Monte Carlo Simulation of Quantum Spin Systems

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A Monte Carlo method applicable to a class of noncommuting spin variables is developed. The technique relies on a stochastic procedure which simulates the dominant vacuum-to-vacuum graphs of quantum many-body theory. Computational speed is only weakly dependent on the dimensionality of the system and is fast enough to handle large lattices. This method is tested on the $S=\frac{1}{2}$ ferromagnetic Heisenberg model in one, two, and three dimensions and on the $S=\frac{1}{2}$ XY model in one dimension where exact results are known.

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Monte Carlo simulation of quantum systems is an important and rapidly growing area of research[1] which is directed towards developing a nonperturbative technique to calculate the properties of interacting quantum systems. Recently[2] a method based on a direct space–imaginary-time representation has been used to treat a number of problems involving fermionic and bosonic degrees of freedom in one dimension (1D) with good results. In this paper we discuss an exact method first mentioned by Handscomb[3] to treat the $S=\frac{1}{2}$ ferromagnetic Heisenberg model. We interpret this method, we believe for the first time, as a simulation of dominant vacuum-to-vacuum processes and extend this so as to be applicable to a class of noncommuting spin variables. The method is then tested on the $S=\frac{1}{2}$ ferromagnetic Heisenberg model in one, two, and three dimensions. This serves to clarify the method, to check its speed, and also to verify the quantitative aspects. It is then applied to $S=\frac{1}{2}$ XY model in one dimension and compared with exact results. At this point we would like to emphasize that by its very nature the method is only weakly dependent on the dimensionality of the system, this being one of its advantages.

An important ingredient in any Monte Carlo simulation is an exhaustive enumeration of states. In Handscomb's method the states are represented by a countably infinite set of ordered integers; later we shall see that this is also the space of all vacuum-to-vacuum graphs of many-body theory. This unconventional enumeration of states is the novelty of this method. Consider now a Hamiltonian H which may be expressed as the sum

$$H=\sum_{i=1}^{N_b} h_i,$$

where N_b is large but finite. Then the expectation value of an operator O may be expressed as

$$\langle O\rangle=\sum_{n=0}^{\infty}\sum_{\{C_n\}} O(C_n)\pi(C_n),$$

where

$$Z\pi(C_n)=[(-\beta)^n/n!]\,\mathrm{tr}(h_{i_1}\cdots h_{i_n})$$

and

$$O(C_n)=\mathrm{tr}(Oh_{i_1}\cdots h_{i_n})/\mathrm{tr}(h_{i_1}\cdots h_{i_n}).$$

In these equations $\{C_n\}$ denotes any sequence of ordered integers $i_1,\ldots,i_n$ in the range $1\le i\le N_b$ and Z denotes the partition function. For $\pi(C_n)$ to define a proper distribution we must have $\pi(C_n)>0$ for all C_n and $\sum_n\sum_{\{C_n\}}\pi(C_n)<\infty$. A naive application of this method to antiferromagnets is not possible since $\pi(C_n)<0$.[4] However, for the nearest-neighbor $S=\frac{1}{2}$ XY model on bipartite lattices, to be discussed below, the sign of the coupling is irrelevant.

A Markov chain is formulated as follows. Given a sequence $\{C_n\}$ a forward direction is chosen, with probability f_n, whereas one tries to insert an index selected uniformly and randomly from the set $1\le i\le N_b$ so as to make a transition $\{C_n\}\rightarrow\{C_n i\}$; the decision to make this move depends on the ratio $\pi(C_n i)/\pi(C_n)$ in a standard way. Similarly if a backward direction is selected with probability $(1-f_n)$, an attempt is made to make the transition $\{i_1 C_{n-1}\}\rightarrow\{C_{n-1}\}$. Exploiting the cyclic invariance of trace, we permute the sequence if a backward move was rejected to improve the sampling rate. If the transition probability is constructed by multiplying $\pi(C_n)$ by an arbitrary set of positive numbers $\lambda_1\lambda_2\cdots\lambda_n$, then the equation[3]

$$f_n=1-n\lambda_n f_{n-1}$$

has to be satisfied to reach the desired limit distribution. A convenient parametrization of f's

