

Finite-lattice extrapolations for a Haldane-gap antiferromagnet

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(Received 21 January 1994)

We present results of exact diagonalizations of the isotropic antiferromagnetic $S = 1$ Heisenberg chain by the Lanczos method, for finite rings of up to $N = 22$ sites. The Haldane gap $G(N)$ and the ground-state energy per site $e(N)$ converge, with increasing N , faster than a power law. By Vanden Broeck-Schwartz and Shanks transformations, the extrapolated values are $G(\infty) = 0.41049(2)$ and $e(\infty) = -1.401485(2)$. The spin-spin correlation function is well fit by $\exp(-r/\xi)/\sqrt{r}$ with $\xi = 6.2$.

I. INTRODUCTION

A great variety of magnetic phenomena can be understood by the study of classical spin systems. However, we know that there are some surprises from quantum mechanics in one-dimensional spin systems. Haldane has conjectured¹ that the properties of the one-dimensional Heisenberg antiferromagnet are qualitatively different depending on whether the spin is integer or half-integer. This intriguing argument applies notably to the simple prototypical antiferromagnetic (AF) $S = 1$ spin chain which, according to Haldane, should exhibit a gap (G) towards spin excitations. This conjecture has been checked experimentally, in particular with the compound NENP $[\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4]$ for which inelastic neutron scattering and susceptibility measurements have clearly shown the existence of a spin gap.²

The Heisenberg AF $S = 1$ spin chain has been studied in many numerical works. In 1973, ten years before the Haldane conjecture, De Neef³ computed the specific heat by exact diagonalizations of the Hamiltonian for chain lengths up to $N = 8$. In 1977, Blöte⁴ diagonalized chains up to $N = 10$. In 1982, Botet and Jullien,⁵ with diagonalizations up to $N = 12$, obtained evidence for a nonvanishing gap in the thermodynamic limit. Their value for the gap was rather imprecise ($G \approx 0.25J$). After this work, other authors used exact diagonalizations with chains of increasing length: in 1984, Glaus and Schneider⁶ and Parkinson and Bonner⁷ with $N = 14$, in 1987, Moreo⁸ with $N = 16$, and in 1990, Lin⁹ with $N = 18$, a length that has also been reached by Haas *et al.*¹⁰ and Takahashi.¹¹ This growth is almost linear: two more spins every three years. In fact, the numerical complexity of an exact diagonalization is 3^N . The exponential growth of computer power is not sufficient to explain these results and much progress has been done in the algorithms. However, it is clear that it is very difficult to continue along this line of study.

With Monte Carlo methods,¹¹⁻¹⁵ longer chains can easily be studied (for example, $N = 64$), but the results have statistical as well as systematic errors (the latter being much more troublesome). In 1985, Nightingale and Blöte¹⁶ obtained a very precise estimate of the Haldane

gap $G = 0.41$ by use of a stochastic implementation of direct iteration. In this case there is a systematic bias, caused by the finite number of "walkers," that is difficult to control.

Real-space renormalization-group methods have also been applied to spin chains. The first works were quite disappointing because of large systematic errors, but in 1988 Lin and Pan,¹⁷ gave the very precise value $G = 0.4097(5)$. In 1992, White and Huse found $G = 0.41050(2)$ and a ground-state energy with a precision of 10^{-12} by an improved method, the density-matrix renormalization-group (DMRG) technique.¹⁸

Let us briefly comment on the most precise measurement of the Haldane gap itself in the present implementation of the DMRG algorithm. These works¹⁸ have used open chains for which momentum is not a good quantum number. As a consequence, it is not possible to simply measure the energy of the Haldane triplet state defined as the lowest-lying $k = \pi$, $S = 1$ state on a periodic chain. Some estimates have looked at the $(S = 1)$ - $(S = 2)$ gap with simple open boundary conditions but the most precise estimate of White and Huse uses a fine tuning of a peculiar boundary condition. In fact, on an open chain, magnon states are reflected by the boundaries to form standing waves. These standing waves can be acted upon by adjusting the boundary conditions. Since from the Affleck-Kennedy-Lieb-Tasaki¹⁹ (AKLT) picture there are effective spins $1/2$ at the end of the open chain, White and Huse have added extra spins $1/2$ coupled to the rest of the spin-1 chain by an adjustable exchange coupling J_{end} . Such a coupling allows some control over the potential energy of the one-magnon states. To select a state with a $k = \pi$ magnon one has to take $J_{\text{end}} = 0.5088$ that makes the spin and energy densities most uniform near the middle of the chain. Then the energy of this state is the Haldane gap and is measured from the ratio of the excess energy density to the spin density near the middle of the chain where effects of the end spins are minimal. The associated systematic errors (choice of J_{end} and uniformity) are not yet well studied but they are apparently small (see Table II of White and Huse). We think it is worth checking the corresponding accuracy by using a method which leads directly to the energy of the one-magnon state such as exact diagonalizations.

