Monte Carlo method for obtaining the ground-state properties of quantum spin systems

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A Monte Carlo method to find the ground-state properties of quantum spin systems is presented. Transforming a quantum spin Hamiltonian in a matrix with non-negative elements, we set up a Markov process whose stationary probability is dominated by the leading eigenvector of this matrix. From the simulation of the Markov process, by means of a Metropolis algorithm, we obtain the properties and the energy of the ground state. The method is applied to the spin-1 isotropic, Heisenberg antiferromagnet chain.

I. INTRODUCTION

The present Monte Carlo method was developed to obtain the properties of the leading eigenvector of non-negative matrices. The method is based on the recognition that any given matrix with non-negative entries can be regarded as the tranfer matrix of a certain statistical mechanical model. Since the properties of the model are dominated by the leading eigenvector of the transfer matrix,[1] then a Monte Carlo method that simulates the model will provide the properties of the leading eigenvector. If the leading eigenvector is also the ground state of a quantum system, then the method is capable of simulating the zero-temperature properties of this quantum system. This is, in fact, the case of several many-body quantum systems. Although the method presented here is general, we will be concerned only with quantum spin sytems.

If the quantum system has dimension d, then the statistical model system to be simulated has dimension $d+1$. In this sense the present method resembles other stochastic methods such as the path integral Monte Carlo method.[2–6] However, there is an essential distinction. In the path integral Monte Carlo method, the simulation is performed at a finite temperature and the ground-state properties of the system must be obtained by a zero-temperature extrapolation. Our method, on the other hand, is a zero-temperature Monte Carlo method.

The method we present is yet distinct from other zero-temperature Monte Carlo methods applied to quantum spin systems such as the Green's function Monte Carlo method[7–13] and the guided random-walk algorithm.[14,15] All these techniques can be viewed as stochastic versions of the power method in which the leading eigenvector of a matrix is projected out by repeated matrix multiplication.

The method present here has been used formerly to obtain the zero-temperature properties of spin-1/2 antiferromagnetic Heisenberg models.[16–18] Here, we generalize the method to be used to any value of spin and apply to the case of the spin-1 isotropic antiferromagnetic Heisenberg chain.

II. MONTE CARLO METHOD

Let T be a non-negative matrix, $T(\mu_1,\mu_2)\geqslant 0$, with μ_1 and μ_2 two suitable indices that take a discrete and finite set of values. For a given integer L, let us define a configuration μ by $\mu=(\mu_1,\mu_2,\ldots,\mu_L)$ and assign to it a probability $P(\mu)$ given by

$$P(\mu)=Z^{-1}T(\mu_1,\mu_2)T(\mu_2,\mu_3)\cdots \times T(\mu_{L-1},\mu_L)T(\mu_L,\mu_1), \tag{1}$$

where Z is a normalization constant. The present method is based on the recognition that the statistical properties of a system described by $P(\mu)$ are dominated by the leading eigenvector of T, for sufficiently large L. Therefore, from the properties of the *statistical mechanical* system defined by $P(\mu)$, obtained, for instance, by the Metropolis algorithm,[19] one gets the properties of the leading eigenvector of the *quantum* system described by the matrix T.

The method is particularly useful to find the properties of the ground state of quantum Hamiltonians whose nondiagonal elements, calculated on an appropriate vector basis, are nonpositive. If $\mathscr{H}$ is such a Hamiltonian and $\{|\mu\rangle\}$ the appropriate vector basis, then the elements of the matrix T are defined by $T(\mu',\mu)=C\delta(\mu',\mu)-\langle\mu'|\mathscr{H}|\mu\rangle$ where C is a positive constant chosen to make $T(\mu,\mu)$ positive. The ground-state energy E_0 and the largest eigenvalue λ_0 of T are related by $\lambda_0=C-E_0$ and the ground state of $\mathscr{H}$ is identified with the leading eigenvector of T.

