PHYSICAL REVIEW D VOLUME 39, NUMBER 12 15 JUNE 1989

Stochastic truncation method for Hamiltonian lattice field theory

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(Received 12 December 1988)

A new Monte Carlo method is presented for estimating the dominant eigenvalue of a matrix Hamiltonian. It is a version of the power method, in which the basis-state amplitudes are stochastically rounded to integers. Its relation to the ensemble projector Monte Carlo method is discussed and some results are demonstrated for the example of the Z_2 gauge model in $2+1$ dimensions.

I. INTRODUCTION

Monte Carlo techniques have become established as the most reliable means of calculation for very large or complicated lattice systems, such as lattice gauge theories in four dimensions. Within the context of Hamiltonian lattice field theory, several approaches of this sort have been presented.[1-5] They can all be said to derive from the Green's-function Monte Carlo (GFMC) method of Kalos and collaborators.[6,7] Heys and Stump[1] adapted the GFMC method directly to study lattice gauge theory. Blankenbecler and Sugar[2] developed a variant called the projector Monte Carlo (PMC) method, which was later improved by DeGrand and Potvin[4] into the ensemble projector Monte Carlo (EPMC) method. Nightingale and Blöte[5] have presented a similar scheme in connection with lattice spin models. Chin, Negele, and Koonin[3] also developed an alternative to GFMC called the guided random walk (GRW).

All these methods are based upon a von Neumann–Ulam "random walk"[8] in the space of basis states. At each step in the walk, one applies a "projection operator" to the current basis state in some stochastic fashion, making a transition to a new state or states. The projection operator is chosen so as to drive the system into its ground state after many iterations: for example, it might be $e^{-H\Delta\tau}$, or H itself, where H is the Hamiltonian. The number of times each basis state is visited during the walk is proportional to its amplitude in the ground-state wave function (multiplied, in general, by some weighting function); by exploiting this fact one may estimate the ground-state energy and ground-state expectation values. In the PMC method, only a single basis state is allowed in the walk. In the other methods "branching" of the walk is allowed, so that extra basis states may appear or disappear, and the total number fluctuates. To improve statistical accuracy, it is useful to guide the random walk toward the more important regions of state space using a trial wave function ("variational guidance"). The GFMC and GRW algorithms depend on this variational guidance for calculating vacuum expectation values and the results may in fact be biased by the variational ansatz chosen. A guided-random-walk algorithm which avoids the problem of bias was discussed by Barnes, Daniell, and Storey.[9]

Now for lattice models of lesser complexity, such as spin models in two dimensions, a deterministic approach will usually be more accurate than a Monte Carlo approach. One can evaluate the ground-state energy exactly on a sequence of finite lattices (using a Lanczos algorithm, for instance) and extrapolate to the bulk limit using finite-size scaling techniques.[10] For larger systems, however, one must truncate the set of basis states to a manageable size in order to implement this approach.[11,12] The truncation may introduce an unacceptable systematic error,[13] in which case the approach breaks down.

We present here a variant Monte Carlo method called "stochastic truncation," which may be viewed as a combination of the two approaches discussed above. Suppose the ground-state eigenvector $|\phi_0\rangle$ is to be represented on a set of basis states $|i\rangle$; then the basis-state amplitudes $\langle i|\phi_0\rangle$ are approximated by a set of integers $n_i^{(k)}$ at the kth iteration. At the next iteration the Hamiltonian H is used as a projection operator to generate a new set of amplitudes or "occupation numbers" $n_i^{(k+1)}$, in a stochastic fashion. This amounts to a Monte Carlo version of the standard "power method" of numerical analysis. The average value of $n_i^{(k)}$ gives the basis-state amplitude $\langle i|\phi_0\rangle$; but at any given iteration, most of the occupation numbers will be rounded to zero, so that the set of basis states has been effectively truncated to a manageable size in a stochastic way, without necessarily introducing any systematic error.

