the lattice is represented by the \( z \) component of the spin sitting on the site. In another representation we named restructured, two spins connected with the coupling \( J \) are rearranged in three triplets and one singlet states. The total number of non-zero coefficients in expansion of \( | \psi_E \rangle \) is 12,870 (8,565) in the normal (restructured) representation.

Table I shows our results up to \( L = 10 \) obtained from \( 10^4 \) samples with \( \epsilon = 0.1 \), together with the exact values. Note that \( \delta \) in (9) is not necessary for \( | \psi_E \rangle \). We see that the results using the restructured representation are in good agreement with the exact ones. Especially for small values of \( L \) the agreement is excellent. The relative errors are in the range from 0.11% \((L=1)\) to 2.8% \((L=10)\). The results from the normal representation are also compatible with the exact values. We, however, observe that the statistical errors are much larger than those in the restructured representation except for very low \( L \). The relative error is 0.12% for \( L = 1 \) but it rapidly increases
as \( L \) grows to reach 113\% \((L = 9)\), where the evaluated value is not meaningful. For larger values of \( \epsilon \) such tendency is more outstanding. With \( \epsilon = 0.2 \) and \( n_{\text{smpl}} = 10^4 \), for example, we cannot obtain reliable values of \( \langle E_{E(\eta)}(L) \rangle_{\text{smpl}} \) \((L \geq 6)\) in the normal representation, while the results from the restructured representation are satisfying up to \( L = 10 \). When the number of samples is increased we are in principle to obtain satisfactory evaluations even in the normal representation. In fact, we observe that for \( 10^5 \) samples with \( \epsilon = 0.1 \) the statistical errors become smaller than those for \( 10^4 \) samples except for \( L = 10 \). \( \langle E_{E(\eta)}(9) \rangle_{\text{smpl}} / J^9 \) and \( \langle E_{E(\eta)}(10) \rangle_{\text{smpl}} / J^{10} \) for \( 10^5 \) samples are \((-0.189 \pm 0.066) \times 10^8 \) and \((-0.120 \pm 0.088) \times 10^9 \), respectively.

Table II presents the numbers of non-zero coefficients measured in the same calculations with \( 10^4 \) samples, which is to show how the number of non-zero coefficients decreases by each operation of the random choice matrix. In both representations we see that \( \langle N^E_a(L) \rangle_{\text{smpl}} \), which denotes the number of the “on” states after the operation, is less than a tenth part of \( \langle N^E_b(L) \rangle_{\text{smpl}} \), the number of non-zero coefficient before the operation. In addition, the data suggest that both \( \langle N^E_a(L) \rangle_{\text{smpl}} \) and \( \langle N^E_b(L) \rangle_{\text{smpl}} \) become constants for large \( L \) in each representation and these constants very weakly depend upon the representation.

Results in Table I strongly indicate that the restructuring is quite effective here. What is the reason for such qualitatively different behaviors in these two representations then? To answer this question we plot in Fig. 2 the distributions of sorted coefficients in the expansion of \( | \psi_E \rangle \) in both representations. The abscissa is the basis number \( i' \) which is reordered so that \( |c_{i'}| \geq |c_{j'}| \) holds for \( i' < j' \). We observe the distributions are different in the region of the small coefficients, where the normal representation has a longer tail. The minimum value of the non-zero coefficients in the normal representation is \( 7.6 \times 10^{-6} \) while it is \( 1.5 \times 10^{-4} \) in the restructured representation. We will return to this issue in an Appendix.

5. Numerical results on a 8×8 lattice

Let us proceed to a larger lattice with 8×8 sites and show that the SSS method is helpful to evaluate the energy of the first excited states. We study the system with the total spin \( S = 0 \) and 1 in the parameter region \( 0.55 \leq J' / J \leq 0.8 \). Here we use

\[
E_{\{\eta\}}(L) = \langle \psi | \hat{H} M_{\{\eta^{(L)}\}} \hat{H} M_{\{\eta^{(L-1)}\}} \cdots \hat{H} M_{\{\eta^{(1)}\}} | \psi \rangle
\]

(15)

instead of (10) in order to decrease the statistical errors. Throughout this section we employ the restructured dimer representation, which is a very powerful technique for the model under investigation. The results we present here are compared to those in ref.17, where we have been successful to obtain approximate values on the energy difference for this system by means of the operator variational (OV) method.

For this lattice size it is necessary to find an approximate state \( | \psi_A \rangle \) without knowing the
exact eigenstate $|\psi_E\rangle$. Here we employ a systematic way using the Lanczos-like method in small vector spaces; we start with a trial state $|\psi_{\text{trial}}\rangle$, calculate the matrix elements of $\hat{H}$ from the basis \{ $|\psi_{\text{trial}}\rangle$, $\hat{H} |\psi_{\text{trial}}\rangle$, $\hat{H}^2 |\psi_{\text{trial}}\rangle$, $\ldots$, $\hat{H}^p |\psi_{\text{trial}}\rangle$ \} with a small integer $p$, numerically diagonalize the matrix to obtain its all energy eigenvalues and define $|\psi_A\rangle$ as the eigenstate which provides the lowest eigenvalue among them. In the following calculations we fix $p = 6$.