The Monte Carlo method is constructed by setting up a Markov process for which the probability $P(\mu)$ given by (1) is the stationary probability. To this end it suffices to define a transition probability $W(\mu\rightarrow\mu')$ which satisfies the detailed balance condition

$$P(\mu)W(\mu\rightarrow\mu')=P(\mu')W(\mu'\rightarrow\mu). \tag{2}$$

In this way, with knowledge of the quotient $P(\mu)/P(\mu')$, it is possible to make a simulation based on the Metropolis algorithm.[19] We choose $W(\mu\rightarrow\mu')$ such that the allowed transitions are those for which the states μ and μ' differ by just one component. If we denote by $w_\ell(\mu_\ell\rightarrow\mu'_\ell)$ the probability of changing the ℓth component from μ_ℓ to μ'_ℓ, then the detailed balance condition is written as

$$T(\mu_{\ell-1},\mu_\ell)T(\mu_\ell,\mu_{\ell+1})w_\ell(\mu_\ell\rightarrow\mu'_\ell) = T(\mu_{\ell-1},\mu'_\ell)T(\mu'_\ell,\mu_{\ell+1})w_\ell(\mu'_\ell\rightarrow\mu_\ell). \tag{3}$$

A possible Monte Carlo algorithm can be set up by choosing

$$w_\ell(\mu_\ell \to \mu'_\ell) = \frac{A}{T(\mu_{\ell-1},\mu_\ell)T(\mu_\ell,\mu_{\ell+1})}, \tag{4}$$

where A is a constant, or

$$w_\ell(\mu_\ell \to \mu'_\ell) = \min\left\{ \frac{T(\mu_{\ell-1},\mu'_\ell)T(\mu'_\ell,\mu_{\ell+1})}{T(\mu_{\ell-1},\mu_\ell)T(\mu_\ell,\mu_{\ell+1})},\ 1 \right\}. \tag{5}$$

III. BASIC FORMULAS

In a Monte Carlo simulation we obtain estimates of quantities that are averages of state functions. Particularly, we are interested in two types of averages:

$$\langle A(\mu_1)\rangle = \sum_\mu A(\mu_1)P(\mu) = \sum_{\mu_1} A(\mu_1)P(\mu_1) \tag{6}$$

and

$$\langle B(\mu_1,\mu_2)\rangle = \sum_\mu B(\mu_1,\mu_2)P(\mu) = \sum_{\mu_1}\sum_{\mu_2} B(\mu_1,\mu_2)P(\mu_1,\mu_2), \tag{7}$$

where

$$P(\mu'_1) = \sum_\mu \delta(\mu'_1,\mu_1)P(\mu) \tag{8}$$

and

$$P(\mu'_1,\mu'_2) = \sum_\mu \delta(\mu'_1,\mu_1)\delta(\mu'_2,\mu_2)P(\mu) \tag{9}$$

are marginal probability distributions.

We consider T to be an irreducible matrix (that is, a matrix that cannot be reduced to block diagonal form by permutation of row and column indices) with non-negative elements, so that the Perron-Frobenius theorem[20] guarantees that its largest eigenvalue λ_0 will be nondegenerated and the corresponding eigenvector ϕ_0 will have positive elements, that is, $\phi_0(\mu_1)>0$. It is easy to prove that, for sufficiently large L,

$$P(\mu_1) = [\phi_0(\mu_1)]^2 \tag{10}$$

and

$$P(\mu_1,\mu_2) = \lambda_0^{-1}\phi_0(\mu_1)T(\mu_1,\mu_2)\phi_0(\mu_2), \tag{11}$$

the error being of the order $(\lambda_1/\lambda_0)^L$ where λ_1 is the second largest eigenvalue of T.