In Sec. II of this paper we formulate this algorithm in detail, and in Sec. III we discuss its relation to other approaches. It is closely related to the EPMC method[4,5] in fact, with the quantity $N^{(k)}=\sum_i n_i^{(k)}$ playing the role of ensemble size. In Sec. IV some preliminary tests of the method are discussed for the case of the Z_2 gauge model in $2+1$ dimensions, and in Sec. V our conclusions are summarized. A full-scale application of the method to lattice QED in $2+1$ dimensions is described in the following paper.[14]

II. THE STOCHASTIC TRUNCATION METHOD

A. The basic algorithm

Our approach is based on the standard power method for calculating a single dominant eigenvalue and associated eigenvector of a matrix. Let H be an $n \times n$ matrix for which the Jordan canonical form is diagonal, and suppose E_0 is its unique dominant eigenvalue:

$$|E_0| > |E_i| \quad \text{for } 1 \le i \le n-1 \ . \tag{1}$$

Next, let $|\psi^{(0)}\rangle$ be an initial guess at the exact eigenvector $|\phi_0\rangle$ corresponding to E_0, which we shall call the "ground state"; then a sequence of improved approximations to $|\phi_0\rangle$ may be obtained simply via successive multiplications by the matrix H. Let

$$|\psi^{(m+1)}\rangle = H|\psi^{(m)}\rangle \quad (m \ge 0) \tag{2}$$

and expand $|\psi^{(0)}\rangle$ in the basis of eigenvectors $|\phi_j\rangle$:

$$|\psi^{(0)}\rangle = \sum_{j=0}^{n-1} \alpha_j |\phi_j\rangle \ . \tag{3}$$

Then

$$|\psi^{(m)}\rangle = E_0^m \left[\alpha_0 |\phi_0\rangle + \sum_{j=1}^{n-1} \alpha_j \left(\frac{E_j}{E_0} \right)^m |\phi_j\rangle \right] . \tag{4}$$

From Eq. (1), $(E_j/E_0)^m \to 0$ as $m \to \infty$, so that the eigenvector $|\phi_0\rangle$ is "projected out":

$$|\psi^{(m)}\rangle \to \alpha_0 E_0^m |\phi_0\rangle \quad \text{as } m \to \infty \ . \tag{5}$$

Hence one can obtain estimates of the eigenvalue E_0 and eigenvector $|\phi_0\rangle$.

Now suppose that all calculations are being carried out in some arbitrary basis of vectors $\{|i\rangle, i = 0, 1, \ldots, n-1\}$. Then the eigenvector $|\phi_0\rangle$ can be expanded

$$|\phi_0\rangle = \sum_{i=0}^{n-1} c_i^0 |i\rangle \ , \tag{6}$$

where for simplicity we shall assume the amplitudes c_i^0 are positive real numbers. In the stochastic truncation scheme, we use the power method to construct a sequence of (un-normalized) approximations to $|\phi_0\rangle$:

$$|\psi^{(m)}\rangle = \sum_{i=0}^{n-1} n_i^{(m)} |i\rangle \ , \tag{7}$$

where the $n_i^{(m)}$ are now integers rather than real numbers. Denote

$$N^{(m)} = \sum_{i=0}^{n-1} n_i^{(m)} \ . \tag{8}$$

The algorithm then runs as follows.

Begin from some initial trial vector $|\psi^{(0)}\rangle$, specified in terms of integer amplitudes $n_i^{(0)}$, and an initial "score" $S^{(0)}$. Then at each succeeding iteration m, a new trial vector $|\psi^{(m)}\rangle$ and score $S^{(m)}$ are generated by the rules

$$n_k^{(m)} = \sum_i R \left[\frac{H_{ki} n_i^{(m-1)}}{S^{(m-1)}} \right] , \tag{9}$$

$$S^{(m)} = \frac{N^{(m)}}{N^{(m-1)}} S^{(m-1)} \ . \tag{10}$$

Here H_{ki} is an element of the matrix H and $R(x)$ is a stochastic "rounding function" defined by the requirement that, for any real argument x,

$$R(x) = \begin{cases} [x] & \text{with probability } 1-\delta \ , \\ [x]+1 & \text{with probability } \delta \ , \end{cases} \tag{11}$$

where $[x]$ is the greatest integer less than or equal to x, and $\delta = x - [x]$ is the remainder. The function $R(x)$ may be implemented by generating a random number ϵ in the range [0,1] and choosing

$$R(x) = \begin{cases} [x] & \text{if } \epsilon > \delta \ , \\ [x]+1 & \text{otherwise} \ . \end{cases} \tag{12}$$