In this work we have used the Lanczos technique on the longest possible chain we could reach which is $N = 22$ spins and then we have applied powerful extrapolation techniques. In this strategy, the only source of error is due to the extrapolation technique while the finite-lattice numbers are limited essentially by machine accuracy.

In Sec. II, we explain the numerical method (in particular the importance of the symmetries and the quantum numbers of the Haldane triplet). The programming techniques useful for a chain length $N = 22$ are described in the Appendix. In Sec. III, we explain our extrapolation method: the Shanks and Vanden Broeck-Schwartz (VBS) transformations and how we quote errors. In Sec. IV, we apply our strategy to the Haldane gap and the ground-state energy. In Sec. V, we compare our results with those of other authors. In particular, the precision for the gap is similar to that of White and Huse¹⁸ with compatible results. In Sec. VI, our results for the correlations functions are presented. They are well described by a correlation length $\xi = 6.2$. Section VII presents our conclusions.

II. NUMERICAL METHOD

The Hamiltonian for a chain of length N is

$$H = \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad (1)$$

where the \mathbf{S}_i are the quantum spin-1 operators. The exchange constant is positive ($J = 1$) in the antiferromagnetic case. The boundary conditions are periodic ($N+1 \equiv 1$) and the length N is even to avoid frustration.

We have computed, by exact diagonalization of the Hermitian matrix H , the ground state $|0\rangle$, its energy E_0 , its spin-spin correlation functions, and the energy of the first excitation E_1 , for finite lengths up to $N = 22$ spins. The Haldane gap $G(N)$ is the difference between E_0 and E_1 , the two lowest eigenvalues. The extrapolation method, which gives an estimation of $G(\infty)$, is explained in the next section. We have used the standard Lanczos method,²⁰ which is well adapted for this problem: The matrix is very sparse and only a few extreme eigenvalues are needed.

The size of the matrix H is $3^N \times 3^N$. With the symmetries of the Hamiltonian, H is block diagonal and only the two interesting blocks, with a size smaller than 3^N , must be diagonalized. The symmetries of the lattice are the translational invariance T , and the left-right reflection Lr (Lr transforms the wave vector k to $-k$; so it reduces the size of blocks only for $k = 0$ or π). The spin symmetries are the global rotation $\mathbf{S} = \sum_i \mathbf{S}_i$ [it seems difficult to implement this symmetry, and in practice, only a subgroup of $SU(2)$ is used]. The matrix elements are computed in the z -axis basis: $\{|s_1, s_2, \dots, s_N\rangle\}$ where $s_i = -1, 0, \text{ or } 1$, are the eigenvalues of S_i^z . In this basis, $T|s_1, \dots, s_N\rangle = |s_2, \dots, s_N, s_1\rangle$ and $Lr|s_i\rangle_i = |s_{N-i}\rangle_i$. The spin symmetries that can be implemented easily are S^z , the magnetization along

the z axis (which is diagonal in the z -axis basis), and the π rotation around the x axis, $R_x = \exp(i\pi S^x)$. In this basis, $R_x|s_i\rangle_i = |{-s_i}\rangle_i$ and the action of R_x is a flip of all the spins. So R_x maps the subspace $S_z = m$ onto $S_z = -m$ and reduces the size of blocks only for $m = 0$.

