

Correlation functions of the antiferromagnetic Heisenberg model using a modified Lanczos method

Eduardo R. Gagliano

*Centro Atómico Bariloche, Comisión Nacional de Energía Atómica e Instituto Balseiro, Universidad Nacional de Cuyo,
8400 San Carlos de Bariloche, Río Negro, Argentina*

Elbio Dagotto and Adriana Moreo

Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801

Francisco C. Alcaraz

Departamento de Física da Universidade Federal de São Carlos, Caixa Postal 616, 13 560 São Carlos, São Paulo, Brazil

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Using a modified Lanczos algorithm, we study the correlation functions in the ground state of the one-dimensional antiferromagnetic Heisenberg model. We obtain numerical results for rings up to 24 sites. There are no indications of the anomalous behavior of these correlation functions recently observed in chains with 16 sites. We also present a pedagogical description of the hashing technique which is an efficient algorithm for searching and storage purposes.

I. INTRODUCTION

Finite-size scaling techniques have been applied to the study of phase diagrams in statistical mechanics^{1,2} and quantum-field theory on a lattice.³ In these methods it is necessary to diagonalize the Hamiltonian (H) for finite lattices of increasing size. An efficient technique for the diagonalization of large matrices is the Lanczos method¹⁻³ in which a tridiagonal representation of H is constructed. The bulk limit results are estimated by means of extrapolation algorithms.⁴

The purpose of this paper is twofold. On the one hand, we apply a new modified Lanczos method to the analysis of a one-dimensional interacting spinless fermion model whose dynamics is described by the following Hamiltonian:

$$H = -t \sum_{i=1}^N (C_i^\dagger C_{i+1} + C_{i+1}^\dagger C_i) + G \sum_{i=1}^N (n_i - \frac{1}{2})(n_{i+1} - \frac{1}{2}), \quad (1)$$

where C_i^\dagger and C_i are the creation and annihilation operators for a fermion on the i th lattice site. They satisfy the usual anticommutation relations. n_i is the number operator. This model is a lattice version⁵ of the massless Thirring model.⁶ We work on a lattice with N (even) sites and $N/2$ fermions (half-filled band). We consider periodic (antiperiodic) boundary conditions for an odd (even) number of fermions. This model has been previously analyzed by Monte Carlo^{7,8} and real-space renormalization-group methods.⁹ We compare our results with them.

The Hamiltonian Eq. (1) has a nontrivial phase structure in the thermodynamic limit. When $0 \leq G/2t \leq 1$ there is no long-range order, the mass gap is zero and $\langle n_i \rangle = \frac{1}{2}$ (where the angular brackets denote ground-state

expectation values). At $G/2t = 1$ the model presents an essential singularity. If $G/2t > 1$ there is long-range order, the mass gap is different from zero and $\langle n_i \rangle \approx 0$ for even sites while $\langle n_i \rangle \approx 1$ for odd sites (or vice versa). When the number of sites is finite there is no phase transition (for example the mass gap is always nonzero) but we can obtain information about the bulk critical behavior from the analysis of systems of increasing size.

Using the Jordan-Wigner transformation the model Eq. (1) can be transformed into the anisotropic Heisenberg model, up to boundary terms,

$$H(\rho) = -2t \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y - \rho S_i^z S_{i+1}^z), \quad (2)$$

where $\rho = G/2t$ and S are spin $\frac{1}{2}$ operators. The properties of this Hamiltonian can be deduced from the antiferromagnetic model studied in Refs. 10 and 11 using the relation

$$UH(\rho)U^{-1} = -H(-\rho), \quad (3a)$$

where

$$U = \exp \left[i\pi \sum_{j=1}^N j S_j^z \right]. \quad (3b)$$

Finally we also know¹¹ that the mass gap of our model vanishes at $\rho = 1$ like

$$m(\rho) \sim \exp \left[-\frac{\pi^2}{2\sqrt{2(\rho-1)}} \right]. \quad (4)$$

In this paper we study the behavior of the correlation function in the isotropic case ($G/2t = 1$) defined as