Suppose one wants to calculate the *quantum* average

$$\langle \phi_0|\mathcal{Q}|\phi_0\rangle = \sum_{\mu_1}\sum_{\mu_2} \phi_0(\mu_1)Q(\mu_1,\mu_2)\phi_0(\mu_2) \tag{12}$$

of a certain operator $\mathcal{Q}$ where $Q(\mu_1,\mu_2)=\langle\mu_1|\mathcal{Q}|\mu_2\rangle$ are the matrix elements of $\mathcal{Q}$ in the $\{|\mu_1\rangle\}$ representation. If $\mathcal{Q}$ is diagonal in this representation, that is, in the case $Q(\mu_1,\mu_2)=Q(\mu_1)\delta(\mu_1,\mu_2)$, then

$$\langle \phi_0|\mathcal{Q}|\phi_0\rangle = \sum_{\mu_1} Q(\mu_1)P(\mu_1) = \langle Q(\mu_1)\rangle. \tag{13}$$

For a generic operator, we use Eq. (11) to get

$$\langle \phi_0|\mathcal{Q}|\phi_0\rangle = \lambda_0 \sum_{\mu_1}\sum_{\mu_2} \frac{Q(\mu_1,\mu_2)}{T(\mu_1,\mu_2)}P(\mu_1,\mu_2) = \lambda_0\left\langle \frac{Q(\mu_1,\mu_2)}{T(\mu_1,\mu_2)} \right\rangle. \tag{14}$$

If we multiply both sides of Eq. (11) by $\delta(\mu_1,\mu_2)$ and sum over μ_1 and μ_2, we get, after using (10),

$$\langle \delta(\mu_1,\mu_2)\rangle = \lambda_0^{-1}\langle D(\mu_1)\rangle, \tag{15}$$

where $D(\mu_1)=T(\mu_1,\mu_1)$, so that

$$\lambda_0 = \frac{\langle D(\mu_1)\rangle}{\langle \delta(\mu_1,\mu_2)\rangle}. \tag{16}$$

If in Eq. (14) we choose $\mathcal{Q}$ to be the identity operator, then we obtain

$$\lambda_0^{-1} = \left\langle \frac{\delta(\mu_1,\mu_2)}{D(\mu_1)} \right\rangle. \tag{17}$$

From the estimates of averages obtained from the Monte Carlo method we can use either formula (16) or (17) to get the largest eigenvalue λ_0 of T and formulas (13) and (14) to get the *quantum* averages $\langle \phi_0|\mathcal{Q}|\phi_0\rangle$ over the leading eigenvector ϕ_0 of T. The use of formula (14) is, however, useful only when the elements $T(\mu_1,\mu_2)$ are strictly positive.

IV. MATRIX *T*

Our interest is to study the ground-state, or zero-temperature, properties of one-dimensional quantum spin systems described by Heisenberg-like Hamiltonians. We consider a spin-S Heisenberg Hamiltonian of the form

$$\mathcal{H} = \mathcal{H}_{xy} + \mathcal{H}_z, \tag{18}$$

where

$$\mathcal{H}_{xy} = -\sum_{(ij)} (S_i^x S_j^x + S_i^y S_j^y), \tag{19}$$

where the summation is over nearest-neighbor pairs of sites and $\mathcal{H}_z$ is a diagonal operator in the basis in which the spin operators S_i^z are diagonal.

Let us define the operator $\mathcal{T}$ by

$$\mathcal{T} = -\mathcal{H} + C, \tag{20}$$

where C is a positive constant. The elements of the matrix T are defined by $T(\sigma',\sigma)=\langle\sigma'|\mathcal{T}|\sigma\rangle$ where $|\sigma\rangle = |\sigma_1\sigma_2\cdots\sigma_N\rangle$, with $\sigma_i = -S, -S+1, \ldots, S-1, S$ vectors of the basis in which the operators S_i^z are diagonal.

The nondiagonal elements of T are given by

$$T(\sigma',\sigma) = -\langle\sigma'|\mathcal{H}_{xy}|\sigma\rangle, \tag{21}$$

and they vanish unless the states $|\sigma'\rangle$ and $|\sigma\rangle$ are of the form

$$|\sigma\rangle=|\sigma_1\cdots\sigma_i\sigma_j\cdots\sigma_N\rangle \tag{22}$$

and

$$|\sigma'\rangle=|\sigma_1\ldots,\sigma_i\pm1,\sigma_j\mp1,\ldots\sigma_N\rangle, \tag{23}$$

where i and j are nearest-neighbor sites. In this case the elements are positive and are given by

$$T(\sigma',\sigma)=\frac{1}{2}\sqrt{(S\mp\sigma_i)(S\pm\sigma_i+1)(S\pm\sigma_j)(S\mp\sigma_j+1)}. \tag{24}$$