We will now explain which blocks contain the ground state $|0\rangle$ and the first excitation $|1\rangle$. Because of the $SU(2)$ symmetry, the eigenvectors can be labeled by the quantum numbers j and m . Each energy level has a degeneracy $2j + 1$ and a representative member in the subspace $m = 0$. On the other hand, the subspace $m = 1$ contains no singlet $j = 0$. With the help of general arguments,²¹ the ground state $|0\rangle$ of an antiferromagnetic model is a singlet $j = 0$, but the first excitation can have $j = 0$ or 1. The full diagonalization of H for short chains shows that the first excitation has $j = 1$: the Haldane triplet. We denote it $|1, m\rangle$ with $m = -1, 0, \text{ or } 1$. The other quantum numbers are obtained by using the transformation²¹

$$U = \exp\left(i\pi \sum_{j \text{ even}} S_j^z\right), \quad (2)$$

which is diagonal in the z -axis basis. The interest of U is that the nondiagonal elements of UHU^{-1} are 0 or -1 . The Perron-Frobenius theorem²² can then be applied in each subspace $S_z = m$. For $m = 0$ or 1, it follows that the components of $U|0\rangle$ and $U|1, 1\rangle$ are strictly positive (in the z -axis basis). In a subspace $S_z = m$, $T \cdot U = (-1)^m U \cdot T$. So $|0\rangle$ has the wave vector $k = 0$ and $|1, 1\rangle$ (and so the entire Haldane triplet $|1, m\rangle$) has $k = \pi$. The left-right reflection Lr commutes with U ; $|0\rangle$ and $|1, 1\rangle$ (therefore all the triplet) are even for Lr . The spin rotation R_x commutes with U ; $|0\rangle$ is even for R_x . But $R_x|1, 1\rangle = \pm|1, -1\rangle$ and only $|1, 0\rangle$ is an eigenvector of R_x . In a triplet, the eigenvalues of S_x are $-1, 0, \text{ and } 1$; so those of R_x are $-1, 1, \text{ and } -1$. The eigenvectors $|1, 1\rangle \pm |1, -1\rangle$ match ± 1 ; necessarily, the eigenvalue of $|1, 0\rangle$ for R_x is -1 . To summarize, the ground state $|0\rangle$ is in the subspace ($S_z = 0, k = 0, Lr = +1, R_x = +1$) and one representative of the Haldane triplet is the ground state of the subspace ($S_z = 0, k = \pi, Lr = +1, R_x = -1$).

The advantage of these symmetries is the reduction of the size of the matrix. The size of the subspace $S_z = m$ is $\sum N!/(n_+! n_0! n_-!)$ with $n_+ + n_0 + n_- = N$ and $n_+ - n_- = m$. When N is large,

$$\dim(S_z = 0) \sim \frac{1}{2} \sqrt{\frac{3}{\pi}} \frac{3^N}{\sqrt{N}}. \quad (3)$$

The translation T reduces this size by a factor N (asymptotically when N is large), the left-right reflection Lr by 2 (N large), and the π rotation R_x by 2 (N large). For $N = 22$, the size is reduced by 851 (1% better than the asymptotic formula) and it is equivalent to $N = 16$ without symmetries.

Certain methods are well adapted to obtain the ground state of a large, unstructured sparse and symmetric (or Hermitian) matrix, for example, the conjugate gradient²³ and the Lanczos²⁰ method. In these iterative methods, by starting with an arbitrarily vector V_0 , the matrix H

acts only in matrix-vector multiplications and remains sparse: The vector V_n is a linear combination of $H \cdot V_{n-1}$ and the previous V_i 's ($i \leq n-1$). Then V_n is in the subspace $\mathcal{K}_n = \text{span}(V_0, H \cdot V_0, \dots, H^n \cdot V_0)$. From a theoretical point of view, the Lanczos method builds an orthogonal basis of \mathcal{K}_n and the projection of H on \mathcal{K}_n is a tridiagonal matrix $n \times n$. After n iterations, the ground state is approximated by the vector of \mathcal{K}_n which minimizes the Rayleigh quotient $R(V) = \langle V|H|V \rangle / \langle V|V \rangle$. So, by construction, it is the fastest convergent method among these one using $H \cdot V$ multiplications. Because computers have a finite precision, the orthogonality of the V_i tends to be lost after many iterations and it is difficult to obtain many eigenvalues. However, as we want only the ground states of some blocks, we used the Lanczos method. For $N = 22$, only 55 iterations (or matrix-vector multiplications) are needed to obtain eigenvalues with a precision which cannot be improved by more iterations. Details on the programming techniques are given in the Appendix.