$$\omega_l(N) = \frac{4}{N} \sum_{i=1}^N \langle S_i^z S_{i+l}^z \rangle, \quad (5)$$

where we use the relation $S_i^z = n_i - \frac{1}{2}$. From Ref. 12 we

expect the behavior

$$\lim_{N \rightarrow \infty} \omega_l(N) = \omega_l(\infty) \approx A \frac{(-1)^l}{l} \quad (6)$$

when $l \gg 1$ (A is an unknown constant). So $l |\omega_l(\infty)|$ should be a constant for large enough values of l . However it has been recently remarked¹³ as an unexpected feature that $l |\omega_l(\infty)|$ goes through a maximum at $l \approx 4-8$. These results have been obtained using chains (open ends) with $N \leq 16$. The correlation functions for rings (periodic boundary conditions) do not show this behavior but the authors of Ref. 13 argued that their rings were small and $N \sim 22-24$ are needed. Using our method we obtain the results for these values of N .

Another unexpected result presented in Ref. 13 corresponds to the behavior of the structure factor

$$S_N(k) = \frac{1}{N} \sum_{j,l=1}^N e^{ikl} (\langle n_j n_{j+l} \rangle - \langle n_j \rangle \langle n_{j+l} \rangle) \quad (7)$$

at $k = \pi$. From Eq. (6) we expect it to diverge as

$$S_N(\pi) \approx \frac{A}{2} \ln N \text{ as } N \rightarrow \infty \quad (8)$$

for a periodic ring. However, a slight deviation from Eq. (8) was found¹³ suggesting that finite-size corrections may affect the divergence of $S_N(\pi)$.

We obtain $\omega_l(N)$ and $S_N(k)$ for $N \leq 24$ using the modified Lanczos algorithm. Our results do not support the speculations of Ref. 13. For $l \sim 4-8$ we observe a monotonic increase of $l |\omega_l(\infty)|$ while $S_N(\pi)$ follows Eq. (8) very closely.

The other purpose of this article is the description of the "hashing" technique¹⁴ which seems to be an appropriate method for the numerical implementation of the Lanczos approach (in standard or modified versions). Recently the hashing technique was successfully applied to the analysis of the Ashkin-Teller model and to the Blume-Emery-Griffiths model.¹⁵

The organization of the paper is as follows. In Sec. II we describe the modified Lanczos algorithm. In Sec. III we present the results. Final comments are included in Sec. IV. The appendix is devoted to a detailed description of the hashing technique.

II. THE METHOD

In this section we describe our modified Lanczos algorithm. Although this method has been previously analyzed by two of the authors in Ref. 16 in the context of lattice gauge theories, we believe that it is worthwhile to present it here for readers mainly interested in statistical mechanics problems.

As in the standard Lanczos method, the technique that we propose requires the selection of an initial trial vector ψ_0 (normalized to one). If ψ_0 has a nonzero projection over the true ground state Φ_0 of the Hamiltonian ($H\Phi_0 = E_0\Phi_0$), the method gives a good approximation to the ground-state properties of H . Otherwise it will converge to an excited state.

Applying H over ψ_0 , we define a state ψ_1 as follows:

$$\psi_1 = \frac{H\psi_0 - \langle H \rangle \psi_0}{(\langle H^2 \rangle - \langle H \rangle^2)^{1/2}}, \quad (9)$$

ψ_1 has norm one and it is orthogonal to ψ_0 . In Eq. (9) we use the notation $\langle H^n \rangle = \langle \psi_0 | H^n | \psi_0 \rangle$. In the standard Lanczos approach it is necessary to construct another state orthogonal to ψ_0 and ψ_1 and so on, in such a way that the matrix H is tridiagonal. The method presented here has the following modification: in the basis ψ_0, ψ_1 we have a (2×2) representation of H which is easily diagonalized. Its lowest eigenvalue (ε_1) and the corresponding eigenvector ($\tilde{\psi}_0$) are better approximations to E_0 and Φ_0 than $\langle H \rangle$ and ψ_0 .