As for the trial state $|\psi_{\text{trial}}\rangle$ we employ one of the states described in the appendix D in ref.17 whose energy eigenvalue is found to be the lowest of all states we tried in the numerical study by means of the OV method. Namely we start from $|\psi_{\text{trial}}\rangle = |\Psi_{nn,0,0,0,0}\rangle$ for $S = 0$ and $|\psi_{\text{trial}}\rangle = |\Psi_{nn,1,0,0,0}\rangle$ for $S = 1$, which are among the two-nearest-neighboring-triplet states with the odd and the even $I_+$ parity, respectively. It should be noted that in our previous study\(^{17}\) the energy eigenvalue for the even $I_+$ is much higher than that for the odd $I_+$ when $S = 0$ while for $S = 1$ the lowest energy is independent of the $I_+$ parity.

Now we present the results. Table III and IV show values of $\langle E_{\text{A}_{\{q\}}}(L) \rangle_{\text{smpl}}$ observed for the $S = 0$ and $S = 1$ cases, where the suffix A represents that $|\psi\rangle$ in (10) is an approximate state $|\psi_A\rangle$. In both tables we see very small errors, which support that the restructuring technique is quite effective. How many non-zero coefficients appear here? When $S = 0$ the number of non-zero coefficients in $|\psi_A\rangle$ is $1,264,256$, while $\langle N^A_b(5) \rangle_{\text{smpl}}$, the number of non-zero coefficients in $\hat{H} M_{\{q(\bar{\eta})\}} \hat{H} M_{\{q(3)\}} \hat{H} M_{\{q(2)\}} \hat{H} M_{\{q(1)\}} |\psi_A\rangle$ in measurements, ranges from $(9.78 \pm 0.03) \times 10^5$ at $J'/J = 0.55$ to $(1.912 \pm 0.004) \times 10^6$ at $J'/J = 0.75$. In the $S = 1$ case $|\psi_A\rangle$ contains $690,624$ components and we observe $\langle N^A_b(5) \rangle_{\text{smpl}}$ is $(2.84 \pm 0.02) \times 10^5 ((1.534 \pm 0.004) \times 10^6)$ at $J'/J = 0.55 (0.8)$. By operating $M_{\{q(\bar{\eta})\}}$ we can reduce it to less than a tenth. In concrete terms, $\langle N^A_b(5) \rangle_{\text{smpl}}$ for $S = 0$ ranges from $(8.35 \pm 0.02) \times 10^4$ at $J'/J = 0.55$ to $(1.657 \pm 0.003) \times 10^5$ at $J'/J = 0.75$ and for $S = 1$ it is $(2.27 \pm 0.01) \times 10^4 ((1.271 \pm 0.003) \times 10^5)$ at $J'/J = 0.55 (0.8)$. Thus we see that we can evaluate expectation values of $\hat{H}^L$ not only for small $J'/J$ but also in the critical region of the parameter space.

How do we extract energy eigenvalues from these data? We try two ways, one is to use the extrapolation formula and another is to do the Lanczos-like calculation with the basis \{ $|\psi_A\rangle$, $\hat{H} |\psi_A\rangle$, $\hat{H}^2 |\psi_A\rangle$ \}, noting that the Hamiltonian matrix elements from this basis are given by $\langle \psi_A | \hat{H}^L | \psi_A \rangle$ up to $L = 5$.

The extrapolation formula is the one discussed in the previous paper,\(^4\)

$$
\langle \psi_A | \hat{H}^L | \psi_A \rangle = E^L (q_0 + \frac{q_1}{L + \alpha + 1}) = F(L, E, q_0, q_1, \alpha).
$$

In process of determining four parameters in this formula, $E$, $q_0$, $q_1$ and $\alpha$, we use two relations

$$
F(0, E, q_0, q_1, \alpha) = q_0 + \frac{q_1}{\alpha + 1} = \langle \psi_A | \psi_A \rangle = 1,
$$

$$
F(1, E, q_0, q_1, \alpha) = E \left( q_0 + \frac{q_1}{\alpha + 2} \right) = \langle \psi_A | \hat{H} | \psi_A \rangle.
$$
so that $q_1$ and $\alpha$ are calculated from $E$ and $q_0$. Note that the value of $\langle \psi_A | \hat{H} | \psi_A \rangle$ is known in the process of generating $| \psi_A \rangle$. Then we look for the values of $E$ and $q_0$ which minimize