III. NUMERICAL RESULTS AND EXTRAPOLATION METHOD

The numerical values are given in Table I with 12 digits after the decimal point, for periodic chains with length up to $N = 22$. We have no direct means to estimate the precision. Some direct iterations have been made with the eigenvector obtained by the Lanczos method and the precision is estimated at better than 10^{-11} for the ground-state energy E_0 and the first excitation E_1 . The sizes $N = 2$ and 4 are added because we will see that they have, surprisingly, a good behavior with respect to the extrapolation method. Results up to $N = 18$ have been published by other authors (see the caption of Table I).

The gap $G(N) = E_1 - E_0$ and the ground-state energy per site $e(N) = E_0/N$ have still not converged. To obtain a good estimate of their thermodynamic limits,

the convergence must be accelerated by an extrapolation method, adapted to their behavior.

For periodic chains, the convergence of the gap has been observed to be exponential. In a theory with a gap, we expect of course exponential convergence towards the thermodynamic limit for a closed chain. This has been shown explicitly in the large- N limit of the nonlinear σ model.¹⁵ We analyze the estimated decay length $\xi(N)$ at the index N as given by

$$\xi(N) = 2 / \ln \left(\frac{a_{N-4} - a_{N-2}}{a_{N-2} - a_N} \right), \quad (4)$$

where a_N represents the sequence $G(N)$ or $e(N)$. If $a_N = A + b \exp(-N/\xi)$, then $\xi(N) = \xi$ exactly for all N . If $a_N = A + b/(N - n_0)^\nu$, then $\xi(N) \sim (N - n_0)/(\nu + 1)$ for N large, and the exponent ν is given by the asymptotic slope of $\xi(N)$.

In Fig. 1, we have plotted $\xi(N)$ for $G(N)$ and $e(N)$. Both curves are concave: The estimated exponent ν increases with N (for $N = 22$, respectively, $\nu \approx 15$ and 11). This figure shows that the gap and the energy per site converge faster than a power law. This is good evidence for the expected exponential behavior of the Haldane conjecture. For this reason, we extrapolate with the Shanks transformation.^{24,25} We explain in some detail this method because we will use it in a different way than Ref. 15 or 26. If the sequence a_N is a sum of k exponentials,

$$a_N = A + b_1 e^{-N/\xi_1} + \dots + b_k e^{-N/\xi_k}, \quad (5)$$

the limit A is one of the $2k + 1$ unknowns and can be obtained by solving the system (5) for $a_{N-2k}, \dots, a_N, a_{N+2}, \dots, a_{N+2k}$. We call $A_N^{(k)}$ this solution, i.e., the limit A extracted from $a_{N-2k}, \dots, a_{N+2k}$ supposing that the sequence a_N is a sum of k exponentials. Of course, if the sequence a_N has not exactly this form, then $A_N^{(k)}$ varies with N . The simplest case of the Shanks transformation is $k = 1$. The solution is

TABLE I. Dimension of the largest block ($S_z = 0, k = 0, L_r = +1, R_x = +1$), ground-state energy E_0 , first excitation energy E_1 , gap $G(N) = E_1 - E_0$, and ground-state energy per site $e(N) = E_0/N$ for chain lengths $N = 2-22$. These results are obtained by exact diagonalization. Previous results for $N = 8$ are given by De Neef (Ref. 3), $N = 10$ by Blöte (Ref. 4), $N = 12$ by Botet and Jullien (Ref. 5), $N = 14$ by Glaus and Schneider (Ref. 6) and Parkinson and Bonner (Ref. 7), $N = 16$ by Moreo (Ref. 8), and $N = 18$ by Lin (Ref. 9).