The diagonal elements of T are given by

$$D(\sigma)=T(\sigma,\sigma)=-\langle\sigma|.\mathscr{H}_z|\sigma\rangle+C. \tag{25}$$

In the case where

$$\mathscr{H}_z=-\sum_{(ij)}S_i^zS_j^z, \tag{26}$$

which will be considered further on, we have

$$D(\sigma)=-\sum_{(ij)}\sigma_i\sigma_j+C. \tag{27}$$

We choose the constant C sufficiently large so that $D(\sigma)$ is positive.

Notice that the operator

$$S^z=\sum_i S_i^z \tag{28}$$

commutes with $\mathscr{H}$ and also with $\mathscr{T}$. Due to this property, the matrix T defined above reduces to a block diagonal form, each one of the $2S+1$ blocks, or sectors, being labeled by the eigenvalue M of S^z. Each block has the important property of being an irreducible matrix.

V. MONTE CARLO ALGORITHM

In this section we present a generalization of the Monte Carlo algorithm developed by de Oliveira[16] which was only suitable for spin-1/2 chains. We set up an algorithm to get the properties of the leading eigenvector of a given sector of T defined in the previous section. The algorithm for a given sector M is defined as follows.

Consider a square lattice of $N\times L$ sites having L columns of N sites each. At each site there is a spin variable $\sigma_{i\ell}$, $i=1,2,\ldots,N$ and $\ell=1,2,\ldots,L$, that takes the values $-S$, $-S+1$, $-S+2$, $\ldots$, $S-1$, S. To make a connection with previous results we use the notation $\mu_\ell=(\sigma_{1\ell},\sigma_{2\ell},\ldots,\sigma_{N\ell})$ and $\mu'_\ell=(\sigma'_{1\ell},\sigma'_{2\ell},\ldots,\sigma'_{N\ell})$ for the present and next configuration of the ℓth column.

We start with a total configuration such that (1) for each column ℓ, $\sigma_{1\ell}+\sigma_{2\ell}+\cdots+\sigma_{N\ell}=M$, and (2) the configurations μ_ℓ and $\mu_{\ell+1}$ of two consecutive columns are either equal to each other or are of the form $\mu_\ell=(\sigma_{1\ell},\ldots,\sigma_{i\ell},\sigma_{i+1,\ell},\ldots,\sigma_{N\ell})$ and $\mu_{\ell+1}=(\sigma_{1\ell},\ldots,\sigma_{i\ell}\pm1,\sigma_{i+1,\ell}\mp1,\ldots,\sigma_{N\ell})$.

The algorithm is constructed in such a way that these two properties are preserved in each step of the simulation.

At each step of the process we try to modify the states of two nearest-neighbor sites that belong to a randomly chosen column by performing the transformations

$$\sigma_{i\ell}\to\sigma_{i\ell}+1 \quad\text{and}\quad \sigma_{i+1,\ell}\to\sigma_{i+1,\ell}-1$$

or

$$\sigma_{i\ell}\to\sigma_{i\ell}-1 \quad\text{and}\quad \sigma_{i+1,\ell}\to\sigma_{i+1,\ell}+1.$$

Of course, these transformations are not performed when the pair of sites are such that $\sigma_{i\ell}=\sigma_{i+1,\ell}=S$ or $\sigma_{i\ell}=\sigma_{i+1,\ell}=-S$. Pairs of this type we call forbidden pairs and the others allowed pairs. We denote by $N(\mu_\ell)$ the number of allowed pairs in the configuration μ_ℓ of the ℓth column.

At each time step of the Monte Carlo simulation we first choose one column at random, say, the ℓth column, and try to modify its configuration according to the following cases.