The improved energy is

$$\varepsilon_1 = \langle H \rangle + b\alpha, \quad (10a)$$

while the improved wave function $\tilde{\psi}_0$ is

$$\tilde{\psi}_0 = \frac{\psi_0 + \alpha\psi_1}{(1 + \alpha^2)^{1/2}}, \quad (10b)$$

where

$$b = (\langle H^2 \rangle - \langle H \rangle^2)^{1/2}, \quad (10c)$$

$$f = \frac{\langle H^3 \rangle - 3\langle H \rangle \langle H^2 \rangle + 2\langle H \rangle^3}{2(\langle H^2 \rangle - \langle H \rangle^2)^{3/2}}, \quad (10d)$$

and

$$\alpha = f - (f^2 + 1)^{1/2}. \quad (10e)$$

The method can be iterated by considering $\tilde{\psi}_0$ as a new initial trial vector and repeating the steps Eqs. (9) and (10). In each iteration we obtain an improved estimation of the wave function and the energy of the ground state of H .

We want to stress that although usually the initial state ψ_0 is selected as the ground state of an unperturbed Hamiltonian H_0 (where $H = H_0 + V$), any other starting vector is acceptable in principle. The choice of the starting vector will only affect the convergence rate. For example it has been shown in Ref. 16 (and also in the model analyzed below) that sometimes it is useful to begin the calculation with a variational trial function whose free parameters are selected such that the variational energy is minimized.

An advantage of the modified Lanczos method is that we may obtain a good approximation to Φ_0 without much effort. In each iteration we only need to store three vectors (say ψ_0 , $H\psi_0$, and $H^2\psi_0$) expanded in the basis of eigenstates of H_0 . If the size of the Hilbert subspace where we work is M , we must store $3M$ coefficients. In the usual Lanczos approach it is also possible to calculate eigenvectors: first evaluate the eigenvector in the tridiagonal basis and then repeat the tridiagonalization technique accumulating the basis vectors with their corresponding weights. In our approach, the eigenvectors are calculated without repeating the process.

Once we have obtained a good approximation to Φ_0 then it is possible to evaluate the ground-state expectation value of any operator. For example we show below that we can calculate correlation functions with high accuracy. We test the method in the quantum one-dimensional model described in the Introduction. Working with lattices up to $N = 24$ we obtain the wave functions and the

energy of the ground and first excited states as well as the correlation functions with great accuracy. Previous results presented in the literature for the correlation functions of the Heisenberg model in the isotropic case have been obtained with $N = 16$ as maximum.^{13,17} This fact illustrates the power of the modified Lanczos approach (supplemented by the hashing technique described in the Appendix).

III. RESULTS

In Table I we show the results for the ground-state energy per unit site (ϵ_N) obtained with the modified Lanczos approach at $G/2t = 1$ [where the Hamiltonian Eq. (1) can be transformed into the isotropic Heisenberg model]. Fitting these results with a polynomial $\epsilon_N = \epsilon_\infty + \alpha/N^2$ we obtained $\epsilon_\infty = -0.8862 \pm 0.0001$. Note the good agreement with the exact value in the thermodynamic limit¹¹ $\epsilon = -0.886294$. The ground-state eigenvector and eigenvalue at $N = 18$ (20, 22, and 24) have been obtained using 20 min, (95 min, 7 h, and 30 h) of CPU (central processing unit) time in a Vax11/780 computer with an accuracy of 10^{-7} . The results for $N \leq 16$ have been evaluated in only a few minutes of CPU time. As an initial trial function we choose the alternate state $|1010 \cdots 10\rangle$, i.e., the ground state of the interaction term. In this calculation we have also exploited the spin inversion symmetry (in the Heisenberg model language) which reduces the number of representatives (r) by a factor of about 2. r is approximately given by the number of states in the half-filled band subspace divided by the number of terms of each representative, i.e.,

$$r \simeq \frac{1}{2N} \binom{N}{N/2}. \quad (11)$$

We remark that the numbers presented in Table II are coincident with the results of Ref. 17 (where the Bethe ansatz was used with $N \leq 16$), Ref. 18 (where a method similar in spirit to our technique was employed), and Ref. 19 (where the standard Lanczos scheme was used for $N \leq 18$). We prove that the approach of Ref. 18 converges slower than our method.