N	Dimension	$-E_0$	$-E_1$	Gap $G(N)$	$-e(N)$
2	2	4.0	2.0	2.0	2.0
4	5	6.0	5.0	1.0	1.5
6	15	8.617423181814	7.896795819190	0.720627362624	1.436237196969
8	59	11.336956077897	10.743400823522	0.593555254375	1.417119509737
10	290	14.094129954932	13.569322004518	0.524807950414	1.409412995493
12	1 728	16.869556139477	16.385359669563	0.484196469914	1.405796344956
14	11 549	19.655133499935	19.196168152997	0.458965346938	1.403938107138
16	82 790	22.446807281171	22.004011719811	0.442795561360	1.402925455073
18	617 898	25.242312007671	24.810090537803	0.432221469868	1.402350667093
20	4 730 966	28.040291720480	27.615081406019	0.425210314461	1.402014586024
22	36 871 567	30.839898879910	30.419383859516	0.420515020394	1.401813585450

TABLE IV. The correlation functions $C_N(r)$, calculated by exact diagonalization for N up to 22. For $N \leq 18$, these results have been published by other authors (Refs. 7–9).

r	$N = 6$	8	10	12	14	16	18	20	22
1	0.47874573	0.47237317	0.46980432	0.46859878	0.46797936	0.46764181	0.46745022	0.46733819	0.46727118
2	0.28844542	0.27210249	0.26392567	0.25918542	0.25622175	0.25429251	0.25300867	0.25214355	0.25155626
3	0.28606604	0.24086913	0.22135314	0.21075706	0.20436261	0.20028789	0.19761348	0.19582835	0.19462472
4		0.21561295	0.18479849	0.16814782	0.15810415	0.15169940	0.14749166	0.14468055	0.14278366
5			0.18180007	0.15402811	0.13824755	0.12849332	0.12220081	0.11804519	0.11526281
6				0.14543474	0.12353893	0.11017252	0.10161828	0.09599964	0.09225227
7					0.12121726	0.10228686	0.09052395	0.08293057	0.07792178
8						0.09842421	0.08305179	0.07322701	0.06679153
9							0.08143053	0.06847270	0.06012605
10								0.06646187	0.05588756
11									0.05479614

energy is more precise and the precision on the gap value is similar. The fact that both methods give results with six and five identical digits is a good argument that they are both quite accurate.

VI. CORRELATION FUNCTIONS

In this section, we present our results for the correlation functions

$$C_N(r) = (-1)^r \langle S_0^z S_r^z \rangle = (-1)^r \langle \mathbf{S} \cdot \mathbf{S} \rangle / 3, \quad (13)$$

for the ground state of an isotropic and periodic chain of length N for $N \leq 22$. Numerical values are given in Table IV. To compute these quantities, the eigenvalue is not sufficient and the eigenvector is required. So the precision for the $C_N(r)$ is less than for the energies. It can be estimated around 10^{-8} , for example, by comparing $C_N(1)$ with $E(N)$, or by direct applications of the matrix H on the Lanczos result.

For an infinite chain, the Haldane conjecture predicts an exponential decrease $C_\infty(r) \sim b \exp(-r/\xi)/\sqrt{r}$ when r is large. This is because the underlying continuum theory is a nonlinear σ model which is *relativistic* in 1+1 dimensions. In fact, if we approximate the nonlinear σ model by free massive bosons, the propagator is the modified Bessel function K_0 which has this asymptotic behavior. The Haldane conjecture does not deal with short-distance details so that there is no *a priori* preferred choice when trying to fit data on the full range of spin-spin separation.

For a periodic chain, one has the equality $C_N(r) = C_N(N-r)$. To extract the correlation length ξ for N and r large, we analyze our data with the guess $C_N(r) = C_\infty(r) + C_\infty(N-r)$, which is reasonable if $\xi \ll N$. For some classical spin systems (one-dimensional Potts model, Ising chain with a magnetic field, etc.) with nonvanishing temperature, the corrections to this formula are of order $\mathcal{O}(C_\infty(N))$.