If we denote the average of any quantity over many trials or iterations by angular brackets we therefore have

$$\langle R(x) \rangle = x \ . \tag{13}$$

B. Equilibrium conditions

Assume that the system settles down after some time to an equilibrium, where $N^{(m)}$ and $S^{(m)}$ fluctuate over successive iterations around some fixed average values. Then the average amplitude or "occupation number" $\langle n_k \rangle$ and the average score are related according to Eq. (9) by

$$\langle n_k \rangle = \sum_i H_{ki} \left\langle \frac{n_i}{S} \right\rangle \simeq \left\langle \frac{1}{S} \right\rangle \sum_i H_{ki} \langle n_i \rangle \tag{14}$$

(the approximation involved here will be discussed below). Comparing this with the eigenvalue equation

$$\sum_k H_{ki} c_i^0 = E_0 c_k^0 \tag{15}$$

we see that Eq. (14) is satisfied if

$$\langle n_k \rangle \propto c_k^0 \ , \tag{16}$$

$$\left\langle \frac{1}{S} \right\rangle = E_0^{-1} \ , \tag{17}$$

so the average occupation number $\langle n_k \rangle$ is proportional to the ground-state amplitude c_k^0, and the average $\langle 1/S \rangle$ gives the ground-state energy.

Thus Eq. (9) implements the power method in a stochastic fashion, and the trial vectors $|\psi^{(m)}\rangle$ at equilibrium provide a discrete, stochastic representation of the ground-state eigenvector $|\phi_0\rangle$. For basis states whose amplitudes c_i^0 are very small, the occupation numbers $n_i^{(m)}$ will usually be zero: thus the less important basis states have been "truncated" out, again in a stochastic fashion. Equation (10) adjusts the score in a way designed[4] to maintain an equilibrium "ensemble size" $N^{(m)}$.

Our discussion of the equilibrium conditions has relied upon the approximation made at Eq. (14), that $n_i^{(m)}$ and

$1/S^{(m)}$ are uncorrelated. This assumption is of course incorrect, in general. But the error should be unimportant, provided one works with a sufficiently large ensemble size $\langle N \rangle$. It would be preferable if the approximation could be avoided entirely, but there seems to be no very straightforward way of doing this. One might try to use a fixed score S, for instance: but insofar as S differs from E_0, the ensemble size $N^{(m)}$ would diverge as $m \to \infty$, or else decrease to zero, and no equilibrium would be attained.

C. Measurements

After equilibrium has been reached, one may obtain estimates of the eigenvalue E_0 at each iteration in two standard ways.[4] One of them, the "growth" estimate, depends on Eq. (17):

$$E_0 \simeq S^{(m)} . \tag{18}$$

The other is called the "trial" estimate, based on Eq. (16):

$$E_0 \simeq \frac{\langle \chi | H | \psi^{(m)} \rangle}{\langle \chi | \psi^{(m)} \rangle} = \sum_{i,j} \frac{H_{ji} n_i^{(m)}}{N^{(m)}} , \tag{19}$$

where $|\chi\rangle$ is a reference vector, called the "broad state," with amplitude $c_i = 1$ for every basis state. The ground-state expectation value of any operator Q which commutes with H can also be estimated, simply replacing H by Q in Eq. (19).

If an operator Q does *not* commute with H, we must use two independent trial states to estimate its expectation value

$$\langle \phi_0 | Q | \phi_0 \rangle \simeq \frac{\langle \psi'^{(m)} | Q | \psi^{(m)} \rangle}{\langle \psi'^{(m)} | \psi^{(m)} \rangle} , \tag{20}$$

where $|\psi'^{(m)}\rangle$ and $|\psi^{(m)}\rangle$ are two independently evolved ensembles. We cannot use the same ensemble $|\psi^{(m)}\rangle$ on either side of Q, because although $\langle n_k \rangle \propto c_k^0$, it does not follow that $\langle n_k^2 \rangle \propto (c_k^0)^2$—in fact that is far from the truth if $\langle n_k \rangle < 1$.