can be used to determine λ's which satisfy the above relation. In order to illustrate the method let us consider the $S=\frac{1}{2}$ ferromagnetic Heisenberg model. In this rather special case the equivalence between $\vec{S}_1\cdot\vec{S}_2$ and $\frac{1}{4}(2P_{12}-1)$, where P_{12} is the permutation operator, can be exploited to rewrite the Hamiltonian as a sum of transposition operators (we consider for simplicity only the nearest-neighbor case). A string of operators $h_{i_1}\cdots h_{i_n}$ then simply induces a permutation on a standard set $(1,2,3,\ldots,N)$, where N is the number of spins on the lattice. For example, the permutation induced by a "time"-ordered sequence of transpositions $P_{56}P_{34}P_{12}P_{23}P_{12}$ shown in Fig. 1(a) can be factored into a cycle of length 3, a cycle of length 2, and $N-5$ trivial cycles of length 1. The nontrivial cycles are shown in Fig. 1(b). Each sequence can be graphically represented in this way. The processes are time ordered within a cycle but not between cycles. The trace of a string of operators is 2^x where $x=n_{C_n}$ is the total number of cycles including the trivial ones. Trace ratios such as $\pi(C_n i)/\pi(C_n)$ are either 2 or $\frac{1}{2}$ depending on whether a cycle was broken up into two parts or two cycles were joined together in the process. Thus the Monte Carlo method simulates the vacuum fluctuations of the system by joining or splitting apart these cycles, thus carrying out a walk

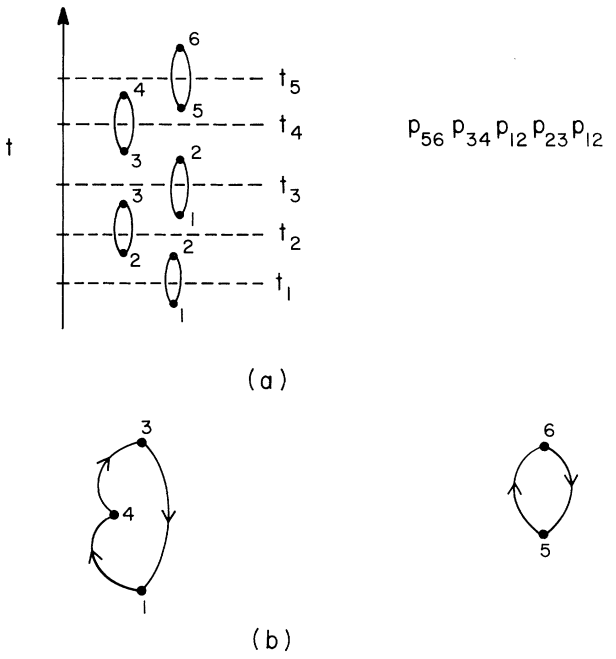

FIG. 1. An example of vacuum-to-vacuum graphs for Heisenberg model.

along the paths connecting dominant processes. The average of an operator is an average over these processes. This procedure enumerates all the graphs only for the $S=\frac{1}{2}$ isotropic Heisenberg model. This becomes evident in trying to simulate the $S=\frac{1}{2}$ XY model which we discuss below. In this case

$$H=-J\sum_{\langle ij\rangle}(S_i^+S_j^-+S_j^+S_i^-),$$

where the sign of J is irrelevant for bipartite lattices and $\langle ij\rangle$ denotes a nearest-neighbor pair. This Hamiltonian can be written as

$$H=\sum_{i=1}^{2N_b}h_i,$$

where N_b is the number of bonds on the lattice. For example, let us say that $h_1=S_1^+S_2^-$. The trace of all odd-order terms in βJ in the expansion of the exponential vanishes, and so it is clear that two indices at a time must be inserted or deleted. However, if Handscomb's original method is used, i.e., $\{C_n\}\rightarrow\{C_n ij\}$ or $\{i_1 i_2 C_{n-2}\}\rightarrow\{C_{n-2}\}$, not all the graphs are generated. We can generate all the graphs only if i and j are inserted at two random locations in the sequence or deleted from two random locations. The difference equation to be satisfied now is as follows:

$$f_{n+2}=1-(n+1)(n+2)\lambda_{n+1}\lambda_{n+2}f_n.$$

Since the h's are no longer equivalent to permutation operators a new method is needed to calculate the trace ratios. If a directed bond such as $S_1^+S_2^-$ is represented by an arrow whose head is on site 1, then a sequence C_n is a collection of graphs consisting of arrows whose tails and heads alternate at a site as time increases, and the number of arrows going into a site is equal to the number going out.[5] Each of these directed ordered graphs can be collapsed so that they are no longer directed or time ordered. This exhibits the connectedness of the lattice by means of bare graphs. The trace of a string of operators is 2^{N-n_v}, where n_v is the total number of sites in the bare graphs. However, for any linked graph there is a corresponding graph obtained by reversing all the arrows. Their traces are the same and both should be included. The Monte Carlo method must sample them equally, but for large graphs this requires unacceptably long sampling times. The solution to this difficulty is to partition the Hamiltonian into bonds such as $h_1=(S_1^+S_2^-+S_2^+S_1^-)$. A linked graph of zero trace is then recognized by the fact that no possible assignments of arrows can satisfy the