$$S_{\text{fit}} \equiv \sum_{L=1}^{5} \left[ 1 - \frac{\langle E_{A\{\eta\}}(L) \rangle_{\text{smpl}}}{F(L, E, q_0, q_1, \alpha)} \right]^2,$$

within the ranges $\langle \psi_A | \hat{H} | \psi_A \rangle - 0.5 \leq E \leq \langle \psi_A | \hat{H} | \psi_A \rangle$ and $0.5 \leq q_0 \leq 1.0$. Results of the fitting for $J'/J > 0.5$ are shown in Tables V ($S = 0$) and VI ($S = 1$). The statistical errors of the measured values,

$$S_{2\text{Er}} \equiv \sum_{L=1}^{5} \left[ \frac{E_r(L)}{\langle E_{A\{\eta\}}(L) \rangle_{\text{smpl}}} \right]^2,$$

are also presented in the tables. The fact that $S_{\text{fit}}$ is smaller than $S_{2\text{Er}}$ means the fitting is statistically acceptable. We see that values of $q_0$ obtained from the fit are close to 1. Since $q_0$ represents the overlapping between the trial state and the exact state, $\langle \psi_A | \psi_E \rangle$, this implies that our way to generate the state $| \psi_A \rangle$ supplies good approximations of the exact eigenstate $| \psi_E \rangle$ for this model. The energy difference from the fit normalized by the intra-dimer coupling, $(E_{\text{fit}} - E_0)/J$, is plotted in Fig. 3 ($S = 0$) and Fig. 4 ($S = 1$) together with those obtained by the OV method. Here $E_0$ denotes the energy of the ground state in the singlet dimer phase, which is $-24.0J$ for the $8 \times 8$ system. We see that the data from the OV method with $L_{\text{max}} = 4$ and the data from the SSS method are in good agreement when $J'/J = 0.55$. For larger coupling ratios the data from the SSS method are below the data from the OV method. Especially near the critical point this tendency is outstanding, suggesting that the SSS method is more suitable to study the phase transition in the SS model. The data by the SSS method also support that an intermediate spin-gap phase exists, because at $J'/J \simeq 0.71$ $E_{\text{fit}} - E_0$ becomes zero for $S = 0$ while $E_{\text{fit}} - E_0 \sim 0.18J$ for $S = 1$ there.

Let us turn to another way we try to extract energy eigenvalues. Based on the observation that $| \psi_A \rangle$ is a good approximate of $| \psi_E \rangle$, we apply the Lanczos-like method to evaluate the eigenvalue $E^{(n)} (n= 1, 2, 3)$ from the matrix $H^{(n)}$ whose matrix elements are calculated from bases $\{ | \psi_A \rangle \}$, $\{ | \psi_A \rangle, \hat{H} | \psi_A \rangle \}$ and $\{ | \psi_A \rangle, \hat{H} | \psi_A \rangle, \hat{H}^2 | \psi_A \rangle \}$, respectively. Substituting $\langle E_{A\{\eta\}}(L) \rangle_{\text{smpl}}$ in Tables III and IV for $E_{A}(L) = \langle \psi_A | \hat{H}^L | \psi_A \rangle$ in

$$\alpha_1 \equiv \langle \psi_A | \hat{H} | \psi_A \rangle,$$

$$\beta_1 \equiv \sqrt{\langle \psi_A | \hat{H}^2 | \psi_A \rangle - \alpha_1^2},$$

$$\alpha_2 \equiv \frac{1}{\beta_1^2} \left( \langle \psi_A | \hat{H}^3 | \psi_A \rangle - \alpha_1^3 \right) - 2\alpha_1,$$

$$\beta_2 \equiv \sqrt{\frac{1}{\beta_1^2} \left( \langle \psi_A | \hat{H}^4 | \psi_A \rangle - 2\alpha_1 \langle \psi_A | \hat{H}^3 | \psi_A \rangle + \alpha_1^2 \langle \psi_A | \hat{H}^2 | \psi_A \rangle \right) - \alpha_2^2 - \beta_1^2},$$

$$\alpha_3 \equiv \frac{1}{\beta_2^2 \beta_1^2} \left( \langle \psi_A | \hat{H}^5 | \psi_A \rangle - 2\alpha_1 \langle \psi_A | \hat{H}^4 | \psi_A \rangle + \alpha_1^2 \langle \psi_A | \hat{H}^3 | \psi_A \rangle \right) - 2\alpha_2.$$
we diagonalize

\[
H^{(1)} \equiv (\alpha_1), \quad H^{(2)} \equiv \begin{pmatrix} \alpha_1 & \beta_1 \\ \beta_1 & \alpha_2 \end{pmatrix}, \quad H^{(3)} \equiv \begin{pmatrix} \alpha_1 & \beta_1 & 0 \\ \beta_1 & \alpha_2 & \beta_2 \\ 0 & \beta_2 & \alpha_3 \end{pmatrix}.
\]