D. Variational guidance

If we already know a good approximation to the ground-state eigenvector, in the form of a vector $|\chi_0\rangle$ say, then this can be used to improve our estimates.[4,15] The eigenvalue E_0, for instance, can be estimated by

$$E_0 \simeq \frac{\langle \chi_0 | H | \psi^{(m)} \rangle}{\langle \chi_0 | \psi^{(m)} \rangle} \tag{21}$$

instead of Eq. (19); this latter equation becomes an exact equality in the case $|\chi_0\rangle = |\phi_0\rangle$.

One way of implementing this[15] is to perform a similarity transformation

$$|\psi'\rangle = U|\psi\rangle , \tag{22}$$

$$H' = UHU^{-1} , \tag{23}$$

where

$$U_{ij} = \langle i | \chi_0 \rangle \delta_{ij} \tag{24}$$

and then to apply the algorithm as before to $|\psi'\rangle$ and H'. It is easy to see that

$$U|\chi\rangle = |\chi_0\rangle , \tag{25}$$

where $|\chi\rangle$ is the "broad state" defined previously and therefore

$$\frac{\langle \chi | H' | \psi' \rangle}{\langle \chi | \psi' \rangle} = \frac{\langle \chi_0 | H | \psi \rangle}{\langle \chi_0 | \psi \rangle} . \tag{26}$$

Thus the estimate (19) in the transformed system is equivalent to (21) in the original system.

III. RELATION TO OTHER APPROACHES

The stochastic truncation technique outlined above is closely related to the EPMC method of DeGrand and Potvin,[4] and that of Nightingale and Blöte.[5] In the EPMC, one works with an "ensemble" $|\psi^{(m)}\rangle$, which merely consists of a set of basis states $|i\rangle$, some of which may be identical with each other. The multiplicity of each basis state in the ensemble is then equivalent to our occupation number $n_i^{(m)}$. The ensemble $|\psi^{(m)}\rangle$ is employed as a stochastic approximation to the ground-state eigenvector in the same way as we have done. The evolution of the ensemble is carried out somewhat differently in the EPMC method, however. At each iteration a state $|i\rangle$ is allowed to "branch" into only one new state $|f\rangle$, although a number of copies of that state may be produced.

DeGrand and Potvin[4] used an operator $\exp(-H\Delta\tau)$ as "projector" onto the ground state, whereas Nightingale and Blöte[5] used H itself as we have done. It is technically easier to use the local operator H as projector, rather than its exponential: it avoids the necessity for expedients such as "checkerboarding" the lattice.[4] One might expect to pay a penalty in increased "equilibration" times from the starting configuration, but in practice we have found that equilibration is quite rapid in any case.

The EPMC method is also restricted in that the multiplicity of each basis state cannot be negative. It is therefore only suitable for cases where the ground-state amplitudes c_i^0 are all real and positive: this is true for a large class of matrix Hamiltonians in physics, but of course it is not universally true. Using stochastic truncation, on the other hand, we can allow the integers $n_i^{(k)}$ to be negative, or even complex, provided some suitable modifications are made in the algorithm. There seems no reason in principle why one cannot handle a general Hamiltonian matrix—although this remains to be demonstrated in practice.

Stochastic truncation appears at first sight to have another advantage, in that each basis state is processed only once at every iteration, whereas in the EPMC there are $n_k^{(m)}$ separate copies to be processed. But this is only a real advantage if the average of $n_k^{(m)}$ over all occupied states (call it $\bar{n}^{(m)}$) is significantly greater than one. The processing of each state will take longer in the stochastic truncation case, and each "output" state has to be looked up in a master file to avoid the duplication accepted in the EPMC case; so there are some disadvantages to be

considered also. The average of $\bar{n}^{(m)}$ over many iterations may be used as a "figure of merit": if $\langle \bar{n} \rangle$ is greater than (say) 2, then the stochastic truncation method is probably more efficient than EPMC, whereas if $\langle \bar{n} \rangle \simeq 1$ the EPMC method will be preferable.