TABLE I. Ground-state energy per unit site ϵ_N obtained with the modified Lanczos approach at $G/2t = 1$. N is the number of sites. We work in the half-filled-band case.

N	$-\epsilon_N$
4	1.000 000
6	0.934 258
8	0.912 773
10	0.903 089
12	0.897 898
14	0.894 792
16	0.892 787
18	0.891 416
20	0.890 438
22	0.889 716
24	0.889 167

TABLE II. The correlation functions $\omega_l(N)$ [Eq. (5)] and the structure factor $S_N(k)$ [Eq. (7)] at $k = \pi$ ($G/2t = 1$).

N				
l	18	20	22	24
0	1.000 000	1.000 000	1.000 000	1.000 000
1	-0.594 278	-0.593 802	-0.593 323	-0.593 048
2	0.246 051	0.245 668	0.245 197	0.244 972
3	-0.209 462	-0.208 178	-0.206 973	-0.206 259
4	0.147 871	0.146 480	0.145 147	0.144 380
5	-0.138 902	-0.136 267	-0.134 023	-0.132 636
6	0.114 486	0.111 576	0.109 102	0.107 594
7	-0.114 241	-0.109 498	-0.105 812	-0.103 485
8	0.102 301	0.096 982	0.092 906	0.090 361
9	-0.107 653	-0.099 378	-0.093 534	-0.089 836
10		0.092 833	0.086 307	0.082 225
11			-0.089 986	-0.084 167
12				0.079 797
$S(\pi)$	1.110 709	1.147 123	1.178 659	1.209 431

We have also evaluated the mass gap defined⁸ as the difference between the ground-state energy in the subspace with $(N/2) + 1$ fermions and the lowest energy in the half-filled band sector. Our results are consistent with Eq. (4).

In Table II, we give the results obtained with our method ($G/2t = 1$; $N = 18-24$) for the correlation functions Eq. (5). Table II can be easily evaluated once we get an accurate approximation to the ground-state wave function of H , i.e., in a single run of our programs we obtained ϵ_N (Table I) and $\omega_l(N)$. We have also evaluated the correlation functions for $N \leq 16$. They are coincident with the values given in Refs. 13 and 17. $\omega_l(N)$ for $N = 18-24$ have not appeared previously in the literature on the Heisenberg model. In Table II we also show the structure factor $S_N(k)$ at $k = \pi$.

In Fig. 1 we show our results for $S(k)$ ($G/2t = 1$, $N = 20$) compared with the Monte Carlo results of Ref. 7 for a 40-site lattice. Both methods give results in close

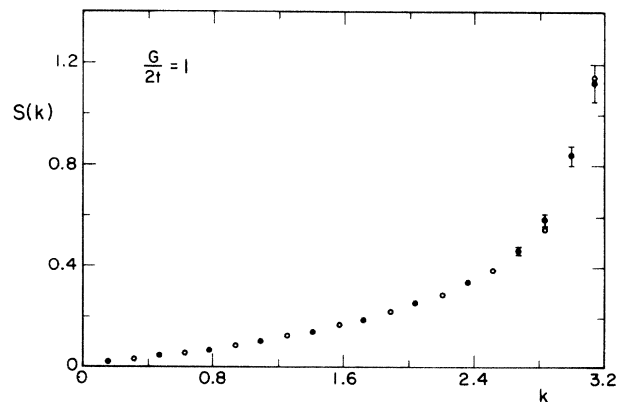


FIG. 1. The structure factor $S(k)$ ($G/2t = 1$). The solid circles (●) denote Monte Carlo results from Ref. 7 using 40 sites while open circles (○) are results from our modified Lanczos technique with $N = 20$.

agreement showing that a good estimation of $S(k)$ can be obtained from the modified Lanczos method.