The results are also in Tables V (S = 0) and VI (S = 1). As we see in tables we obtain better estimates by \( E^{(2)} \) than by \( E^{(1)} \). Note that values of \( E^{(2)} \) are in good accordance with \( E_{\text{fit}} \) in Tables III and IV, which indicates that the fits are reliable. We could not, on the other hand, obtain trustworthy values of \( E^{(3)} \) from the present data. It is mainly because of the insufficient statistical precision, which we can cope with by increasing the number of samples, or by decreasing the parameter \( \epsilon \). It seems that the latter is much more effective than the former. In the \( S = 0 \) and \( J'/J = 0.7 \) case, for instance, we observe that we cannot obtain any \( E^{(3)} \) from \( 9 \times 10^4 \) samples with \( \epsilon = 0.001 \) while \( E^{(3)} \) calculated from \( 10^4 \) samples with \( \epsilon = 0.0005 \) is \(-23.928J\), which is slightly lower than the value of \( E^{(2)} \) in Table V.

6. **Summary and Discussions**

In this paper we calculated the expectation values of \( \hat{H}^L \) (\( L = 1, 2, \cdots \)) of the two-dimensional SS model\(^8\) using the SSS method.\(^4\) Comparing our results on a \( 4 \times 4 \) lattice with exact values we demonstrated that the method is applicable even to this strongly frustrated quantum spin system. We also showed that deviations of the evaluated values are much less in the restructured representation than in the normal representation. In the normal representation of the SS model we observed rapid increase of the statistical errors for large values of \( L \), which is in contrast with our previous study of the \( 4 \times 4 \) spin one-half Heisenberg model.\(^4\) A qualitative discussion on the reason why such increase occurs is given in the appendix.

In study of the \( 8 \times 8 \) SS system we concentrated our attention on an intermediate phase reported in refs.11-17. We examined energy eigenvalues of the lowest excited states with the total spin \( S = 0 \) and \( S = 1 \) for several values of the coupling ratio. It should be emphasized that the method is powerful even in the critical region of the model, where the negative sign problem prevents us from obtaining statistically meaningful results by means of the standard quantum Monte Carlo techniques.\(^20\) In order to numerically extract the energy eigenvalues from the observed \( \langle \hat{H}^L \rangle \) we tried two ways, a fitting within some parameter space and a Lanczos-like diagonalization. We see results from these two ways are consistent to give us reliable estimate of energy eigenvalues. It should be kept in mind that employing highly qualified trial states in the SSS method is a key for the success. Thus we see that the critical value of \( J'/J \) is less than 0.71 for the phase transition.
from the singlet dimer phase to the intermediate phase, which is compatible with the value in ref.12. Note that this upper bound is obtained with a non-perturbative method. The spin gap at the critical point, \( \sim 0.18J \), is about one-half of the one reported in ref.12, however. More intensive investigations should be made in future work before we establish physical properties of this phase.

**Appendix: Large Variances**

In this appendix we discuss the reason why very large variances are observed in the normal representation of the SS model. As we have seen in Fig. 2 much more terms with very small coefficients appear in the expansion of the wave function \( |\psi_A\rangle \) in the normal representation compared to the restructured representation. So we analyze the expression for the variance paying our attention to contributions from those terms.

Let us examine \( \sigma^2_{\langle \eta \rangle}(L) \), the variance of \( \langle \langle E_{\langle \eta \rangle}(L) \rangle \rangle \) introduced in ref. 4,

\[
\sigma^2_{\langle \eta \rangle}(L) \equiv \langle \langle E_{\langle \eta \rangle}(L)^2 \rangle \rangle - \langle \langle E_{\langle \eta \rangle}(L) \rangle \rangle^2 \\
= \sum_{i,i',j,j'} \cdots \sum_{k,k',l,l'} c_i h_{ij} \cdots h_{kl} c_{i'} h_{i'j'} \cdots h_{kl'} c_{l'} \\
\times \langle \langle \eta_i^{(1)} \eta_i^{(1)} \rangle \rangle \langle \langle \eta_j^{(2)} \eta_j^{(2)} \rangle \rangle \cdots \langle \langle \eta_k^{(L)} \eta_k^{(L)} \rangle \rangle \langle \langle \eta_{l'}^{(L+1)} \eta_{l'}^{(L+1)} \rangle \rangle - E(L)^2 \\
= \sum_{i,i',j,j'} \cdots \sum_{k,k',l,l'} c_i h_{ij} \cdots h_{kl} c_{i'} h_{i'j'} \cdots h_{kl'} c_{l'} \cdot \{1 + \delta_{ii'}(\langle \langle \eta_i^2 \rangle \rangle - 1)\} \\
\times \{1 + \delta_{jj'}(\langle \langle \eta_j^2 \rangle \rangle - 1)\} \cdots \{1 + \delta_{kk'}(\langle \langle \eta_k^2 \rangle \rangle - 1)\} \{1 + \delta_{l'l'}(\langle \langle \eta_{l'}^2 \rangle \rangle - 1)\} \\
- E(L)^2. \quad \text{(A.1)}
\]