Stochastic truncation may also be compared with deterministic truncation schemes, such as those discussed by Irving and Hamer,[11] or Patkos and Rujan.[12] In deterministic schemes, one works within a specified subset of the full space of basis states, and then calculates the exact ground-state eigenvector and eigenvalue within that truncated subspace. If the matrix H is not too large, or if the ground-state eigenvector is dominated by a relatively few basis states, then this will clearly be the most precise and economical method. In other circumstances, however, the truncation may introduce an unacceptably large systematic error: this is likely to occur, for instance, at weak couplings in a lattice gauge theory.[13]

In the stochastic scheme, the truncation does not *a priori* introduce any systematic error. The ensemble size is limited, but if one averages over sufficiently many iterations, every basis state will be sampled from time to time. On the other hand, there will be a substantial random error to contend with. As usual, we expect the Monte Carlo method to win out for very large matrices, and for lattice Hamiltonians in higher dimensions.

IV. SOME NUMERICAL TESTS

We have carried out some preliminary numerical tests of the algorithm outlined above for the case of the Z_2 gauge model in 2+1 dimensions. This is a relatively simple lattice gauge model, and its Hamiltonian eigenvalues can be calculated exactly for small lattice sizes.[13,16] It is dual[17] to the 2+1 Ising model, and so its phase structure is well understood.

The Hamiltonian for the model is[17]

$$H = \sum_l [1-\sigma_3(l)] - x \sum_p \sigma_1(l_1)\sigma_1(l_2)\sigma_1(l_3)\sigma_1(l_4) , \tag{27}$$

where l labels the links on a two-dimensional (2D) square lattice, p labels the plaquettes, and the $\{l_i, i=1,\ldots,4\}$ are the four links surrounding the plaquette p. The $\sigma_k(l)$ are Pauli matrices acting on a two-state spin vector at each link l of the lattice, and x is the coupling variable. Periodic boundary conditions are assumed. The model undergoes a second-order phase transition at[13] $x_c = 3.04$.

Two sets of calculations were performed, for lattices of 2×2, 3×3, and 4×4 sites. First, exact values of the ground-state energy and the axial string tension were calculated using standard Lanczos methods.[13,16] Second, the stochastic truncation method was used to obtain Monte Carlo estimates of the same quantities. This allows us to check the accuracy of the stochastic truncation scheme.

In order to apply the algorithm, one needs to arrange matters so that the ground-state eigenvalue is largest in magnitude ("dominant"). This we did by using $(E_s I - H)$ as projection operator, where I is the identity matrix and E_s is a sufficiently large energy shift. Within reasonable limits, the accuracy of the algorithm is insensitive to E_s. The calculations were performed in a "symmetrical" basis, i.e., a basis of states symmetric under translations, rotations, and reflections. The total number of basis states is then only a few hundred for the 4×4 lattice.

A. Approach to equilibrium

The approach to equilibrium was rapid: in most cases equilibrium appeared to be achieved within 10 to 20 iterations. Figure 1 shows the worst case: namely, the ground-state energy for a 4×4 lattice at $x=3$ (close to the critical point). Even here, it appears that equilibrium has been attained after about 50 iterations. In general, one may expect the problem of "critical slowing down" to become more serious for larger lattices near a critical point, where the exponential decay of the higher state correction terms in Eq. (4) becomes slow.

For very small ensemble sizes ($N^{(m)} < 50$, say), equilibrium appears difficult to achieve. Some peculiar problems of iteration schemes of the present sort at small ensemble sizes have been discussed by Hetherington.[18]

The score $S^{(m)}$ as given by Eq. (10) has been chosen (following DeGrand and Potvin[4]) so as to "correct" any fluctuations in ensemble size, and produce a trend toward equilibrium. In practice, we have found that this prescription usually produces an overcorrection, so that successive scores tend to be anticorrelated. Other prescriptions are possible, such as

