Exact diagonalization of quantum-spin models

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We have developed a technique to replace hashing in implementing the Lanczös method for exact diagonalization of quantum-spin models that enables us to carry out numerical studies on substantially larger lattices than previously studied. We describe the algorithm in detail and present results for the ground-state energy, the first-excited-state energy, and the spin-spin correlations on various finite lattices for spins $S=\frac{1}{2}$, 1, $\frac{3}{2}$, and 2. Results for an infinite system are obtained by extrapolation. We also discuss the generalization of our method to other models.

I. INTRODUCTION

Studies of quantum-spin models have been an important subject in many-body physics for a long time. Experimental and theoretical studies have shown, in many magnetic materials, electrons are quite localized because of strong Coulomb repulsion, and from first-principles calculations it can be shown that the interaction between electrons may be well represented by model Hamiltonian describing a set of interacting spins $\mathbf{S}_i$.[1] An important class of such interacting spin models consists of spins coupled bilinearly to their nearest neighbors on a finite lattice of size N. The Hamiltonian for such a system takes the form:

$$H=\sum_{\langle i,j\rangle}(J_x S_i^x S_j^x+J_y S_i^y S_j^y+J_z S_i^z S_j^z)\ , \tag{1}$$

where $\langle i,j\rangle$ denotes all nearest-neighbor pairs on a lattice. S_i^α is spin operator on site i and has the value of $S_i^a=-S,\ -S+1,\ldots,S$. This Hamiltonian describes the antiferromagnetic (ferromagnetic) Heisenberg model when $J_x=J_y=J_z\equiv J>0(<0)$, the XY model when $J_z=0$ and $J_x=J_y$, and the XXZ model when $J_x=J_y$. In one dimension the XXZ model has been diagonalized analytically by means of the Bethe Ansatz.[2] However, the use of the Bethe Ansatz solution is quite limited. Using exact diagonalization techniques, quantum-spin models have been studied numerically by many people. The pioneering calculations on finite lattices in one dimension were performed by Bonner Fisher[3] in 1964 for the Ising-Heisenberg model and in two dimensions by Oitmaa and Betts[4] in 1978 for the antiferromagnetic Heisenberg model the XY model with spin $S=\frac{1}{2}$. Later many exact diagonalization studies were carried out[5] for spin-$\frac{1}{2}$ and higher spins, especially for spin-1 chains to test Haldane's conjecture[6] that for integer-spin chains there is a gap in the excitation spectrum whereas for half-integer-spin chains the gap is absent. The biggest lattices studied by exact diagonalization techniques in previous studies have been[5] 27 sites for $S=\frac{1}{2}$, 14 sites for $S=1$, 12 sites for $S=\frac{3}{2}$, and 10 sites for $S=2$, etc. Using our new coding technique, we have been able to perform exact diagonalizations on 32 sites (square lattice) and 30 sites (ring) for $S=\frac{1}{2}$, 18 sites for $S=1$, 14 sites for $S=\frac{3}{2}$, and 12 sites for $S=2$.

In the following section we describe in detail the new coding technique we have developed for diagonalizing quantum-spin models and illustrate the method by an example. In Sec. III we study the ground-state energy and spin-spin correlations on various lattices and give our estimates for the infinite system. Finally, we discuss the generalization of our technique to other models in Sec. IV.

II. METHODOLOGY

The simplest way to study the model Hamiltonian defined by Eq. (1) numerically is simply to obtain the matrix elements of H in a basis of $\{S_i^z;i=1,2,\ldots,N\}$, where we chose the z axis as the quantization direction, and then diagonalize the H matrix by using standard eigenvalue routines on computer. For a spin-S system of size N the number of degrees of freedom is $(2S+1)^N$. To date the biggest matrix that can be diagonalized by this direct approach on a modern computer is about $10\,000\times10\,000$, which corresponds to a spin-$\frac{1}{2}$ system of size 13. In order to be able to study the model Hamiltonian on larger lattices certain methodological improvements must be made.