TABLE I. Susceptibility for $S=\frac{1}{2}$ Heinsenberg model in 1D.

kT/J	Padé	$N=8$	$N=32$	$N=128$
1.0	1.869	1.867 ± 0.004	1.869 ± 0.004	1.869 ± 0.004
0.6	2.324	2.299 ± 0.007	2.324 ± 0.008	2.328 ± 0.007
0.4	2.835	2.694 ± 0.008	2.841 ± 0.012	2.841 ± 0.010
0.2	4.172	3.202 ± 0.008	4.199 ± 0.024	4.210 ± 0.022

TABLE II. Energy and specific heat for $S=\frac{1}{2}$ XY model in 1D.

	Energy		Specific heat	
$kT/\|J\|$	Exact	MC	Exact	MC
2.5	−0.1924	−0.192 ± 0.001	0.071	0.071 ± 0.001
1.5	−0.3010	−0.299 ± 0.002	0.163	0.166 ± 0.002
1.0	−0.4058	−0.402 ± 0.003	0.263	0.265 ± 0.004
0.5	−0.5589	−0.558 ± 0.001	0.307	0.305 ± 0.028
0.35	−0.6000	−0.590 ± 0.010	0.229	0.233 ± 0.010

rules mentioned earlier. The trace of a string of operators is $2^{N-n_v}2^{n_d}$, where n_v is again the number of sites in the collapsed bare graphs and n_d the number of linked parts. More details will be discussed elsewhere.[6]

For any model it is easy to show that the internal energy (except for a constant) satisfies $E/N_b|J| = -\langle n\rangle_{MC}/\beta|J|N_b$; i.e., the Monte Carlo average of the length of the sequences gives the internal energy. The specific heat can be computed from $C_v/Nk_B = (\langle n^2\rangle_{MC} - \langle n\rangle_{MC}^2 - \langle n\rangle_{MC})$, a result that is easily proved. The reduced susceptibility for the $S=\frac{1}{2}$ Heisenberg model is given above the transition temperature (if there is one) by

$$\chi T/N\mu^2 = N^{-1}\langle\textstyle\sum_i l_i^2\rangle_{MC}.$$

This sum runs over the squares of the lengths of all the cycles including the trivial ones.

The comparison of susceptibility for the $S=\frac{1}{2}$ Heisenberg model with Padé results[7] in 1D is shown in Table I. In Table II the internal energy and specific heat for the $S=\frac{1}{2}$ XY model in 1D are compared with the exact results for 40 spins. Our numbers are different from those in Ref. 2 since we use a grand canonical ensemble. The results for the $S=\frac{1}{2}$ XY model in higher dimensions will be discussed elsewhere.[6] In Fig. 2 we show the susceptibility of the two-dimensional Heisenberg model. This is to be compared with the results in 3D shown in Fig. 3 and the data presented for 1D in Table I. The dependence of susceptibility on the lattice size in 2D is similar to that of 1D and different from that in 3D. This leads us to believe that these results are consistent with the general belief that a transition in 2D is unlikely. In Fig. 4 the results for internal energy and specific heat are plotted for the 3D

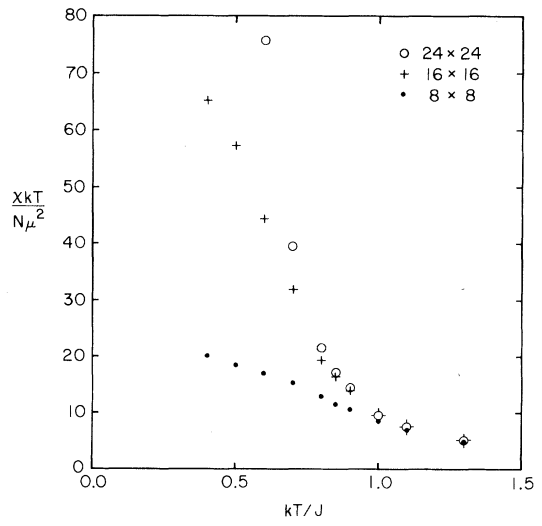

FIG. 2. Susceptibility for 2D Heisenberg model.