(1) The chosen column is identical to the preceding and following columns. Then, we choose at random one of the allowed pairs of spins of the chosen column with probability $1/N(\mu_\ell)$. Let the states of the pair be α and β. Then, the chosen column could be modified according to the two possibilities

$$\begin{pmatrix}\alpha&\alpha&\alpha\\ \beta&\beta&\beta\end{pmatrix}\to\begin{pmatrix}\alpha&\alpha+1&\alpha\\ \beta&\beta-1&\beta\end{pmatrix} \tag{29}$$

and

$$\begin{pmatrix}\alpha&\alpha&\alpha\\ \beta&\beta&\beta\end{pmatrix}\to\begin{pmatrix}\alpha&\alpha-1&\alpha\\ \beta&\beta+1&\beta\end{pmatrix}. \tag{30}$$

We choose one of the possibilities with equal probability. If $|\alpha|=S$ or $|\beta|=S$, there is just one possibility. Then, the new configuration will be accepted with probability

$$p_\ell=\frac{N(\mu_\ell)}{[D(\mu_\ell)]^2}. \tag{31}$$

(2) The preceding column is identical to the following and distinct from the chosen column which differs from the other two by just one pair of sites whose states are $\alpha-1$ and $\beta+1$. The two possibilities of changing the states are

$$\begin{pmatrix}\alpha&\alpha-1&\alpha\\ \beta&\beta+1&\beta\end{pmatrix}\to\begin{pmatrix}\alpha&\alpha&\alpha\\ \beta&\beta&\beta\end{pmatrix} \tag{32}$$

and

$$\begin{pmatrix}\alpha&\alpha-1&\alpha\\ \beta&\beta+1&\beta\end{pmatrix}\to\begin{pmatrix}\alpha&\alpha+1&\alpha\\ \beta&\beta-1&\beta\end{pmatrix}. \tag{33}$$

We choose one of them with equal probability. If $\alpha=S$ or $\beta=-S$, there is just one possibility. In this case the new configuration is accepted with probability

$$p_\ell=\frac{1}{[T(\mu_\ell,\mu_{\ell+1})]^2}. \tag{34}$$

(3) The preceding column is identical to the chosen column and distinct from the following column. There is just one possibility of changing the state which is

$$\begin{pmatrix} \alpha & \alpha & \alpha+1 \\ \beta & \beta & \beta-1 \end{pmatrix} \rightarrow \begin{pmatrix} \alpha & \alpha+1 & \alpha+1 \\ \beta & \beta-1 & \beta-1 \end{pmatrix}. \quad (35)$$

The new configuration is accepted with probability equal to

$$p_{\ell} = \min\left\{ \frac{D(\mu_{\ell})}{D(\mu_{\ell-1})}, 1 \right\}. \quad (36)$$

(4) The following column is identical to the chosen column and distinct from the preceding column. There is just one possibility of changing the state which is

$$\begin{pmatrix} \alpha & \alpha+1 & \alpha+1 \\ \beta & \beta-1 & \beta-1 \end{pmatrix} \rightarrow \begin{pmatrix} \alpha & \alpha & \alpha+1 \\ \beta & \beta & \beta-1 \end{pmatrix}. \quad (37)$$

The new configuration is accepted with probability

$$p_{\ell} = \min\left\{ \frac{D(\mu_{\ell-1})}{D(\mu_{\ell})}, 1 \right\}. \quad (38)$$

(5) The three columns are distinct by just one pair:

$$\begin{pmatrix} \alpha+1 & \alpha & \alpha-1 \\ \beta-1 & \beta & \beta+1 \end{pmatrix}. \quad (39)$$

In this case we cannot make any change in the chosen column.