The first thing one can do is to use various symmetry operators in order to write the H matrix as a direct product of several smaller matrices. Usually, these symmetries consist of conservation of total magnetization along a chosen quantization direction, say, the z direction (S_z conservation); translational invariance (if we impose periodic boundary conditions); rotational invariance; and reflection invariance of the system. Use of these symmetry operators one can reduce the size of the H matrix significantly. For example, the biggest size of the H matrix of a 4×4 periodic square lattice with spin $S=\frac{1}{2}$ is 153 when all symmetries are applied. Obviously this is much smaller than $2^{16}=65\,536$. One can also use total spin S to reduce further the size of the H matrix. However, this constraint is rather complicated to program, especially if one intends to vectorize the code to take advantage of the architecture of certain machines. Moreover

the total spin S is a conserved quantity only when the Hamiltonian is rotationlly invariant in spin space and that is a severe restriction on the parameter space ($|J_x|=|J_y|=|J_z|$ at least). So we will usually not use this symmetry.

The second thing one can do is to calculate the eigenvalues and eigenvectors of only a few states, say, the ground state and the first excited state. By doing so, one needs not to store the whole H matrix, which requires a memory of $M\times M$ words where M is the size of the Hilbert space, but only a few vectors of length M. In applications, we usually need at most three vectors of length M. Nevertheless, this forms a strong limit on the maximum system size one can study. There exist several well-documented algorithms for obtaining the largest or the smallest eigenvalue and eigenvector; the Lanczös method[7] is one of them. Using symmetries and the Lanzös method, we have been able to calculate properties of the ground state and the first excited state for a spin-$\frac{1}{2}$ system on a two-dimensional square lattice of size 32.[8] Needless to say, the direct approach, leading to matrix of size 2^{32}, is unfeasible.

We are in position to describe the new coding technique we used in diagonalizing quantum-spin models on finite lattices. For clarity, we will describe our method in two subsections. For purposes of illustration, we will use a six-site spin-$\frac{1}{2}$ system with total magnetization zero as an example to explain things in detail when necessary. The total number of spin configurations of the system is $6!/3!3!=20$.

A. Coding with only total S_z conservation

We start with our method for the case in which no symmetries except total S_z conservation are used. This not uncommon in practice. For instance, periodic boundary conditions cannot be imposed when the interactions between spins are different on different bonds that connect spin pairs. Consider a system with spin-S of size N and total z-component of spin S_z^t. The Hilbert space is composed by all possible spin configurations $\{S_i^z; i=1,\ldots,N\}$ consistent with the given value of total magnetization $S_z^t=\sum_{i=1}^{N}S_i^z$, and its dimension is M ($M\ll(2S+1)^N$). Note that the choice of the labeling of the basis state is quite arbitrary, but once the basis states have been labeled, it must be treated consistently. Any vector is a linear combinations of these basis states,

$$\phi=\sum_{j=1}^{M}C_j|j\rangle\ , \tag{2}$$

where C_j are the coefficients. To implement numerical calculations we need to know how to represent efficiently both a given spin configuration and the action of H on this spin configuration. The first part is readily solved by the widely used method of defining an integer I according to

$$I=\sum_{i=1}^{N}s(i)(2S+1)^{i-1}\ , \tag{3}$$

where $s(i)\equiv S_i^z+S=0,\ 1,\ldots,2S$, as the representative of the spin configuration $\{S_z^1,S_z^2,\ldots,S_z^N\}$. This is a one-to-one correspondence between a single integer and a spin configuration. If there were no restriction on S_z^t, then all I's from 1 to $(2S+1)^N$ would be allowed. Since we are considering only the restricted subspace of fixed S_z^t, only M of the I's actually occur and we to have to introduce a "storage/lookup table" labeling them in an arbitrary way $|1\rangle,|2\rangle,\ldots,|M\rangle$. When the Hamiltonian H operates on one such configuration, many other configurations are generated because of the spin-flip terms in Eq. (1). The problem is to find the locations of these configurations in the storage table. A naive way of performing search is to introduce a vector defined by $J(I)$=position of the configuration represented by integer I in the storage table, as shown in Table I for our example. However, one immediately sees that the length of this vector $J(I)$ can be as long as $(2S+1)^N$ and will, in general, contain many null entries. For a spin-$\frac{1}{2}$ system of size 24, the length of the vector $J(I)$ already exceeds memory space of the most advanced present computers. Hence this is certainly not an appropriate approach, especially when studies on large lattices are desired.