$$S^{(m)} = aS^{(m-1)} + (1-a)S^{(m-1)}\frac{N^{(m)}}{N^{(m-1)}} , \tag{28a}$$

where $a \in [0,1]$ is a parameter to be varied, or

$$S^{(m)} = S^{(m-1)}\left[\frac{N^{(m)}}{N^{(m-1)}}\right]^{1/2} . \tag{28b}$$

We have found that these definitions can sometimes give

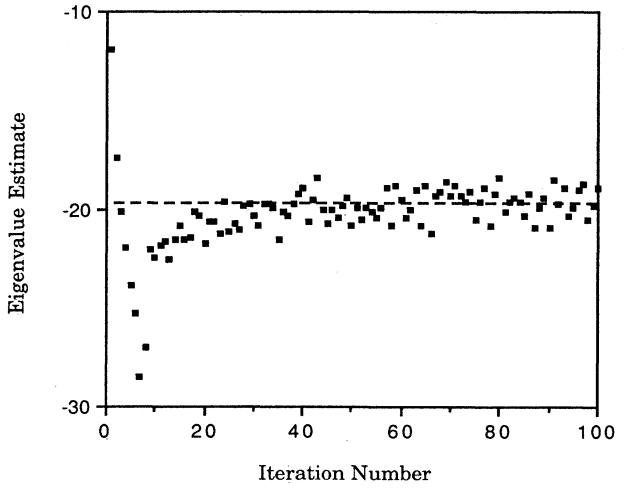

FIG. 1. The eigenvalue estimate against iteration number for the ground state in the vacuum sector on a 4×4 lattice at $x=3$. The dashed line is the eigenvalue averaged over the region from the 100th to the 1000th iteration.

much smoother sequences of eigenvalue estimates and substantially reduce the statistical error of the final result. For the time being, however, we continue with the prescription (10).

B. Error estimates

The simple "growth" estimate, $E_0 = \langle S \rangle$, was used for the energy eigenvalue in each sector. To find the expected statistical error in the result, the "blocking" method[19] was used, in which the data are split into blocks, and the average $\langle S \rangle_\nu$ is computed for each block ν. The standard error obtained by treating these block averages as independent estimates of $\langle S \rangle$ should then be a constant for all block sizes N', provided that N' is greater than the correlation length among the raw data, and the number of blocks is sufficiently large. This constant value is taken as the estimate of the statistical error.

The error in the final result was found to decrease with the number of iterations N_I in the equilibrium region as $1/\sqrt{N_I}$. This is of course the expected statistical behavior.

The behavior as a function of ensemble size is illustrated in Fig. 2. For the cases discussed here, the statistical error decreases as $1/\langle N \rangle$, where $\langle N \rangle$ is the average ensemble size. This is easily understood: because of the stochastic integerization, the basis-state amplitudes $n_i^{(m)}$ differ from the true values c_i^0 by amounts of ~ 1. The relative error in these amplitudes will thus be $O(1/\langle N \rangle)$; and this relative error will feed through to the final estimate. In this situation, it is clearly more advantageous to decrease the error by increasing the ensemble size, rather than increasing the number of iterations.

The argument in the above paragraph only holds, however, if the set of basis states is "well covered," i.e., the figure of merit $\langle \bar{n} \rangle \gg 1$. If the ensemble size is small and $\langle \bar{n} \rangle \simeq 1$, one would expect each state in the ensemble to perform an independent random walk, so that the statistical error should go as $1/\sqrt{\langle N \rangle}$.

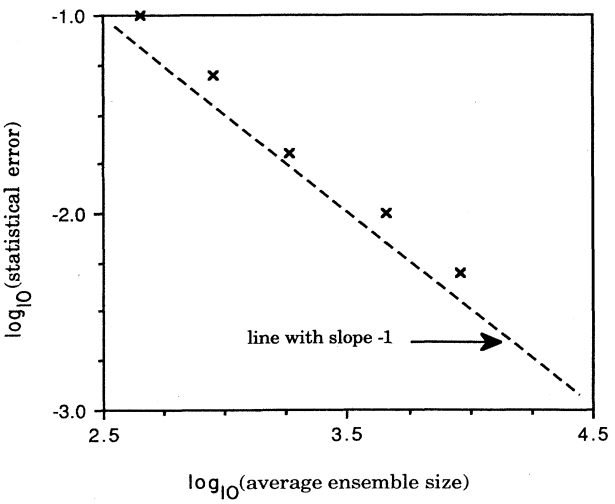

FIG. 2. Logarithm of the statistical error against logarithm of the average ensemble size N_E (base 10), for a 4×4 lattice at $x=2$ in the vacuum sector.