Now we analyze the behavior of $\omega_l(N)$ in the limit $N \rightarrow \infty$ to test the hypothesis of Ref. 13. For l fixed we assume

$$|\omega_l(N)| = |\omega_l(\infty)| + \alpha_l/N^2, \quad (12)$$

and using our numerical results for $N=22$ and 24 we obtain the results shown in Fig. 2. Note the different behavior for l even and odd (this detail was remarked previously in many papers¹⁰). Between $l=4$ and 8 we do not observe a maximum for $l|\omega_l(\infty)|$. Our results suggest that the relation Eq. (6) is valid with A around 0.6 and 0.7 . Note that the results for $l=9,10$ would suggest the existence of a broad maximum for $l \approx 8$. We prefer to attribute this behavior to the uncertainty in the extrapolation $N \rightarrow \infty$. In fact, it is clear that for l around $N/2$ the errors in this extrapolation are appreciable.

Another evidence supporting our conclusions can be obtained from $l|\omega_l(N)|$ for N fixed, say $N=24$. There are no indications of a maximum. We also remark that a fit of our data using a polynomial with a term β_l/N^4 also agrees with our conclusions. Summarizing, we obtain no evidence for the existence of a maximum in $l|\omega_l(\infty)|$. Of course it may be possible that due to errors in our extrapolations we are not able to observe a broad maximum around $l=8$. Numerical results for $N=26-30$ are needed to check without ambiguities whether there is a strange behavior of $l|\omega_l(\infty)|$ or not.

Finally we study $S_N(\pi)$ as a function of $\ln N$ (see Fig. 3). The results for $N \sim 18-24$ suggest a straight line behavior with slope around $0.33-0.35$. This is consistent with Eq. (8) using our estimation for A quoted above, i.e.,

$$S_N(\pi) \sim (0.3-0.35)\ln N.$$

So if finite-size corrections affect the logarithmic divergence of $S_N(\pi)$, they are very small.

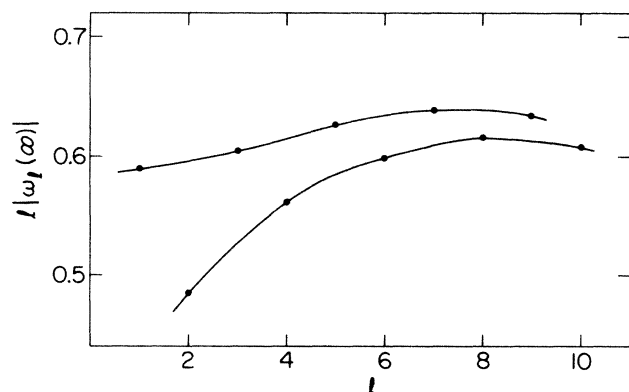


FIG. 2. Extrapolated correlation function $l|\omega_l(\infty)|$ as a function of l . To guide the eye we connect the even- l points using a continuous line (the same for odd l).

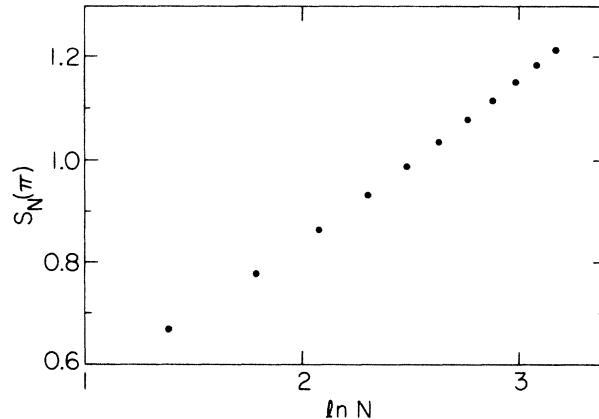


FIG. 3. The structure factor $S_N(\pi)$ as a function of $\ln N$.