A better way of searching is to use the "hashing technique." The main idea is to construct a hashing function $h(I)$ which gives a correspondence between the representatives $\{I\}$ and a position vector $h(I)$. For example, we can define a hashing function by

$$h(I)=[I(\mathrm{mod}K)]+1\ ,$$

which is commonly used in practice.[9] It is easy to see that the size of memory to be used is about K, which is the order of M (in practice, one usually picks K to be the smallest prime number that larger than M). In general, it may occur that different representatives $I_1,I_2,\ldots,$ corresponding to the same value of the hashing function, a phenomena called "collisions;" this is shown in Table I for $I=26$ and 49 if $K=23$, for example. Although one can try hard to find a good hashing function so as to minimize the number of collisions, it is almost impossible to construct a hashing function that has no collisions at all. Readers interested in using the hashing technique can find a detailed description of this algorithm in most books of computer science, say Ref. 9. Gagliano *et al.* have used the hashing technique in finite lattice calculations for rings up to 24 sites.[10]

It is obvious that calculations can be more efficient if one can construct an algorithm that is both a one-to-one correspondence between a representative I and its position in the storage table and also requires very little memory space. A hint for how to develop such an algorithm comes from observing that the length of vector $J(I)$ is so long because we are in effect doing a one-dimensional sequential search. Therefore, it is naturally to try a two-dimensional (2D) search. Let us divide the lattice into two parts A and B and define two integers by

$$\begin{aligned} I_a&=\sum_{i=1}^{[N/2]}s(i)(2S+1)^{i-1}\ ,\\ I_b&=\sum_{i=1}^{[N+1/2]}s(i+[N/2])(2S+1)^{i-1}\ , \end{aligned} \tag{4}$$

TABLE I. Spin configurations, their representations I, their positions in the storage table $J(I)$ by using a naive way of searching (see the text) for a spin-$\frac{1}{2}$ system of size 6. A hashing function $h(I)=[I(\mathrm{mod}K)]+1$ with $K=23$ is also shown.

Configuration	I	$J(I)$	$h(I)$	Configuration	I	$J(I)$	$h(I)$
0 0 0 1 1 1	7	1	8	1 0 0 0 1 1	35	11	13
0 0 1 0 1 1	11	2	12	1 0 0 1 0 1	37	12	15
0 0 1 1 0 1	13	3	14	1 0 0 1 1 0	38	13	16
0 0 1 1 1 0	14	4	15	1 0 1 0 0 1	41	14	19
0 1 0 0 1 1	19	5	20	1 0 1 0 1 0	42	15	20
0 1 0 1 0 1	21	6	22	1 0 1 1 0 0	44	16	22
0 1 0 1 1 0	24	7	2	1 1 0 0 0 1	49	17	4
0 1 1 0 0 1	25	8	3	1 1 0 0 1 0	50	18	5
0 1 1 0 1 0	26	9	4	1 1 0 1 0 0	52	19	7
0 1 1 1 0 0	28	10	6	1 1 1 0 0 0	56	20	11

where $[X]$ means the integer part of number X. Correspondingly, we define two vectors $J_a(I_a)$ and $J_b(I_b)$ so that the position of the configuration represented by integer I is given by

$$J=J_a(I_a)+J_b(I_b)\ . \tag{5}$$

We show this method of coding for our example in Table II. Note that this division can be applied to an arbitrary lattice. It is easy to see that

$$I=(2S+1)^{[N/2]}I_a+I_b$$

and that (J_a,J_b) behaves just like a two-dimensional coordinate (x,y); thus we call one of the J's the "base vector" and the other the "position vector." The advantage of introducing vector J_a and J_b is that the maximum length of $J_a(I_a)$ and $J_b(I_b)$ is $(2S+1)^{[(N+1)/2]}$ which is about the square root of that of $J(I)$. This is certainly a considerable improvement, since for a spin-$\frac{1}{2}$ system of size 32 this number is only $2^{16}=65\,536$. When a configuration represented by I is changed to another configuration represented by $\tilde{I}$ due to spin-flip operator, we can find $\tilde{I}_a$ and $\tilde{I}_b$, and then $\tilde{J}$ easily. It is easy to see that this method of coding gives a one-to-one correspondence between configurations and their position in the storage table and uses very little memory space for searching. It is also automatically vectorized on a vector machine. One can reduce still further the memory space used for searching by generalizing this method to three or higher-dimensional searches. In principle, the minimum amount of computer memory space needed is $(2S+1)N$. However, one needs more computations to accomplish such a

TABLE II. Spin configurations, their representations I_a and I_b, their base vectors $J_a(I_a)$ and position vectors $J_b(I_b)$ and their positions in the storage table $J(I)$ by using the new coding technique for unsymmetrized basis (see the text) for a spin-$\frac{1}{2}$ system of size six.

