not the velocity autocorrelation function.

[6]The algebra required to obtain the friction coefficient is formidable. I include the expression here because it was obtained by a completely independent calculation from that of Ref. 5 and follows the notation of Refs. 2 and 3. The many differences in notation between Ref. 5 and Refs. 2 and 3 make comparison difficult. Also I hope to simplify the task of comparing the results for "stick" boundary conditions to those of "slip" boundary conditions obtained in Ref. 2.

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Quantum-Statistical Monte Carlo Method for Heisenberg Spins

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(Received 23 March 1982)

An exact Monte Carlo method for calculating thermodynamic properties of quantum spin systems is described. Results for one-dimensional ferromagnetic and antiferromagnetic systems and for three-dimensional ferromagnetic systems show that the method can be used to study quantum spin systems as extensively as classical spin systems are studied with conventional Monte Carlo methods.

PACS numbers: 05.30.Ch

In the last decade Monte Carlo calculations have proven to be a very valuable tool in deepening our understanding of classical spin systems.[1] This cannot be said for quantum systems. Recently, however, there has been considerable interest in the development of Monte Carlo procedures for these systems.[2] These methods use the fact that a d-dimensional quantum system can be mapped onto a $(d+1)$-dimensional classical system through the use of Trotter's formula.[3] This mapping is exact only when the additional "time" dimension is infinite, which of course cannot be realized on a computer. This means that for a Monte Carlo calculation one has in addition to the limited size of the physical system also the problem of a finite time dimension.

A method which does not possess this difficulty was proposed by Handscomb[4] for the ferromagnetic Heisenberg system. In this Letter I generalize the method and demonstrate its usefulness for both ferromagnetic and antiferromagnetic interactions.

I study the spin-$\frac{1}{2}$ Heisenberg Hamiltonian

$$\mathcal{H} = -2J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} - g\beta H \sum_{i=1}^{N} S_i^z,$$

or, expressed in terms of permutation operators $E(i,j) = (1 + 4\vec{S}_i \cdot \vec{S}_j)/2$,

$$\mathcal{H} = -J \sum_{i=1}^{dN} E(i, i+1) - g\beta H \sum_{i=1}^{N} S_i^z + \frac{d}{2} JN,$$

where (dN) is the number of interactions. In neglecting the constant I write this as

$$\mathcal{H} = \mathcal{H}^0 - J \textstyle\sum_i E_i .$$

The partition function can be expanded as follows:

$$Z_{\pm} = \mathrm{Tr} e^{-\mathcal{H}/kT} = \sum_{n=0}^{\infty} (\pm)^n \frac{(\beta|J|)^n}{n!} \sum_{C_n} \mathrm{Tr}\{E_{i_1} \ldots E_{i_n} \exp(-\mathcal{H}^0/kT)\},$$

where $\sum_{C_n}$ denotes the sum over all possible sequences $(i_1 \ldots i_n)$. The $\pm$ signs correspond to the ferromagnetic and antiferromagnetic cases. With the definition

$$\pi(C_n) = \frac{(\beta|J|)^n}{n!} \mathrm{Tr}\{E_{i_1} \ldots E_{i_n} \exp(-\mathcal{H}^0/kT)\}$$

we have $Z_{\pm} = \sum_n \sum_{C_n} (\pm)^n \pi(C_n)$. Similarly we write

$$\mathrm{Tr}\{O e^{-\mathcal{H}/kT}\} = \textstyle\sum_n \sum_{C_n} \Omega(C_n) \pi(C_n)$$

with

$$\Omega(C_n) = \frac{(\pm)^n \mathrm{Tr}\{O E_{i_1} \ldots E_{i_n} \exp(-\mathcal{H}^0/kT)\}}{\mathrm{Tr}\{E_{i_1} \ldots E_{i_n} \exp(-\mathcal{H}^0/kT)\}}.$$

With these definitions we have for the quantum mechanical expectation value

$$\langle O\rangle = \frac{\mathrm{Tr}\{Oe^{-\mathcal{H}/kT}\}}{\mathrm{Tr}\{e^{-\mathcal{H}/kT}\}} = \frac{\langle\Omega\rangle_{\mathrm{cl}}}{\langle(\pm)^n\rangle_{\mathrm{cl}}},$$

where the angular brackets with subscript "cl" denote a classical expectation value over the distribution $\pi(C_n)$.

The usefulness of this mapping is strongly dependent, in general, on the form of the Ω's and π. For the Heisenberg Hamiltonian it is easy to calculate that

$$\pi(C_n) = \frac{(\beta|J|)^n}{n!}\prod_{j=1}^{k(C_n)} 2\cosh\frac{g\beta H a_j}{2kT}.$$

Here $k(C_n)$ is the number of cycles in $\{E_{i_1}\ldots E_{i_n}\}$ and a_j is the length of a cycle. The energy operator can be incorporated into the distribution $\pi(C_n)$ and therefore calculated as the average number of permutations

$$E(H) = -HM(H) - \langle n\rangle_{\mathrm{cl}}/\beta + \tfrac{1}{2}dJN.$$

The magnetization is given by

$$M(H) = \langle\textstyle\sum_j (g\beta/2)a_j \tanh\{a_j g\beta H/2kT\}\rangle_{\mathrm{cl}}.$$

The zero-field susceptibility and specific heat are somewhat more complicated, but reduce at zero field to

$$\chi_0 = (kT)^{-1}\langle\textstyle\sum_j(\frac{1}{2}g\beta a_j)^2\rangle_{\mathrm{cl}},$$

$$C_v = k[\langle n^2\rangle_{\mathrm{cl}} - \langle n\rangle_{\mathrm{cl}}^2 - \langle n\rangle_{\mathrm{cl}}].$$

To realize a Markov chain with limiting distribution $\pi(C_n)$ we need to define the transition probabilities. Starting from a random sequence of permutation operators $\{E_{i_1}\ldots E_{i_n}\}$, we add a randomly chosen permutation operator at a randomly chosen position in the sequence or remove a randomly chosen permutation from the sequence. This is a modification of Handscomb's procedure in which an operator is added only at the end and removed from the beginning. In case of nonacceptance of a removal, cyclic permutation was applied to provide a better covering of sample space. This procedure destroys the structure of the sequence faster and should be better, particularly for longer sequences. Because the trace is invariant under cyclic permutation, this is still a proper Markov chain.