For \( L \geq 2 \) this variance contains one or more terms that might blow up with small non-zero coefficients, because the statistical average \( \langle \langle \eta^2 \rangle \rangle = \epsilon/|c_s| \), which follows from (4) and (9), becomes huge if a non-zero coefficient \( c_s \) in (8) is much less than \( \epsilon \). The most dangerous term among them is

\[
T \equiv \sum_{i,i',k,k',l,l',m,n} c_i^2 c_i'^2 (h_{ij})^2 (h_{jk})^2 \cdots (h_{lm})^2 (h_{mn})^2 \\
\times (\langle \langle \eta_i^2 \rangle \rangle - 1)(\langle \langle \eta_j^2 \rangle \rangle - 1)(\langle \langle \eta_k^2 \rangle \rangle - 1) \cdots (\langle \langle \eta_m^2 \rangle \rangle - 1)(\langle \langle \eta_n^2 \rangle \rangle - 1).
\]

For \( L = 1 \) this term is harmless since in this case

\[
T = \sum_i c_i^2 (\langle \langle \eta_i^2 \rangle \rangle - 1) \sum_j c_j^2 (\langle \langle \eta_j^2 \rangle \rangle - 1)(h_{ij})^2 \\
= \sum_{c_i \neq 0} c_i^2 \left[ \max \left(1, \frac{\epsilon}{|c_i|}\right) - 1 \right] \sum_{c_j \neq 0} c_j^2 \left[ \max \left(1, \frac{\epsilon}{|c_j|}\right) - 1 \right] (h_{ij})^2 \\
= \sum_{0 < |c_i| < \epsilon} (\epsilon |c_i| - c_i^2) \sum_{0 < |c_j| < \epsilon} (\epsilon |c_j| - c_j^2)(h_{ij})^2.
\]
Actually we observe on a $4 \times 4$ lattice that the measured variances of $\langle E_{\{i\}}(1) \rangle$, which are defined by (12), are comparable in both representations. They are $0.153J^2$ and $0.135J^2$ when $\epsilon = 0.1$ and $n_{\text{sampl}} = 10^4$ for the normal representation and the restructured representation, respectively.

Let us then consider the case $L = 2$, where

$$T = \sum_{i} c_i^2(\langle h_i^2 \rangle - 1) \sum_{k} c_k^2(\langle h_k^2 \rangle - 1) \sum_{j} (h_{ij})^2(h_{jk})^2(\langle \eta_j^2 \rangle - 1)$$

$$= \sum_{0 <|c_i| <|\epsilon>} (\epsilon|c_i| - c_i^2) \sum_{0 <|c_k| <|\epsilon>} (\epsilon|c_k| - c_k^2) \sum_{0 <|c_j| <|\epsilon>} (h_{ij})^2(h_{jk})^2(\langle \eta_j^2 \rangle - 1)$$

$$\sim \sum_{0 <|c_i| <|\epsilon>} (\epsilon|c_i| - c_i^2) \sum_{0 <|c_k| <|\epsilon>} (\epsilon|c_k| - c_k^2) \sum_{0 <|c_j| <|\epsilon>} (h_{ij})^2(h_{jk})^2 \frac{\epsilon}{|c_j|}.$$}

If the Hamiltonian matrix is positive-definite ($h_{jk} \geq 0$) and all coefficients of the eigen state are non-negative ($c_k \geq 0$),

$$0 \leq h_{jk}c_k \leq \sum_{l} h_{jl}c_l = Ec_j$$

holds for any $k$. In this case it follows that

$$T \sim \sum_{0 <|c_i| <|\epsilon>} (\epsilon|c_i| - c_i^2) \sum_{0 <|c_k| <|\epsilon>} (\epsilon - c_k) \sum_{0 <|c_j| <|\epsilon>} (h_{ij})^2h_{jk} \cdot h_{jk}c_k \cdot \frac{\epsilon}{c_j}$$

$$\leq \sum_{0 <|c_i| <|\epsilon>} (\epsilon|c_i| - c_i^2) \sum_{0 <|c_k| <|\epsilon>} (\epsilon - c_k) \sum_{0 <|c_j| <|\epsilon>} (h_{ij})^2h_{jk} \cdot Ec_j \cdot \frac{\epsilon}{c_j}$$

$$= \epsilon E \sum_{0 <|c_i| <|\epsilon>} (\epsilon|c_i| - c_i^2) \sum_{0 <|c_k| <|\epsilon>} (\epsilon - c_k) \sum_{0 <|c_j| <|\epsilon>} (h_{ij})^2h_{jk},$$

which gives a safe upper bound of $T$. This means that the positive-definite systems are free from unacceptably large variances caused by the smallness of the coefficients. For the frustrated systems with the negative sign problem, on the contrary, there is no guarantee that they can escape from this difficulty. It is very likely, therefore, that the frustration and a lot of small coefficients would be responsible together to such behavior of the statistical errors in the measurement. Clearly similar discussions are possible for $L \geq 3$.