Configuration A	I_a	$J_a(I_a)$	Configuration B	I_b	$J_b(I_b)$	$J=J_a+J_b$
1 1 1	7	1	0 0 0	0	0	1
0 1 1	3	1	0 0 1	1	1	2
1 0 1	5	2	0 0 1	1	1	3
1 1 0	6	3	0 0 1	1	1	4
0 1 1	3	1	0 1 0	2	4	5
1 0 1	5	2	0 1 0	2	4	6
1 1 0	6	3	0 1 0	2	4	7
0 1 1	3	1	1 0 0	4	7	8
1 0 1	5	2	1 0 0	4	7	9
1 1 0	6	3	1 0 0	4	7	10
0 0 1	1	1	0 1 1	3	10	11
0 1 0	2	2	0 1 1	3	10	12
1 0 0	4	3	0 1 1	3	10	13
0 0 1	1	1	1 0 1	5	13	14
0 1 0	2	2	1 0 1	5	13	15
1 0 0	4	3	1 0 1	5	13	16
0 0 1	1	1	1 1 0	6	16	17
0 1 0	2	2	1 1 0	6	16	18
1 0 0	4	3	1 1 0	6	16	19
0 0 0	0	1	1 1 1	7	19	20

high-dimensional search, so there is a balance between use of computer time and memory. Recalling that the real limitation is the ability to store a few vectors of length M, we think that two-dimensional search is good enough in practice.

B. Coding with translational symmetry

The method described in the previous subsection is simple. The way of dividing the lattice into two parts is arbitrary. However, this is not the case when additional symmetries are used. Suppose we impose periodic boundary conditions and use translational symmetry to reduce the size of the H matrix by a factor of N. For the example we are using, the total number of independent basis states under the translation operator is four. As we can see from Table II, several configurations correspond to the same basis under the translation operator. The vectors J_a and J_b are different for these configurations, so the relation between the translationally invariant basis and its position in the storage table is not unique unless one can find a way to overcome this difficulty. Fortunately, we have found a way of dividing the lattice that can utilize fully periodic boundary conditions and other symmetries such as reflection; we call it "sublattice coding." For simplicity we illustrate this approach on a bipartite lattice. Let us divide the lattice into the two natural sublattices so that each point in a sublattice has all its nearest neighbors in the other sublattice. Then for a given total magnetization in one sublattice, say the sublattice B, we distribute all possible spin configurations and record them as position vector J_b. Correspondingly, for spin configuration in sublattice A we record only those configurations that are distinct under the translation operator in its own sublattice and record them as base vector J_a. We show all these for our example in Table III, where the symmetrized basis states are printed in bold. Note that the total magnetization in one sublattice is fixed once it is fixed in the other sublattice and that it ranges from $-(N/2)S$ to $(N/2)S$. However, when translated by one lattice spacing, the two sublattices exchange with each other so we only need to do half the work. As we can see from Table III, for our example, the relation between the translationally invariant basis and its position in the storage table specified by J_a+J_b is a unique one.

Another consideration is that one has to record W, the weight of the translationally invariant basis. Interesting enough for a spin-$\frac{1}{2}$ system with total magnetization zero and size $2P$, where P is an prize integer, the weight of all translational basis state is the same ($W=2P$), except for the two Néel states ($W=2$). This property reduces the amount of computation somewhat. For more general cases, we usually do not have such nice properties and we need to store the weight of the translationally invariant basis. We may have to do a little more computations but we do not need more memory space. We can simply put W into the same word in which we put I, since for most computers each word is of 32 or 64 bits long.