(6) The preceding and following columns are distinct in two pairs that have one site in common. Here we distinguish two cases which are

$$\begin{pmatrix} \alpha & \alpha-1 & \alpha-1 \\ \beta & \beta+1 & \beta \\ \gamma & \gamma & \gamma+1 \end{pmatrix} \rightarrow \begin{pmatrix} \alpha & \alpha & \alpha-1 \\ \beta & \beta-1 & \beta \\ \gamma & \gamma+1 & \gamma+1 \end{pmatrix} \quad (40)$$

and

$$\begin{pmatrix} \alpha & \alpha-1 & \alpha-1 \\ \beta & \beta+1 & \beta+2 \\ \gamma & \gamma & \gamma-1 \end{pmatrix} \rightarrow \begin{pmatrix} \alpha & \alpha & \alpha-1 \\ \beta & \beta+1 & \beta \\ \gamma & \gamma-1 & \gamma+1 \end{pmatrix}. \quad (41)$$

In the first case the states of the three sites are modified whereas in the second case we change the states of two the external sites only. In both cases, however, the new state is accepted with probability

$$p_{\ell} = \min\left\{ \frac{T(\mu_{\ell-1},\mu'_{\ell})T(\mu'_{\ell},\mu_{\ell+1})}{T(\mu_{\ell-1},\mu_{\ell})T(\mu_{\ell},\mu_{\ell+1})}, 1 \right\}. \quad (42)$$

(7) The preceding and following columns are distinct in two pairs that do not overlap:

$$\begin{pmatrix} \alpha & \alpha-1 & \alpha-1 \\ \beta & \beta+1 & \beta+1 \\ \gamma & \gamma & \gamma-1 \\ \delta & \delta & \delta+1 \end{pmatrix} \rightarrow \begin{pmatrix} \alpha & \alpha & \alpha-1 \\ \beta & \beta & \beta+1 \\ \gamma & \gamma-1 & \gamma-1 \\ \delta & \delta+1 & \delta+1 \end{pmatrix}. \quad (43)$$

In this case we make the transition with probability 1.

It is straightforward, although tedious, to verify that the transition probabilities defined by this algorithm satisfy the detailed balance condition.

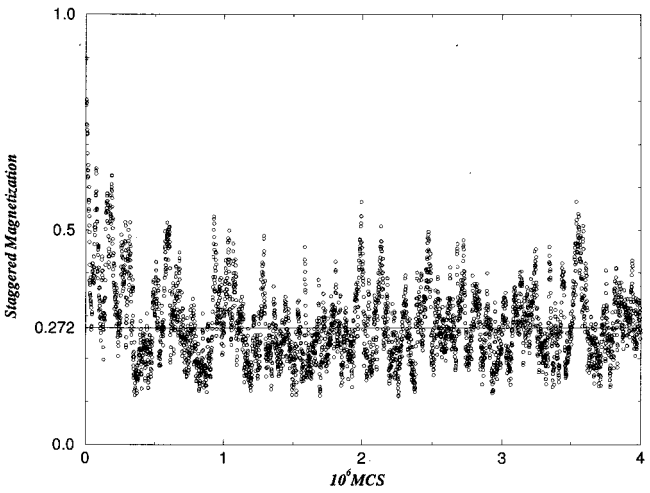

FIG. 1. Time evolution of the staggered magnetization for the case of a chain with $N=32$ sites. Each point represents an average over 10^3 MCS. The line represents the average value over the last 3×10^6 MCS.

VI. APPLICATION

To show the usefulness of the method we present a simulation made in a quantum spin system described by the isotropic antiferromagnetic Heisenberg Hamiltonian given by

$$\mathscr{H} = \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}, \quad (44)$$

where $\vec{S} = (S_i^x, S_i^y, S_i^z)$ are spin-1 operators, with periodic boundary conditions. This model is particularly interesting due to the prediction by Haldane that isotropic antiferromagnetic Heisenberg chains, with integer spin, have an energy gap.[21]

Performing rotations on the spins operators of the odd sites by an angle π around the z axis, that is, making the transformations $S_i^x \rightarrow -S_i^x$, $S_i^y \rightarrow -S_i^y$, and $S_i^z \rightarrow S_i^z$ if i is odd, we obtain a Hamiltonian of the form (18), namely,

$$\mathscr{H} = -\sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \sum_{i=1}^{N} S_i^z S_{i+1}^z. \quad (45)$$