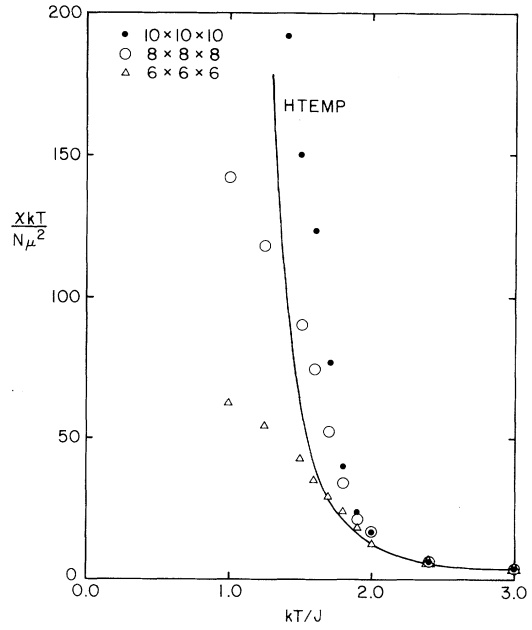

FIG. 3. Susceptibility for 3D Heisenberg model. HTEMP corresponds to a truncated high-temperature series (Ref. 8).

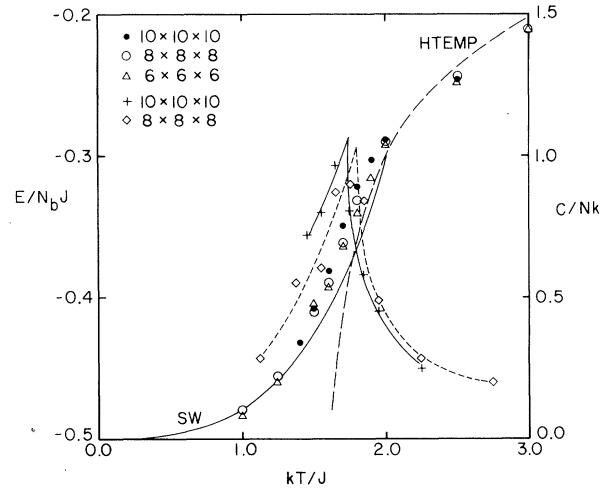

FIG. 4. Results for 3D Heisenberg model. Crosses and diamonds denote specific heat. The lines are drawn to guide the eyes.

$S=\frac{1}{2}$ Heisenberg model. SW is the spin-wave theory containing terms up to T^4 and is plotted from the results quoted in Ref. 8. HTEMP corresponds to a truncated eight-term high-temperature series.[8]

The number of iterations was between 6×10^4 and 5×10^6, depending on the individual case. The *statistical* errors as determined by calculating the standard deviation of block averages were generally kept to less than 1%. As always, errors computed by this procedure are not strict bounds.

Our emphasis here has been on developing a general method and estimating its speed and its potential. We have shown that Handscomb's method, neglected for nearly twenty years, is very powerful and lends itself to generalizations, provided sufficient care is taken to make all graphs accessible. Interesting problems[9] involving quenched or annealed disorder in the XY model are now possible and will be considered in the near future.

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[1]F. Fucito, E. Marinari, G. Parisi, and C. Rebbi, Nucl. Phys. B180, 369 (1981); D. J. Scalapino and R. L. Sugar, Phys. Rev. Lett. 46, 519 (1981); D. Weingarten and D. Petcher, Phys. Lett. 49B, 333 (1981); R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981); A. Duncan and M. Furman, Nucl. Phys. B140, 767 (1981); J. Kuti, Institute for Theoretical Physics Report No. NSF-ITP-81-151 (unpublished); H. De Raedt and A. Lagendijk, Phys. Rev. Lett. 46, 77 (1981).

[2]J. E. Hirsch, D. J. Scalapino, R. L. Sugar, and R. Blankenbecler, Phys. Rev. Lett. 47, 1628 (1981).

[3]D. C. Handscomb, Proc. Cambridge Philos. Soc. 58, 594 (1962), and 60, 115 (1964).

[4]In a recent paper [J. W. Lyklema, Phys. Rev. Lett. 49, 88 (1982)] data for very high temperatures have been presented for the $S=\frac{1}{2}$ isotropic Heisenberg antiferromagnet in 1D. This method fails for temperatures lower than those presented.

[5]D. D. Betts, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

[6]S. Chakravarty and D. B. Stein, to be published.

[7]G. A. Baker, G. S. Rushbrooke, and H. E. Gilbert, Phys. Rev. 135, A1272 (1964).

[8]See G. S. Rushbrooke, G. A. Baker, and P. J. Wood in the volume quoted in Ref. 5.

[9]An example is the motion of tricritical point in ^{3}He-^{4}He mixture as presented by J. del Cueto, R. L. Johnson, T. Rohde, F. H. Wirth, and E. H. Graf, J. Phys. (Paris), Colloq. 41, C-7, 133 (1980).