For the procedure described above I define the following transition probabilities:

$$\mathcal{P}(C_n \to C_{n+1}) = p(i)f(n)T(C_{n+1}),$$

$$\mathcal{P}(C_{n+1} \to C_n) = [1 - f(n+1)]T(C_n).$$

Here $f(n)$ is the probability of adding a permutation to a sequence of length n and $p(i)$ is the probability of choosing permutation i. For the acceptance $T(C_{n+1})$ we find[5]

$$T(C_{n+1}) = \min\left(1, \frac{1-f(n+1)}{p(i)f(n)}\frac{\pi(C_{n+1})}{\pi(C_n)}\right).$$

In the calculations presented I have taken $p(i) = 1/N$ and $f_n = (1+\lambda n)^{-1}$. Other possibilities are $(f_n = \frac{1}{2}, f_0 = 1)$ or $(1-f_n)/nf(n-1) = \lambda$. Test runs with these choices showed that all forms gave equally good results. The constant λ is an estimate for $1/\langle n\rangle_{\mathrm{cl}}$ and is recalculated in the program. If $n \cong \langle n\rangle_{\mathrm{cl}}$ and $\lambda \cong 1/\langle n\rangle_{\mathrm{cl}}$ we have $f_n \cong \frac{1}{2}$ so the probability of adding or removing a permutation operator is practically equal around $\langle n\rangle_{\mathrm{cl}}$.

These one-dimensional results are compared with those of Bonner and Fisher,[6] who diagonalized the Hamiltonian for small systems numerically. For the ferromagnetic case I calculated the energy, specific heat, and the susceptibility at zero field for several temperatures. The results for both open and closed chains are in

TABLE I. Ferromagnetic energy, susceptibility, and specific heat in one dimension for several system sizes. The temperature is $J/kT = 1$ and the magnetic field is zero. The last line gives the exact value obtained by Bonner and Fisher for $N = 10$. For other values, cf. Figs. 10 and 11 in Ref. 6.

N	$-E/NJ$	$2kT\chi/g^2\beta^2N$	C_v/kN
3	0.450	0.802	0.135
4	0.412	0.881	0.170
5	0.389	0.913	0.156
6	0.379	0.926	0.140
8	0.376	0.933	0.133
10	0.375	0.934	0.129
BF	0.375	0.934	0.129

TABLE II. Susceptibility for a one-dimensional ferromagnetic ring ($N = 8$) at $J/kT = 1$. Compare with Fig. 22 of Ref. 6.

$g\beta H/2kT$	$2kT\chi/g^2\beta^2N$
0.25	0.711
0.50	0.381
0.75	0.195
1.00	0.104

TABLE III. The antiferromagnetic energy and susceptibility for several temperatures at zero field. The numbers in parentheses are from Ref. 6.

$kT/\|J\|$	$-E/\|NJ\|$	$\|J\|\chi/Ng^2\beta^2$
5.0	0.163 (0.162)	0.040 (0.040)
2.6	0.314 (0.318)	0.061 (0.061)
2.0	0.415 (0.409)	0.068 (0.068)
1.5	0.52 (0.516)	0.07 (0.073)

complete agreement with their results. As an example I show in Table I the N dependence of the various quantities. Excellent agreement was also obtained for the susceptibility in a magnetic field (Table II).

For the antiferromagnetic case, the alternating signs in the expressions for the observable raise additional problems. The results for the energy and susceptibility are given in Table III. For high temperature there is good agreement with exact results. At lower temperatures, however, it becomes more difficult to obtain good statistics.

In three dimensions, I have studied the disordered phase for ferromagnetic spins on a simple cubic lattice. I compare the results for $J/kT = 0.3$ with high-temperature series expansions.[7] This temperature is chosen such that the truncated series (eight or ten terms) is still accurate. For the energy and susceptibility the agreement is excellent. Just as for classical spins the specific heat is somewhat harder to calculate. Also, calculations for higher and lower temperatures have been made. In these cases as well, the agreement with the series expansions is excellent as long as no truncation errors occur.

The results presented here show clearly that the method provides the possibility for studying quantum systems as extensively as their classical counterparts. Generalization to a nonconstant coupling parameter is trivial and the application to fermion lattice models through the use of a Jordan-Wigner transformation is straightforward. In contrast to the approximate methods based on Trotter's formula, the present method yields, in principle, numerically exact results for a chosen system size N. A more extensive account of the method and further results will be published elsewhere.

TABLE IV. The susceptibility, energy, and specific heat for a three-dimensional ferromagnetic system of size N. The temperature is $J/kT = 0.3$. RBW denotes the series-expansion results (Ref. 7).

N	$-E/NkT$	$2kT\chi/g^2\beta^2N$	C_v/kN
27	0.195	1.431	0.187
64	0.173	1.532	0.157
125	0.168	1.547	0.134
216	0.168	1.554	0.137
343	0.167	1.553	
512	0.167	1.556	
729	0.168	1.551	
1000	0.168	1.554	
RBW	0.167	1.550	0.137

The author thanks Professor K. Binder for stimulating discussions.

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