IV. CONCLUSIONS

In this paper we have analyzed the Heisenberg model using a modified Lanczos method (supplemented by the hashing technique). We obtain accurate results for rings with $N \leq 24$ using a VAX11/780 computer. As far as we know there are only two previous papers^{20,21} where $N=20$ was studied for this model.

Regarding the specific physical problem that we analyze in this paper, i.e., the behavior of $l|\omega_l(\infty)|$, we conclude that there is no evidence of an anomalous behavior of this magnitude for rings with $N \leq 24$.

In Fig. 1 we show that the modified Lanczos technique can be used for the analysis of the structure factor giving results as accurate as those provided by the Monte Carlo method of Ref. 7. Since this technique has been recently criticized^{13,22} it is worthwhile to develop alternative methods.

The approach analyzed in this paper can be further improved as follows.

(i) To speed up the programs we may write the hashing subroutine in assembly language. This would reduce the computing time by a factor of about 2 (see Ref. 2).

(ii) The number of states may be reduced by using valence-bond diagrams.^{21,23}

(iii) If enough storage facilities are available it may be possible to diagonalize matrices 3×3 or 4×4 in each iteration instead of 2×2 steps described here. This modification would speed up the convergence of the method.

Finally we remark that we may improve our numerical method using initial variational trial functions [ψ_0 in Eq. (9)] with free parameters chosen such that the energy is a minimum. We test this idea using functions recently proposed in lattice gauge theories.²⁴ We observe that the use of this modification is worthwhile only when a few iterations can be performed or when great accuracy is unnecessary. In general, selecting ψ_0 as the ground state of an unperturbed Hamiltonian H_0 is a good starting point. Similar conclusions have been obtained in Ref. 25.

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APPENDIX: HASHING TECHNIQUE

In this appendix we describe some programming techniques which we believe are useful in practice when the standard or modified Lanczos approach is used. Some methods are well known but we also describe them here for completeness.

Due to the boundary conditions used in our Hamiltonian Eq. (1), we may work with translationally invariant states. For example in $N=4$ one of these states is

$$|\phi\rangle = \frac{1}{\sqrt{4}}(|1100\rangle + |0110\rangle + |0011\rangle + |1001\rangle), \quad (\text{A1})$$

where $|1100\rangle$ means $C_1^\dagger C_2^\dagger |0\rangle$ (if we order the sites from left to right) and $|0\rangle$ is the state of zero fermions. $|\phi\rangle$ is stored as follows. We select one of the terms of $|\phi\rangle$ as a "representative" following an arbitrary convention. Then we write it as an integer because the combination of ones and zeros which denote a state can be thought of as a binary number. The advantage of this method is that we can store one state in a single word and the action of the quantum operators on the states can be implemented by logical functions.

Now we describe the hashing technique which is an efficient algorithm for searching and storage purposes. Suppose that we want to apply the Hamiltonian H on the state ψ_0 . The state is usually given as a linear combination of representatives (we denote them by $\{|\bar{n}\rangle\}$) which are eigenstates of H_0

$$\psi_0 = \sum_n C_n |\bar{n}\rangle. \quad (\text{A2})$$

When the potential term V acts on $|\bar{n}\rangle$ many other representatives are generated. Let us consider one of them, say $|\bar{m}\rangle$. It may have appeared previously so we need to search for it in the storage place (described below) and change its coefficient. If $|\bar{m}\rangle$ has not appeared before we must put it in an unoccupied place. These are the basic operations which must be efficiently implemented.

A naive method to store the representatives is by using two vectors of length M . In one of them, denoted by $I(i)$ ($1 \leq i \leq M$), we put the integers $\{K\}$ which indicate the representatives. In the other vector, say $C(i)$, we store the corresponding coefficients. When a state is generated in an iteration we have to search for it in the vector $I(i)$ beginning at $i=1$. If the state is present we change its coefficient. Otherwise we put it in the first empty place. Of course this technique is not the most appropriate one when M is a large number [e.g., when $N=20$ in the Hamiltonian Eq. (1), $M \sim 5000$], because in this process the number of tested numbers grows linearly with M . It is necessary to use a more elaborate method to deal with this situation. Here, the hashing algorithm, which is a well-known method for specialists in programming techniques

but has not been widely used in the context of finite-size scaling calculations, appears.