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19) For each \( i \), all of \( \eta_i^{(m)} \) \((m = 1, 2, \cdots, L + 1)\) are generated by the on-off probability function (8) with the same
   \( a_i \) in (9), which is related to the expansion of the initial state (5).
20) For example, we observe that the \( r \)-ratio of the 8 \( \times \) 8 SS system with \( \beta J = 4 \) in the Suzuki-Trotter method,
   where \( \beta \) denotes the inverse temperature, is \( r \sim 0.7 \) at \( J'/J = 0.5 \) while it drops to \( r \sim 0.15 \) at \( J'/J = 0.635 \)
   even in the restructured representation. Here the \( r \)-ratio is defined by
   \( r \equiv (N_+ - N_-)/(N_+ + N_-) \), \( N_+ \) (\( N_- \))
   being the number of configurations with positive (negative) weight, respectively.
The Stochastic State Selection Method for Energy Eigenvalues in the Shastry-Sutherland Model

| $L$ | $E_E(L)/J^L$ | Normal | $\langle \langle E_{\{\eta\}}(L) \rangle \rangle_{\text{smpl}}/J^L$ | Restructured |
|-----|---------------|--------|---------------------------------|--------------|
| 1   | $-0.63502 \times 10^1$ | $-(0.63484 \pm 0.00078) \times 10^1$ | $-(0.63486 \pm 0.00073) \times 10^1$ |
| 2   | $0.40325 \times 10^2$ | $(0.40336 \pm 0.00071) \times 10^2$ | $(0.40298 \pm 0.00063) \times 10^2$ |
| 3   | $-0.25607 \times 10^3$ | $-(0.25580 \pm 0.00096) \times 10^3$ | $-(0.25601 \pm 0.00052) \times 10^3$ |
| 4   | $0.16261 \times 10^4$ | $(0.1619 \pm 0.0023) \times 10^4$ | $(0.16277 \pm 0.00052) \times 10^4$ |
| 5   | $-0.10326 \times 10^5$ | $-(0.1056 \pm 0.0052) \times 10^5$ | $-(0.10307 \pm 0.00053) \times 10^5$ |
| 6   | $0.65576 \times 10^5$ | $(0.692 \pm 0.043) \times 10^5$ | $(0.6568 \pm 0.0042) \times 10^5$ |
| 7   | $-0.41642 \times 10^6$ | $-(0.425 \pm 0.053) \times 10^6$ | $-(0.4148 \pm 0.0035) \times 10^6$ |
| 8   | $0.26443 \times 10^7$ | $(0.277 \pm 0.081) \times 10^7$ | $(0.2655 \pm 0.0034) \times 10^7$ |
| 9   | $-0.16792 \times 10^8$ | $-(0.06 \pm 0.19) \times 10^8$ | $-(0.1701 \pm 0.0025) \times 10^8$ |
| 10  | $0.10663 \times 10^9$ | $(0.107 \pm 0.048) \times 10^9$ | $(0.1048 \pm 0.0030) \times 10^9$ |

Table I. Results on $\langle \langle E_{\{\eta\}}(L) \rangle \rangle_{\text{smpl}}$ ($L = 1, 2, \cdots, 10$) obtained for the $4 \times 4$ Shastry-Sutherland (SS) model by the Statistic State Selection (SSS) method. The number of samples is $10^4$ and $\epsilon = 0.1$ for both of the normal and the restructured representations. Exact values of $E_E(L)$ are also presented for comparison.
| $L$ | $\langle N_b^E(L) \rangle_{\text{smpl}}$ | $\langle N_a^E(L) \rangle_{\text{smpl}}$ | $\langle N_b^E(L) \rangle_{\text{smpl}}$ | $\langle N_a^E(L) \rangle_{\text{smpl}}$ |
|-----|-----------------|-----------------|-----------------|-----------------|
| 1   | 12870           | 577.7           | 8565            | 641.0           |
| 2   | 7250.2          | 486.5           | 7464.7          | 532.8           |
| 3   | 6353.7          | 468.0           | 6494.0          | 502.8           |
| 4   | 6159.0          | 463.3           | 6189.0          | 492.8           |
| 5   | 6110.6          | 462.4           | 6079.7          | 488.9           |
| 6   | 6101.0          | 462.2           | 6037.5          | 487.5           |
| 7   | 6097.7          | 462.3           | 6020.0          | 487.0           |
| 8   | 6099.1          | 461.9           | 6015.6          | 486.6           |
| 9   | 6097.0          | 462.0           | 6010.9          | 486.5           |
| 10  | 6097.7          | 462.0           | 6009.5          | 486.3           |