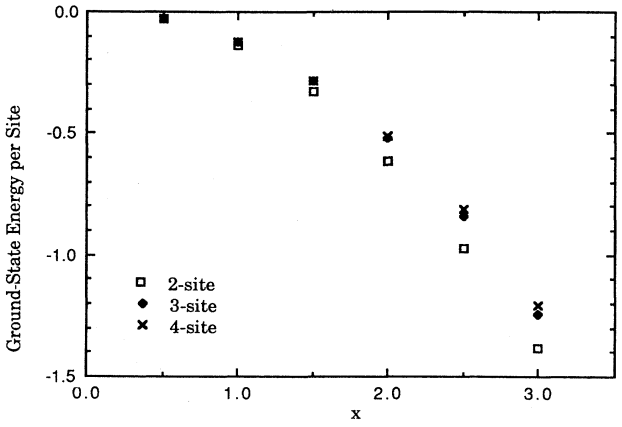

FIG. 3. Stochastic truncation estimates of ω_0/M^2 against coupling x for $M\times M$ lattices with $M=2$, 3, and 4. The errors, both statistical and actual, are too small to be shown.

No sign of systematic error was apparent in the results. The actual error (i.e., the difference between the Monte Carlo estimate and the exact eigenvalue) fluctuated in sign and was consistent with the statistical error in magnitude in most cases. Only for the 4×4 lattice near the critical point did the actual errors become significantly larger than the estimated statistical errors: this is presumably a residue of the "critical slowing-down" effect. For very small ensemble sizes, one would certainly expect to see some systematic effects; but as mentioned above, we were unable to obtain equilibrium in such cases anyway.

C. Results

Estimates for the lowest-energy eigenvalues in the vacuum and axial string vectors ω_0 and ω_1, respectively, were obtained for the 2×2, 3×3, and 4×4 lattices at $x=0.5$, $1.0, \ldots, 3.0$ using runs of 1000 iterations with initial en-

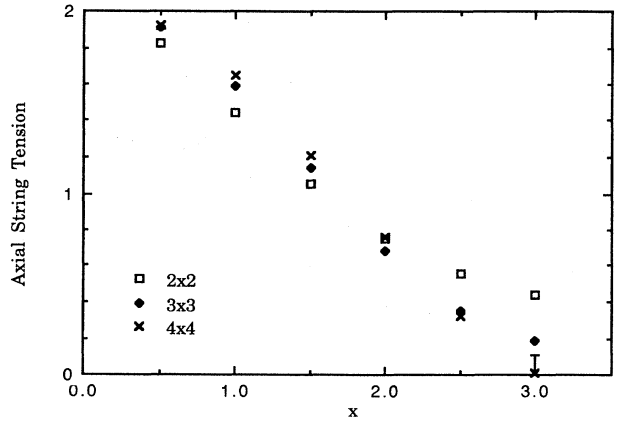

FIG. 4. Stochastic truncation estimates of the axial string tension against coupling x for $M\times M$ lattices. The errors are too small to be shown except for the 4×4 lattice at $x=3$ where the actual error is indicated by a bar.

semble size $N^{(0)}=1000$. The first 100 iterations were discarded in each case to allow for equilibration. The vacuum energy per site is graphed in Fig. 3; and in Fig. 4 is plotted the axial string tension

$$T_a=(\omega_1-\omega_0)/M \tag{29}$$

for each $M\times M$ lattice.

The statistical error in all of the points plotted is below the resolution of the graphs (of order 10^{-5}, 10^{-4}, and 10^{-2} for the 2×2, 3×3, and 4×4 lattices, respectively). The actual error is equally small, except in the case of T_a for the 4×4 lattice at $x=3$, where it is represented as an error bar.

The results clearly show the crossover of the finite lattice string tensions at around $x=2$, and the scaling toward zero near the critical point at $x\simeq3$. The accuracy would be sufficient to permit a finite-size scaling analysis[10] of the critical parameters; but our aim here is simply to establish that the stochastic truncation method is capable of giving accurate eigenvalue estimates.