In addition to periodic boundary conditions, there are other symmetries that we can use to reduce further the size of matrices to be diagonalized. Use of these symmetries may complicate actual programming, but we still have a one-to-one correspondence between the representatives of symmetrized basis and their positions in the storage table and have used very little central processing unit (CPU) time and memory space in searching. The way of dividing the lattice depends on the structure of the

TABLE III. Spin configurations, their representations I_a and I_b, their base vectors $J_a(I_a)$ and position vectors $J_b(I_b)$ and their positions in the storage table $J(I)$ by using the "sublattice coding" method for symmetrized basis (see the text) for a spin-$\frac{1}{2}$ system of size six.

Configuration A	I_a	$J_a(I_a)$	Configuration B	I_b	$J_b(I_b)$	$J=J_a+J_b$
1 1 1	**7**	**1**	**0 0 0**	**0**	**0**	**1**
0 0 0	0		1 1 1	7		
0 1 1	**6**	**1**	**0 0 1**	**4**	**1**	**2**
1 0 0	1		0 1 1	6		
1 0 1	5		1 0 0	1		
0 1 0	2		1 0 1	5		
1 1 0	3		0 1 0	2		
0 0 1	4		1 1 0	3		
0 1 1	**6**	**1**	**0 1 0**	**2**	**2**	**3**
0 0 1	4		0 1 1	6		
1 0 1	5		0 0 1	4		
1 0 0	1		1 0 1	5		
1 1 0	3		1 0 0	1		
0 1 0	2		1 1 0	3		
0 1 1	**6**	**1**	**1 0 0**	**1**	**3**	**4**
0 1 0	2		0 1 1	6		
1 0 1	5		0 1 0	2		
0 0 1	4		1 0 1	5		
1 1 0	3		0 0 1	4		
1 0 0	1		1 1 0	3		

TABLE IV. Dimension of the Hilbert space, the ground-state energy, the first-excited-state energy, and spin-spin correlations of the one-dimensional antiferromagnetic Heisenberg model for spin $S=1$, $N=16$ and 18; spin $S=\frac{3}{2}$, $N=14$; spin $S=2$, $N=12$.

	$S=1$		$S=\frac{3}{2}$	$S=2$
	$N=18$	$N=16$	$N=14$	$N=12$
M	1 228 686	168 181	904 274	818 836
E_0/N	−1.402 351	−1.402 925	−2.839 815	−4.784 014
E_1/N	−1.378 338	−1.375 251	−2.813 935	−4.751 456
$\langle S_0^\alpha S_1^\alpha \rangle$	−0.467 459	−0.467 642	−0.946 605	−1.594 671
$\langle S_0^\alpha S_2^\alpha \rangle$	0.253 017	0.254 293	0.634 030	1.178 345
$\langle S_0^\alpha S_3^\alpha \rangle$	−0.197 618	−0.200 288	−0.556 226	−1.075 912
$\langle S_0^\alpha S_4^\alpha \rangle$	0.147 493	0.151 699	0.483 503	0.980 035
$\langle S_0^\alpha S_5^\alpha \rangle$	−0.122 197	−0.128 493	−0.455 502	−0.952 506
$\langle S_0^\alpha S_6^\alpha \rangle$	0.101 611	0.110 173	0.430 433	0.929 418
$\langle S_0^\alpha S_7^\alpha \rangle$	−0.090 514	−0.102 287	−0.429 266	
$\langle S_0^\alpha S_8^\alpha \rangle$	0.083 041	0.098 424		
$\langle S_0^\alpha S_9^\alpha \rangle$	−0.081 420			

lattice. One needs some practice to discover the way that can most efficiently utilize all the symmetries of the system and extra work may be needed in some cases.

We have performed exact diagonalizations of the *XXZ* model on various lattices by using the standard Lanczös method[7] and the coding technique we have just described. The largest lattice sizes we have been able to study are 32 sites (square lattice) and 30 sites (ring) for $S=\frac{1}{2}$, 18 sites for $S=1$, 14 sites for $S=\frac{3}{2}$, and 12 sites for $S=2$. The accuracy in our calculations is within 10^{-12} for the eigenvalues and 10^{-6} for the eigenvectors and expectation values, such as spin-spin correlation functions. As a check, the normalization of the wave function at the final iteration step is 1 to within 10^{-12} and the total spin S, a conserved quantity when the Hamiltonian is rotational invariant in spin space, is accurate to 10^{-18}. (For the case of spin-$\frac{1}{2}$ and spin 1 the accuracies are better than those cited). Different symmetries are used such as total momentum in the initial states to obtain the ground state and the excited states. The reason we did not do calculations on still larger lattices is not CPU time but the lack of memory space. For example, the size of the H matrix for a 6×6 spin-$\frac{1}{2}$ system after use of all symmetries is about 32 million, and we usually need at least two vectors of this size in order to calculate the ground-state energy. We do not at present have an available computer with this large memory space.