Table II. Numbers of non-zero coefficients before and after operating the random choice matrix $M_{\{q(L)\}}$ to the state $\hat{H}M_{\{q(L-1)\}} \cdots \hat{H}M_{\{q(1)\}} | \psi_E \rangle$ for the $4 \times 4$ SS model obtained from $10^4$ samples with $\epsilon = 0.1.$
Table III. $S = 0$ results on $\langle \langle E_{A_{\eta}}(L) \rangle \rangle_{\text{amp}}/J^L$ obtained for the $8 \times 8$ SS model by the SSS method with $n_{\text{amp}} = 10^4$, $\epsilon = 0.001$ and $\delta = 0.00001$.  

| $L$ | $J'/J = 0.55$ | $J'/J = 0.60$ | $J'/J = 0.65$ | $J'/J = 0.70$ | $J'/J = 0.75$ |
|-----|----------------|----------------|----------------|----------------|----------------|
| 1   | $(0.23268865 \pm 0.00000027) \times 10^2$ | $(0.23467222 \pm 0.00000030) \times 10^2$ | $(0.23680656 \pm 0.00000033) \times 10^2$ | $(0.24149807 \pm 0.00000039) \times 10^2$ | $(0.24149807 \pm 0.00000039) \times 10^2$ |
| 2   | $(0.5414619 \pm 0.0000011) \times 10^3$ | $(0.5507468 \pm 0.0000012) \times 10^3$ | $(0.5608338 \pm 0.0000014) \times 10^3$ | $(0.5833748 \pm 0.0000016) \times 10^3$ | $(0.5833748 \pm 0.0000016) \times 10^3$ |
| 3   | $(0.12600061 \pm 0.00000047) \times 10^5$ | $(0.12925980 \pm 0.00000050) \times 10^5$ | $(0.13283432 \pm 0.00000055) \times 10^5$ | $(0.14095261 \pm 0.00000067) \times 10^5$ | $(0.14095261 \pm 0.00000067) \times 10^5$ |
| 4   | $(0.2932180 \pm 0.0000036) \times 10^6$ | $(0.3033880 \pm 0.0000032) \times 10^6$ | $(0.3146405 \pm 0.0000031) \times 10^6$ | $(0.3406212 \pm 0.0000035) \times 10^6$ | $(0.3406212 \pm 0.0000035) \times 10^6$ |
| 5   | $(0.682344 \pm 0.000021) \times 10^7$ | $(0.712097 \pm 0.000032) \times 10^7$ | $(0.745321 \pm 0.000023) \times 10^7$ | $(0.782349 \pm 0.000028) \times 10^7$ | $(0.823245 \pm 0.000029) \times 10^7$ |
Table IV. $S = 1$ results on $\langle \langle E_{\Lambda(\eta)}(L) \rangle \rangle_{\text{smpl}}$ for the $8 \times 8$ SS model by the SSS method with $n_{\text{smpl}} = 10^4$, $\epsilon = 0.001$ and $\delta = 0.00001$. 