The main idea of the hashing technique is that we may construct a function $i=h(k)$ ("hash function") which gives a correspondence between the representatives $\{K\}$ and a position i in the vectors I and C . If the correspondence is one-to-one the problem of searching is solved because when a state is generated we only need to evaluate $h(k)$ in order to know where it has been stored. However it is almost impossible to construct such a one-to-one function (furthermore the integers $\{K\}$ are unknown *a priori*). In general it may occur that different states K_1, K_2, \dots , have the same index, i.e., $h(K_1) = h(K_2) \dots$. In this case we say that there will be "collisions" and we need an algorithm to deal with this problem. A good hash function minimizes the number of collisions.

It has been shown¹⁴ in many examples that the function

$$h(K) = [K \pmod{M}] + 1 \quad (\text{A3})$$

works very well in practice (in this case, in order to minimize the collisions, it is convenient to choose M , a prime number). We use this hash function in the treatment of the Hamiltonian Eq. (1).

Now we describe the algorithm which deals with the problem of collisions. We need a new vector $L(i)$ of size M . By convention if $L(i) = -1$ the position i is empty. We also need an auxiliary variable R which is used to help find empty places.

Suppose that a representative K has been generated and we want to store it.

(a) First we evaluate the position index i corresponding to the state K by means of the hash function Eq. (A3).

(b) If $L(i) = -1$ the position is empty and we can store the state K here. We proceed as in step (f). Otherwise the position is occupied and we must continue the algorithm.

(c) If $I(i) = K$, then in position i we have just stored the integer K in a previous step. The algorithm finishes successfully. If $I(i) \neq K$ we continue the search.

(d) If $L(i) > 0$ set $i = L(i)$ and go back to step (c) [i.e., we continue the search using the position indicated in $L(i)$].

(e) If $L(i) = 0$, the state K has not appeared previously. We must store it in an empty place as follows: decrease R by one unit. If $L(R) = -1$ then we store K here. Otherwise decrease R another unit until an empty place is found (of course if R becomes zero the table is full and we must begin again by increasing the size M). Set $L(i) = R$. In such a way on the next occasion that K appears it will be localized in steps (c) and (d). Then set $i = R$ and go to step (f).

(f) Change $L(i) = 0$ and $I(i) = K$.

In Table III we show a simple example of the hashing technique where we consider $N=6$, $M=5$, and as initial state the representative $|\overline{101010}\rangle$. Note that in order to evaluate scalar products care should be taken with the possible degeneracy of the representatives. For example the representatives $|\overline{101010}\rangle$ and $|\overline{110100}\rangle$ are

TABLE III. An example of the hashing technique. In the vectors L , I , and C we store the initial vector ψ_0 , while in L' , I' , C' (L'' , I'' , C'') the vector $H\psi_0$ ($H^2\psi_0$) is stored. We consider $G/2t = 1$.

i	L	I	C	L'	I'	C'	L''	I''	C''
1	-1	0	0	0	50	-0.7071	0	50	4.2426
2	-1	0	0	-1	0	0	0	56	1.4142
3	0	42	0.2357	5	42	-0.7071	5	42	3.5355
4	-1	0	0	-1	0	0	-1	0	0
5	-1	0	0	0	52	-0.7071	0	52	4.2426

$$|\overline{101010}\rangle = 3|101010\rangle + 3|010101\rangle, \quad (\text{A4})$$

$$|\overline{110100}\rangle = |110100\rangle + |011010\rangle + |001101\rangle \\ + |100110\rangle + |010011\rangle + |101001\rangle. \quad (\text{A5})$$

The norm of state Eq. (A4) is 18 but the norm of state Eq. (A5) is 6. This fact does not represent a problem because the degeneracy of a given state is easily evaluated.

Finally we want to remark that in order to save computer time it is convenient to apply first the unperturbed Hamiltonian H_0 and then the potential term V .

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