III. NUMERICAL RESULTS

In this section we present some of our results of finite lattice studies. In one dimension the spin-$\frac{1}{2}$ *XXZ* model can be solved analytically by the Bethe Ansatz,[2] and in two dimensions we have previously done extensively exact diagonalization studies,[8] so we will not present the numerical results in detail in this paper. We have also studied the spin-1 *XXZ* model in two dimensions.[11] We list the ground-state energy, the first-excited-state energy, and spin-spin correlation functions for the one dimensional antiferromagnetic Heisenberg model for systems of $S=1$, $N=16$ and 18; $S=\frac{3}{2}$, $N=14$; and $S=2$, $N=12$ in Table IV. In Table V we list similar results for spin-$\frac{1}{2}$ system in 1D for $N=28$ and 30, and in Table VI for a 2D 32 sites square lattice. We also list the size of the H matrix there for reference. Periodic boundary conditions and reflection symmetry were used in these calculations. To the best of our knowledge, results on systems of this size have not previously appeared in the literature.

Although we cannot obtain results for an infinite lattice directly, we can estimate them by extrapolation from results on various finite lattices. Usually the ground-state energy is the easiest quantity to estimate. Fortunately, we can obtain an upper and a lower bound for the

TABLE V. Dimension of Hilbert space, the ground-state energy, the first-excited-state energy, and spin-spin correlations of the one-dimensional spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model for $N=28$ and 30.

	$N=30$	$N=28$
M	2 587 018	718 146
E_0/N	−0.888 131	−0.888 403
E_1/N	−0.878 321	−0.877 164
$\langle S_0^\alpha S_1^\alpha \rangle$	−0.148 022	−0.148 067
$\langle S_0^\alpha S_2^\alpha \rangle$	0.060 973	0.061 018
$\langle S_0^\alpha S_3^\alpha \rangle$	−0.050 988	−0.051 100
$\langle S_0^\alpha S_4^\alpha \rangle$	0.035 450	0.035 571
$\langle S_0^\alpha S_5^\alpha \rangle$	−0.032 177	−0.032 377
$\langle S_0^\alpha S_6^\alpha \rangle$	0.025 821	0.026 037
$\langle S_0^\alpha S_7^\alpha \rangle$	−0.024 409	−0.024 716
$\langle S_0^\alpha S_8^\alpha \rangle$	0.021 000	0.021 331
$\langle S_0^\alpha S_9^\alpha \rangle$	0.020 400	−0.020 842
$\langle S_0^\alpha S_{10}^\alpha \rangle$	0.018 322	0.018 798
$\langle S_0^\alpha S_{11}^\alpha \rangle$	−0.018 189	−0.018 809
$\langle S_0^\alpha S_{12}^\alpha \rangle$	0.016 844	0.017 514
$\langle S_0^\alpha S_{13}^\alpha \rangle$	−0.017 053	−0.017 916
$\langle S_0^\alpha S_{14}^\alpha \rangle$	0.016 179	0.017 119
$\langle S_0^\alpha S_{15}^\alpha \rangle$	−0.016 701	

TABLE VI. Dimension of the Hilbert space, the ground-state energy, the first-excited-state energy, and spin-spin correlations of the two-dimensional spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on a 32-site lattice.