| $L$ | $J'/J = 0.55$ | $\langle \langle E_{\Lambda(\eta)}(L) \rangle \rangle_{\text{smpl}}/J^L$ | $J'/J = 0.60$ | $J'/J = 0.65$ | $J'/J = 0.70$ | $J'/J = 0.75$ | $J'/J = 0.80$ |
|-----|----------------|---------------------------------|----------------|----------------|----------------|----------------|----------------|
| 1   | $-(0.23403813 \pm 0.00000013) \times 10^2$ | $-(0.23504307 \pm 0.00000016) \times 10^2$ |
| 2   | $(0.54774476 \pm 0.00000056) \times 10^3$ | $(0.55246007 \pm 0.00000065) \times 10^3$ |
| 3   | $-(0.12819601 \pm 0.00000026) \times 10^5$ | $-(0.12985518 \pm 0.00000029) \times 10^5$ |
| 4   | $(0.3000356 \pm 0.00000021) \times 10^6$ | $(0.3052268 \pm 0.00000022) \times 10^6$ |
| 5   | $-(0.702218 \pm 0.000023) \times 10^7$ | $-(0.717444 \pm 0.000027) \times 10^7$ |
| 1   | $-(0.23622014 \pm 0.00000019) \times 10^2$ | $-(0.23762394 \pm 0.00000024) \times 10^2$ |
| 2   | $(0.55801950 \pm 0.00000081) \times 10^3$ | $(0.5647149 \pm 0.0000010) \times 10^3$ |
| 3   | $-(0.13182375 \pm 0.00000034) \times 10^5$ | $-(0.13421698 \pm 0.00000042) \times 10^5$ |
| 4   | $(0.3114219 \pm 0.00000023) \times 10^6$ | $(0.3190188 \pm 0.00000023) \times 10^6$ |
| 5   | $-(0.735702 \pm 0.000014) \times 10^7$ | $-(0.758308 \pm 0.000017) \times 10^7$ |
| 1   | $-(0.23936605 \pm 0.00000029) \times 10^2$ | $-(0.24150001 \pm 0.00000036) \times 10^2$ |
| 2   | $(0.5731340 \pm 0.0000012) \times 10^3$ | $(0.5835473 \pm 0.0000015) \times 10^3$ |
| 3   | $-(0.13726176 \pm 0.00000049) \times 10^5$ | $-(0.14106434 \pm 0.00000057) \times 10^5$ |
| 4   | $(0.3287936 \pm 0.0000028) \times 10^6$ | $(0.3411166 \pm 0.0000030) \times 10^6$ |
| 5   | $-(0.787688 \pm 0.000021) \times 10^7$ | $-(0.825086 \pm 0.000022) \times 10^7$ |
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| $J'/J$ | $S_{2Er}$ | $S_{fit}$ | $q_0\ fit$ | $E_{fit}/J$ | $E^{(1)}/J$ | $E^{(2)}/J$ | $E^{(3)}/J$ |
|--------|-----------|-----------|------------|-------------|-------------|-------------|-------------|
| 0.55   | 1.1 $\times 10^{-9}$ | 3.7 $\times 10^{-10}$ | 0.995 | -23.276 | -23.269 | -23.272 | -23.273 |
| 0.60   | 2.1 $\times 10^{-9}$ | 8.4 $\times 10^{-11}$ | 0.994 | -23.478 | -23.467 | -23.473 | -23.476 |
| 0.65   | 1.1 $\times 10^{-9}$ | 8.5 $\times 10^{-11}$ | 0.988 | -23.700 | -23.681 | -23.691 | -58.851 |
| 0.70   | 1.6 $\times 10^{-9}$ | 1.7 $\times 10^{-10}$ | 0.979 | -23.942 | -23.909 | -23.927 | - |
| 0.75   | 1.3 $\times 10^{-9}$ | 3.6 $\times 10^{-10}$ | 0.975 | -24.196 | -24.150 | -24.178 | -24.183 |

Table V. Results from the fit and from the Lanczos-like evaluation for S=0 data in Table III.

| $J'/J$ | $S_{2Er}$ | $S_{fit}$ | $q_0\ fit$ | $E_{fit}/J$ | $E^{(1)}/J$ | $E^{(2)}/J$ | $E^{(3)}/J$ |
|--------|-----------|-----------|------------|-------------|-------------|-------------|-------------|
| 0.55   | 1.1 $\times 10^{-9}$ | 4.9 $\times 10^{-11}$ | 0.986 | -23.410 | -23.404 | -23.408 | - |
| 0.60   | 1.4 $\times 10^{-9}$ | 5.4 $\times 10^{-12}$ | 0.994 | -23.509 | -23.504 | -23.506 | -23.507 |
| 0.65   | 4.2 $\times 10^{-10}$ | 2.7 $\times 10^{-10}$ | 0.995 | -23.629 | -23.622 | -23.626 | -23.626 |
| 0.70   | 5.6 $\times 10^{-10}$ | 4.9 $\times 10^{-11}$ | 0.991 | -23.780 | -23.762 | -23.776 | - |
| 0.75   | 8.2 $\times 10^{-10}$ | 2.2 $\times 10^{-10}$ | 0.978 | -23.982 | -23.937 | -23.967 | -23.969 |
| 0.80   | 8.1 $\times 10^{-10}$ | 3.8 $\times 10^{-10}$ | 0.971 | -24.223 | -24.150 | -24.205 | -24.209 |

Table VI. Results from the fit and from the Lanczos-like evaluation for S=1 data in Table IV.
Fig. 1. A schematic view of the Shastry-Sutherland (SS) model on a $8 \times 8$ lattice. Solid lines represent the inter-dimer coupling ($J'$) and other lines do the intra-dimer coupling ($J$).

Fig. 2. Distributions of coefficients for the $4 \times 4$ SS model in the normal representation (the dashed line) and in the restructured representation (the solid line). The ordinate is the absolute values of each coefficient $c'_{i'}$ while the abscissa denotes the basis number $i'$ reordered so that $|c'_{i'}| \geq |c'_{j'}|$ holds for $i' < j'$.
The dotted line is the spin gap estimated by the perturbation theory up to the fifth order.$^{17}$

Fig. 3. Results for $S = 0$ energy difference for the $8 \times 8$ SS model obtained by the Stochastic State Selection (SSS) method with the fit and the Operator Variational (OV) method.$^{17}$ Here $E_0 = -24.0J$ is the ground state energy in the singlet dimer phase.

Fig. 4. Results for $S = 1$ energy difference for the $8 \times 8$ SS model obtained by the SSS method with the fit and the OV method.$^{17}$ The dotted line is the spin gap estimated by the perturbation theory up to the fifth order.$^{17}$