V. CONCLUSIONS

The "stochastic truncation" scheme which we have presented in this paper is basically a simple Monte Carlo version of the power method for calculating a single dominant eigenvalue and associated eigenvector of a matrix. As such, it may have applications beyond the arena of lattice Hamiltonian field theory which we have envisaged here. If the matrix in question is large or infinite, and cannot be truncated deterministically without introducing unacceptable systematic errors, then a Monte Carlo scheme of this sort may be useful.

The method is closely related to the EPMC method of DeGrand and Potvin,[4] and a similar method of Nightingale and Blöte.[5] We have defined a "figure of merit": namely, the average occupation number $\langle\bar{n}\rangle$, which should indicate the preferred method in a given situation. If $\langle\bar{n}\rangle$ is greater than (say) 2, stochastic truncation should be more efficient; but if $\langle\bar{n}\rangle\simeq1$, then the EPMC method will be preferable, because it will be quicker to process an individual basis state. For lattice gauge theory in a strong-coupling basis, for example, the ground-state eigenvector will be dominated by a few basis states in the strong-coupling region, and stochastic truncation will be most accurate. At weak couplings, more and more basis states will contribute, and $\langle\bar{n}\rangle$ will decrease toward unity. This is the region of more physical interest, of course; and here EPMC probably has the advantage. Nevertheless, we feel that the approach discussed here provides a useful new perspective and insight into Hamiltonian Monte Carlo methods. Furthermore, our approach is not necessarily limited to cases where the ground-state amplitudes are positive definite. So it may be useful, for instance, in lattice gauge theories involving dynamical fermions.

We have performed some preliminary numerical tests of the method using the Z_2 gauge model in $2+1$ dimensions. It was shown that the method was capable of giving accurate estimates of eigenvalues; and it was also demonstrated that in general one should work with an ensemble size as large as can be comfortably accommodated.

ACKNOWLEDGMENTS

The authors are grateful to Professor M. N. Barber, Professor J. Oitmaa, Professor W. Selke, and Dr. F. C. Alcaraz for helpful discussions regarding Monte Carlo methods. The work of C.R.A. was supported by the Commonwealth Postgraduate Research Program, and that of C.M.Y. by the Australian National University Postgraduate Program.

[1]D. W. Heys and D. R. Stump, Phys. Rev. D **28**, 2067 (1983).
[2]D. Blankenbecler and R. L. Sugar, Phys. Rev. D **27**, 1304 (1983).
[3]S. A. Chin, J. W. Negele, and S. E. Koonin, Ann. Phys. (N.Y.) **157**, 140 (1984).
[4]T. A. DeGrand and J. Potvin, Phys. Rev. D **31**, 871 (1985).
[5]M. P. Nightingale and H. W. J. Blöte, Phys. Rev. B **33**, 659 (1986).
[6]M. H. Kalos, Phys. Rev. **128**, 1791 (1962).
[7]D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979).
[8]J. Kuti, in *Monte Carlo Methods in Quantum Mechanical Problems*, edited by M. H. Kalos (NATO Advanced Studies Institute Series B: Physics, Vol. 125) (Plenum, New York, 1984).
[9]T. Barnes, G. J. Daniell, and D. Storey, Nucl. Phys. **B265**, 253 (1986).
[10]M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8.
[11]A. C. Irving and C. J. Hamer, J. Phys. A **16**, 829 (1983).
[12]A. Patkos and P. Rujan, J. Phys. A **18**, 1765 (1985).
[13]C. J. Hamer and A. C. Irving, Nucl. Phys. **B225**, 289 (1983).
[14]C. M. Yung, C. R. Allton, and C. J. Hamer, following paper, Phys. Rev. D **39**, 3778 (1989).
[15]F. Alcaraz, M. Barber, A. Kennedy, J. Kuti, and B. Pendleton (unpublished).
[16]A. C. Irving and A. Thomas, Nucl. Phys. **B200**, 424 (1982).
[17]E. Fradkin and L. Susskind, Phys. Rev. D **17**, 2637 (1978).
[18]J. H. Hetherington, Phys. Rev. A **30**, 2713 (1984).
[19]K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 5b.