We have verified that $\exp(-r/\xi)/\sqrt{r}$ fits the data better than $\exp(-r/\xi)$ or $\exp(-r/\xi)/r$. From these three forms, the estimated values for ξ are respectively 6.2, 4.5, and 10, for $N = 22$. In Fig. 2, we compare the Bessel function $K_0(r/\xi)$ and $\exp(-r/\xi)/\sqrt{r}$. Both fits are comparable in quality. But the estimated correlation lengths ξ are slightly different: 5.9 versus 6.2 for $N = 22$. For

$N = 10$, they are respectively 5.4 and 6.2. We notice that the optimal ξ is 6.2, for all $N \leq 22$, with $\exp(-r/\xi)/\sqrt{r}$, whereas the estimations for ξ with the Bessel function vary with N . For this reason, we prefer the former but we keep in mind that both laws have the same asymptotic behavior and that only an exact solution of the model can give the correlations for short range.

It is interesting to compare the correlation length ξ [obtained with $C_N(r)$] and the decay length $\xi(N)$ [Eq. (4)] of the gap $G(N)$ (Table II) and energy $e(N)$ (Table III). In Fig. 1, we see that it is not excluded that $\xi = 6.2$ is the limit of $\xi(N)$. The extrapolation of $\xi(N)$ with the Shanks transformation gives 5.5 for the gap and 4.6 for the energy, but the columns of the Shanks table are nonmonotonic and these results are only qualitative. Of course, by analyzing the convergence of the $G(N)$ and $e(N)$ with an exponential corrected by a power law (as $1/\sqrt{N}$), the estimations of $\xi(N)$ are greater, and the extrapolations are closer from 6.2. Then this comparison is only qualitative and requires longer chains. Our value ($\xi = 6.2$) is equal to the estimate quoted by Nomura¹³ ($\xi = 6.25$) and by Liang¹⁴ ($\xi = 6.2$) with Monte Carlo methods for $N = 64$. It is comparable with the results of Takahashi¹² ($\xi = 5.5 \pm 2.$) with a Monte Carlo method for $N = 64$, by Kubo³³ ($\xi = 6.7$) with a transfer-matrix method, and by White and Huse¹⁸ ($\xi = 6.03$) with the real-space renormalization-group method.

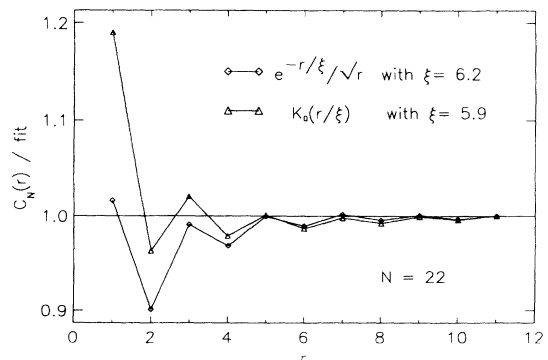


FIG. 2. The ratio of the correlation function $C_N(r) = (-1)^r \langle \mathbf{S}_0^z \cdot \mathbf{S}_r^z \rangle$ and two proposed laws vs r . The $C_N(r)$ have been exactly computed for $N = 22$. The ratios are normalized to 1 for $r = N/2$.

VII. CONCLUSION

The main limitation of exact diagonalizations is, of course, the small lengths that can be studied. The numerical complexity grows as the exponential $[S(S+1)]^N$ for N spins S and the limits of computer power are fastly reached. The length N of the system must be compared with the physical correlation length ξ , and in fact, the situation for the $S=1$ AF spin chain is quite favorable. Within the Haldane conjecture, ξ is finite for integer spins and shortest for small S . We have shown that some quantities can be measured with excellent accuracy: the gap and the ground-state energy. On the other hand, the correlations $C_\infty(r)$ (and thus the correlation length ξ) clearly need longer chains.

The main advantages of exact diagonalizations are that they depend only on one parameter (the size N) and give exact results (i.e., with machine precision). One has to deal only with the thermodynamic limit. By comparison, methods based on Trotter-Suzuki decomposition have three parameters (number of slices, temperature, and length of the chain) and systematic errors which decrease by extrapolating in the number of slices. Monte Carlo methods have their own parameters (number of walkers or length of simulations, etc.) which must be tuned, and the results have statistical fluctuations as well as systematic errors. Real-space renormalization-group methods have to extrapolate with respect to the number of basis states and the chain length.