M	2 357 871
E_0/N	−1.360 358
E_1/N	−1.340 671
r/a	$\langle S_0^a S_r^a \rangle$
0	0.250 000
1	−0.113 363
$\sqrt{2}$	0.069 670
2	0.062 469
$\sqrt{5}$	−0.060 989
$2\sqrt{2}$	0.057 801
3	−0.056 794
$\sqrt{10}$	0.055 484
4	0.053 884

ground-state energy at fixed N. It is easy to show that for chains with open boundary conditions the energy per site $E(N)/N$ gives an *upper* bound and the energy per bond $E(N)/(N-1)$ gives a *lower* bound for the infinite chain. We prove this result by using a variational approach. To simplify the proof we restrict ourselves to the isotropic case, i.e., $J_x=J_y=J_z\equiv J$. Generalization to the *XXZ* model is straightforward. Consider an open chain of size $2N$, and set $J=1$,

$$H=\sum_{i=1}^{2N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}=\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\sum_{i=N+1}^{2N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\mathbf{S}_N\cdot\mathbf{S}_{N+1}$$
$$+H_1+H_2+\mathbf{S}_N\cdot\mathbf{S}_{N+1}\ . \tag{6}$$

Let the variational wave function be a direct product of eigenfunctions of systems $\{\mathbf{S}_1,\mathbf{S}_2,\ldots,\mathbf{S}_N\}$ and $\{\mathbf{S}_{N+1},\mathbf{S}_{N+2},\ldots,\mathbf{S}_{2N}\}$,

$$\Psi_{\rm var}=\Psi(\mathbf{S}_1,\ldots,\mathbf{S}_N)\Psi(\mathbf{S}_{N+1},\ldots,\mathbf{S}_{2N})\ . \tag{7}$$

Then by the variational principle we have,

$$E_{2N}<\langle\Psi_{\rm var}|H_1+H_2+\mathbf{S}_N\cdot\mathbf{S}_{N+1}|\Psi_{\rm var}\rangle$$
$$=E_N+E_N+\langle\Psi_{\rm var}|\mathbf{S}_N\cdot\mathbf{S}_{N+1}|\Psi_{\rm var}\rangle=2E_N\ , \tag{8}$$

and this leads to $E_{2N}/2N<E_N/N$, hence $\lim_{N\to\infty}E_N/N<E_N/N$. Similarly we can use the eigenfunctions of system $\{\mathbf{S}_1,\mathbf{S}_2,\ldots,\mathbf{S}_{2N}\}$ as the variational wave function to show that

$$\lim_{N\to\infty}[E_N/(N-1)][E_N/(N-1)]\ .$$

These upper and lower bounds help us to determine the ground state energy more accurately. In Figs. 1–3 we plot the ground-state energy per site and per bond as functions of $1/N$ for various finite-size chains with open boundary conditions for spin $S=1$, $\frac{3}{2}$, and 2. We also show the ground-state energy per bond for chains with periodic boundary conditions (rings) there. Using least-squares approximation, our estimates of the ground-state energy for the infinite system are the following:

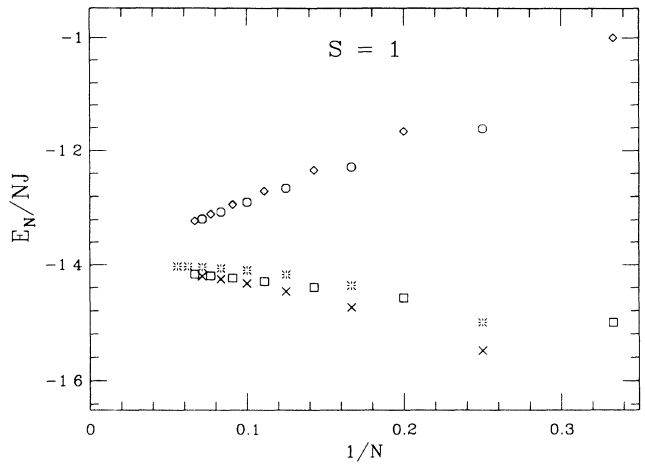

FIG. 1. Spin $S=1$ antiferromagnetic Heisenberg model. Plot of the ground-state energy per site E_N/NJ for chains of odd N (diamonds), chains of even N (octagons), and rings (bursts); and the ground state per bond $E_N/(N-1)J$ for chains of odd N (squares), and chains of even N (crosses).

$E(S=1)=-1.4051-0.0002$, $E(S=3/2)=-2.0987\pm0.0005$, and $E(S=2)=-4.8965\pm0.0002$. As a check, we have used the same procedure for the case of spin-$\frac{1}{2}$ chains and obtained $E(S=\frac{1}{2})=-0.4434\pm0.0003$, compared with the exact value 0.4431. We believe that our estimated values are within 0.1% accuracy of the exact values.