The operator $\mathscr{T}$ is defined by

$$\mathscr{T} = \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - \sum_{i=1}^{N} S_i^z S_{i+1}^z + (N+1). \quad (46)$$

We performed simulations within the sectors with $M=0$ and $M=1$ to get the ground-state energy E_0 and the energy of the first excited state E_1. In this way it is possible to find the energy gap $\Delta E = E_1 - E_0$ of the system. We have also measured the staggered magnetizations per site m_N, defined by

$$m_N = \frac{1}{N} \langle \phi_0 || \mathscr{M} || \phi_0 \rangle, \quad (47)$$

and the staggered susceptibility per site χ, defined by

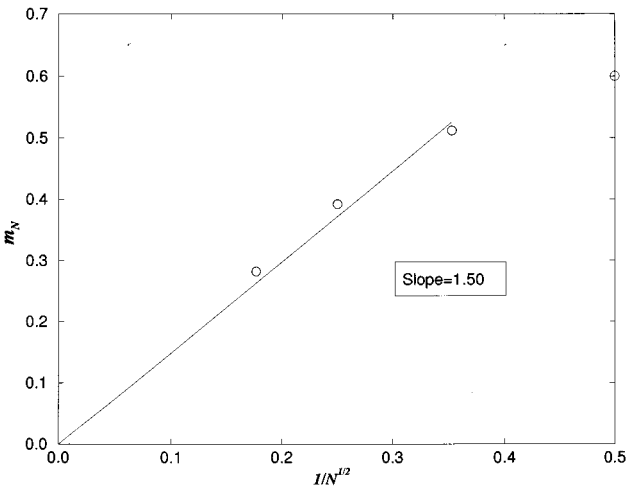

FIG. 2. Staggered magnetization m_N versus $1/\sqrt{N}$.

$$\chi_N=\frac{1}{N}\{\langle\phi_0|\mathscr{M}^2|\phi_0\rangle-\langle\phi_0||\mathscr{M}||\phi_0\rangle^2\}, \tag{48}$$

where

$$\mathscr{M}=\sum_{\ell=1}^{N}(-1)^{\ell}S_{\ell}^{z} \tag{49}$$

and ϕ_0 is the ground state.

The Monte Carlo simulations were performed starting from a configuration corresponding to a saturated Néel state and we used chains of sizes ranging from $N=4$ up to $N=48$ and a number of columns, $L=1000$. We obtained the average estimates using a number of Monte Carlo steps (MCS) of the order of 10^6. One MCS is defined as L trials of changing the state of a column.

Figure 1 shows the time evolution of the staggered magnetization m_N for the case of $N=32$. There is a transitory period, of about 10^6 MCS after which the system reaches the stationary state. Taking the average over the next 3×10^6 MCS, we get the result $m_{32}=0.272\pm0.007$. Figure 2 shows

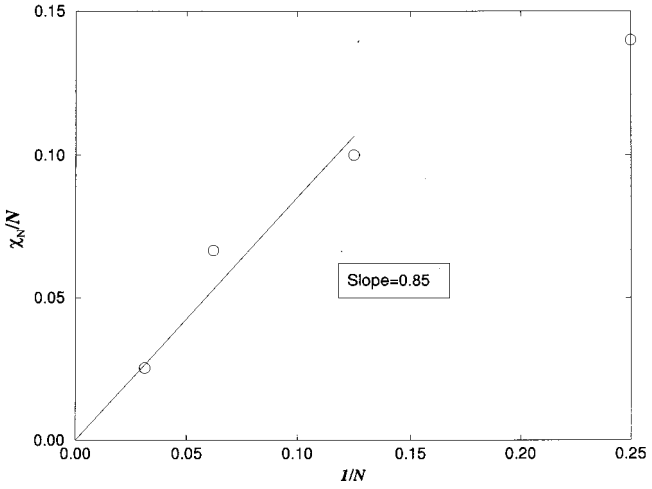

FIG. 3. Staggered susceptibility χ_N over N versus $1/N$. The slope at the origin gives the susceptibility for the infinite chain.