The high precision allows the use of sophisticated extrapolation methods and we are able to validate some assumptions on the asymptotic behavior. Figure 1 suggests that the use of the Shanks transformation is optimal concerning gap extrapolation. In fact the parameter α of the more general VBS transformation can vary only in a small interval around $\alpha = 1$. This shows that our choice is not arbitrary but dictated by the data. The results of exact diagonalizations combined with a careful extrapolation can give physical quantities in the thermodynamic limit with a good precision.

APPENDIX: PROGRAMMING TECHNIQUES

We used a Cray 2 of the CEA with a central memory of 256 megawords of 64 bits. Some details of our program are useful only for this kind of machine in particular and are not described here. The algorithm has two main parts, the building of the sparse matrix H (and its storage on disks) and the matrix-vector $H \cdot V$ multiplication, needed for the Lanczos iterations.

We consider first the matrix multiplication. The matrix H is very sparse. For $N = 22$, its order is $\approx 37 \times 10^6$ and the number of nonvanishing elements is (on average) $8N/9$ per rows (when N is large). We use the classical storage by rows with only the nonvanishing elements of H (values and column number) stored. In practice, 1 bit is needed for the value (± 1) and 26 bits for the column number. So two elements are stored in a 64-bit word and 3.5 gigabytes are used for H . The matrix-vector multipli-

cation is done by an indirect addressing of the elements of the vector, where the address is the column number. This indirect addressing is the most time consuming part of the program and it is intrinsic to this sparse storage method. For $N = 22$, a multiplication needs 190 s of one Cray 2 CPU.

The most difficult part of the algorithm is the building of the matrix with use of symmetries. Each z -axis basis state $|s_1, \dots, s_N\rangle$ is described by the number $\sum_r (s_r + 1)3^{r-1}$. First, the list of the symmetrized basis states is obtained. Each symmetrized state is represented by the state of the z -axis basis, which contributes and has the smallest number. Then the Hamiltonian H operates on this list and generates other states. The problem is to find the corresponding symmetrized states (and their phases). Possible methods are (a) each generated state is symmetrized by action of all the symmetries operators or (b) a storage table gives, for each z -axis state, the symmetrized one and the generated state is searched in this table. The first method is too time consuming and the second one uses too much memory.

We use an intermediate method with a decomposition in two sublattices,⁹ $A = \{s_{2r}\}$ and $B = \{s_{2r+1}\}$. The symmetries R_x , L_r , and T^{2k} do not exchange A and B . We call them sublattice symmetries. On the other hand, symmetries T^{2k+1} exchange A and B . Then, each symmetry is the product of a sublattice symmetry and possibly T . Since a sublattice is described only by $3^{N/2}$ states, we can use a storage table which gives for each sublattice state the symmetrized one. For all the chain, A symmetrization consists of symmetrized A and to operate on B with the same operator. Since a storage table of size $3^{N/2}$ is available, it does not require much time or memory. The last step is the action of T , which exchanges A and B , and S_z , which imposes $S_z(A) + S_z(B) = 0$. By symmetrizing by T , the number of the A -symmetrized states (around 78×10^6 for $N = 22$ and $S_z = 0$) is divided by 2 (for N large). On our computer, we keep on memory the list which gives the fully symmetrized state for each A -symmetrized one. This list has some properties of factorization, as well explained in Ref. 9, and the location of each state is easily obtained by considering each sublattice. To summarize, a generated state is, in a first step, symmetrized by R_x , L_r , and T^{2k} (which keep invariant the sublattices), and in a last step by T . The first step needs only short lists ($3^{N/2}$) and the final one a big list, for which the length is 2 times the order of the fully symmetrized block. For $N = 22$, our program needs 2200 s of one Cray 2 CPU to build the matrix H .

For one block ($|0\rangle$ or $|1, 0\rangle$), with the Lanczos method, the precision cannot be improved after 55 iterations (for $N = 22$). To compute eigenvectors, the Lanczos method is not optimal because all the intermediate vectors must be stored. To do that, 16 gigabytes are required. Then, a first Lanczos calculation gives the eigenvalues and the coordinates of eigenvectors on the Lanczos basis. A second Lanczos calculation is needed to generate the eigenvectors.

The computations of this paper have used 12 h of one Cray 2 CPU.

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