IV. DISCUSSION

In preceding sections we have described explicitly the new coding technique we used in the exact diagonalization of quantum-spin models on finite lattices. Using what we call sublattice coding" method, we were able to carry out exact diagonalizations for lattices up to 32 sites for spin-$\frac{1}{2}$ system, 18 sites for spin-1 system, 14 sites for

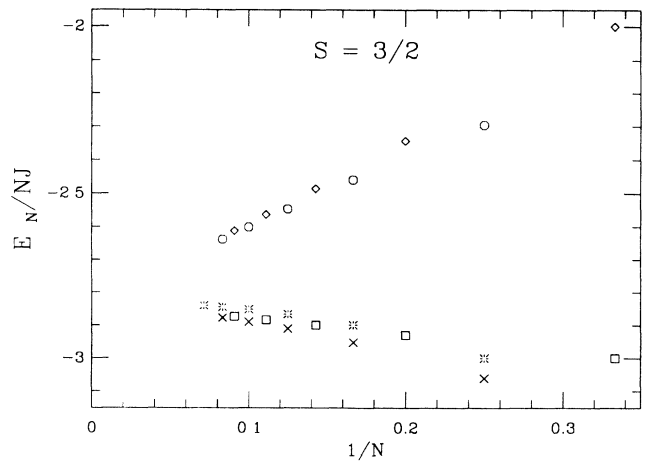

FIG. 2. Same as Fig. 1 for spin $S=\frac{3}{2}$.

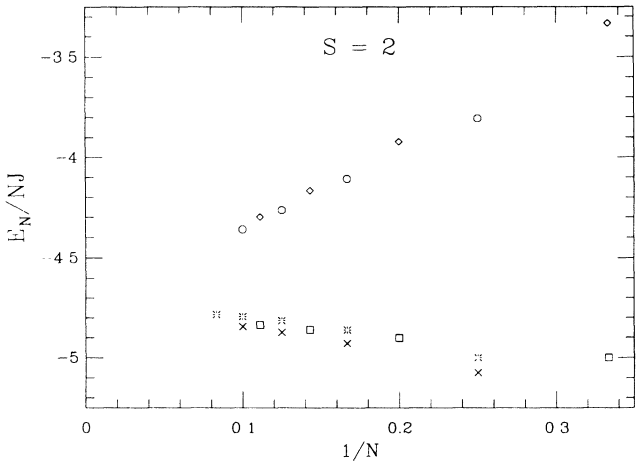

FIG. 3. Same as Fig. 1 for spin $S=2$.

spin-$\frac{3}{2}$ system, and 12 sites for spin-2 system. As we pointed out at the end of Sec. II B, our method is not limited by the CPU time but by the computer memory. One may hope that many configurations give such small contributions to the wave function that one may throw them away and store only "important configurations." If this is the case, then one may perform numerical calculations on much bigger lattices and the "sublattice coding" method is still useful.

We can apply the idea of "sublattice coding" method in finite lattice studies of other model Hamiltonians. For example, for a many-body model Hamiltonian with fermions, such as Hubbard model, we can either treat fermions as a spin-$\frac{3}{2}$ object on each site or use a binary number representing the spin up electrons configuration as the base vector and that for spin down electrons as the position vector. By doing so we again have a one-to-one correspondence between the representatives of basis and its position in the storage table, and the computer cost of searching is again very little. However, we would like to point out that when dealing with fermions one should be careful about the sign because of the Pauli principle, and the way of dividing the lattice depends on the problem one is trying to solve.

We can certainly use our method to study more general quantum-spin models, such as those containing the terms $D\sum_i(\mathbf{S}_i)^2$ or $\lambda\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j)^2$ in Eq. (1). The parameter spaces of such model Hamiltonians are obviously very large, but they contain much more interesting physics. Finite lattice exact diagonalization is a very useful tool to explore these interesting physics models. One may argue that there is always a limit for numerical calculations on finite lattices and that wrong answers may be deduced if the lattice is not big enough. However, this only tells us that one must be very careful in interpreting numerical results. Recently there has been a claim that one can deal with logarithmic corrections on chains of moderate length,[12] say a 20-site spin-$\frac{1}{2}$ chain. With the help of a correct finite-size scaling scheme, we should be able to obtain the correct physics from finite lattice studies.

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