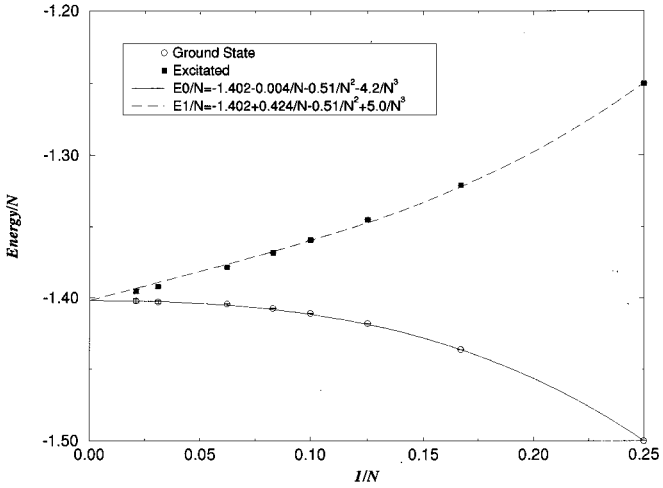

FIG. 4. Energy densities E_0/N and E_1/N, of the ground state and the first excited state versus $1/N$.

m_N as a function of $1/\sqrt{N}$. The extrapolation $N\to\infty$ gives a vanishing staggered magnetization per site for the infinite chain, which is the expected result. Figure 3 shows χ_N/N as a function of $1/N$. The slope at the origin gives the susceptibility for the infinite chain, namely, $\chi=0.85\pm0.03$.

Figure 4 shows a plot of the energy densities E_0/N and E_1/N, corresponding to the ground state and first excited state, respectively, versus $1/N$. The extrapolation $N\to\infty$ gives the result, for the ground-state energy per site, $\epsilon=-1.402\pm0.005$. Figure 5 displays the gap energy $\Delta E=E_1-E_0$ versus $1/N^2$ from which we obtain $\Delta E=0.414\pm0.005$. This is in agreement with the prediction by Haldane[21] and previous numerical results.[6,8,22–24]

The simulations were made in a HP Apollo. The CPU time required in the longest chain was about 48 h.

VII. CONCLUSIONS

We have presented a Monte Carlo method to find the ground properties of quantum spin systems. The method was used to obtain the properties of the ground state of the spin-1

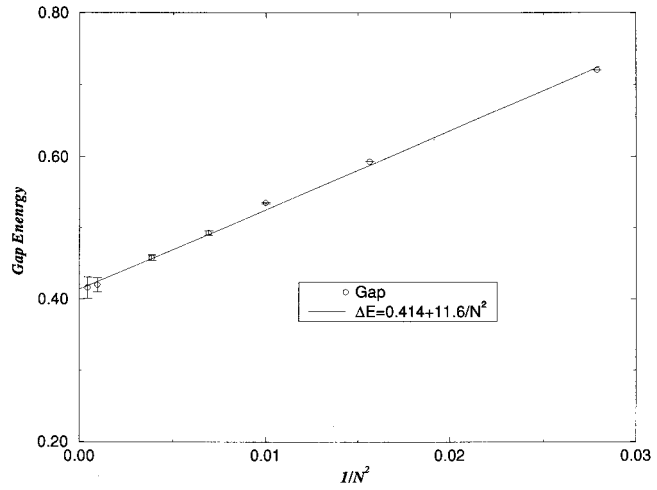

FIG. 5. Gap energy $\Delta E=E_1-E_0$ versus $1/N^2$.

isotropic Heisenberg antiferromagnet chain. The energy gap was found with a precision which is comparable with other Monte Carlo methods. The method was also capable of giving the ground-state averages of quantum operators, especially those which are diagonal in the representation used in the simulation such as the staggered magnetization and the susceptibility in the z direction. The algorithm presented here is valid for Heisenberg-like Hamiltonians of any value of spin, defined on a chain. However, the algorithm can be generalized to be used in the case of any dimension. Due to the general validity of the method it is suitable for studying more complex spin systems.

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