Application of the Green's-function Monte Carlo method to the Hamiltonian XY model

David W. Heys and Daniel R. Stump
Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824
(Received 12 September 1983)

An application of the Green's-function Monte Carlo method to the Hamiltonian XY model is described. Importance sampling is implemented with two trial wave functions—one corresponding to a disordered state and one which incorporates the correlations derived from the spin-wave approximation of the model. Optimal trial functions are obtained from the variational principle. The Monte Carlo results are interpreted with regard to the Kosterlitz-Thouless phase transition.

I. INTRODUCTION

The Green's-function Monte Carlo (GFMC) method is a numerical technique for studying properties of the ground state of a quantum system with many degrees of freedom. It was originally developed for application to quantum many-body problems.[1,2] We described an application of this method to the Kogut-Susskind Hamiltonian formulation of the compact U(1) lattice gauge theory in 2 and 3 spatial dimensions in a previous paper.[3] In this paper we shall describe similar calculations for the Hamiltonian formulation of the XY model.

The XY model, also called the classical planar spin model, describes classical two-dimensional spins located on a two-dimensional cubic lattice with a nearest-neighbor interaction energy proportional to $\vec{S}\cdot\vec{S}'$. The aim of classical statistical mechanics is to compute the partition function

$$Z=\sum_{\text{states}}\exp\left[-\beta\sum_{\vec{x},k}\vec{S}(\vec{x})\cdot\vec{S}(\vec{x}+\hat{k})\right]. \tag{1.1}$$

An important feature of this model is the Kosterlitz-Thouless phase transition,[4] which separates a phase in which the sum over states is dominated by spin-wave fluctuations of an ordered state, so that the spin directions are highly correlated, and a disordered phase in which the correlation between spin directions is small. This phase transition is driven by an interesting mechanism: *vortices* in the spin field, which are coupled in pairs at low temperatures, unbind to produce a disordered state at a critical value of β. Topological configurations that produce long-range disorder of the fields may also be relevant to the transition from an ordered to a disordered vacuum state in lattice gauge theories.[5] The XY model is important to the lattice gauge theorist as the simplest example of this mechanism. In this work we are interested in this model as a testing ground for the GFMC method.

The Metropolis Monte Carlo algorithm has been applied to the computation of the partition function (1.1).[6]

The Hamiltonian formulation of the XY model consists of a *quantum* Hamiltonian that describes a one-dimensional chain of interacting spins.[7] The second dimension is time. The connection between this formulation and that of Eq. (1.1) is that the partition function is a lattice approximation of the Feynman path integral of the quantum system. For the sake of completeness we derive this connection in the Appendix of this paper.

It is the quantum Hamiltonian to which we apply the GFMC method.

An important, and even essential, aspect of the GFMC method is the use of importance sampling. An importance function, which should resemble the ground-state eigenfunction, is used to bias the Monte Carlo sampling in favor of regions of configuration space where the wave function is greatest. The variational principle provides a way to construct useful importance functions. In the XY-model calculations, as in the U(1)-gauge-theory calculations presented in our previous paper, we use two importance functions. The first describes a disordered state; importance sampling with this function is good at weak coupling, but becomes increasingly worse as the coupling increases. The second is derived from the spin-wave approximation of the ground state, and yields good importance sampling at both strong and weak couplings. The variational calculation that optimizes the trial function is done analytically for the disordered state, but numerically for the spin-wave state, by the Metropolis Monte Carlo method. The variational results are interesting in their own right as they give some indication of the nature of the ground state as a function of the coupling constant. Then the GFMC calculations extend the accuracy of the variational calculations.

The outline of this paper is as follows. We define the Hamiltonian XY model and explain our application of the GFMC method in Sec. II. We describe the variational calculations that yield trial functions for the GFMC importance sampling in Sec. III. We discuss the GFMC results in Sec. IV, and make some summarizing remarks in Sec. V.

II. DEFINITION OF THE MODEL

The Hamiltonian of the XY model is[7]

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial\theta_i^{\,2}}-\lambda\sum_{i=1}^{N}[1+\cos(\theta_i-\theta_{i+1})], \tag{2.1}$$

with the periodic boundary condition $\theta_{N+1}=\theta_1$. Here θ_i is an angle variable that defines the direction of the ith

spin; thus its range is $(-\pi,\pi)$, and wave functions are periodic in θ_i with period 2π. H is defined such that the ground-state energy is negative; we let $-Q^2$ denote this energy. In the calculations to be discussed, we formulate the eigenvalue problem in the space of variables conjugate to θ_i; specifically, we write the ground-state eigenfunction as

$$\psi(\vec{\theta})=\sum_{\vec{n}}\phi(\vec{n})\exp\left[i\sum_{i=1}^{N}n_i(\theta_i-\theta_{i+1})\right], \tag{2.2}$$

where periodicity in θ_i requires that the variable n_i be an integer. Then the $\vec{n}$-space eigenfunction $\phi(\vec{n})$ obeys the equation

$$-Q^2\phi(\vec{n})=S(\vec{n})\phi(\vec{n})-\lambda\sum_{\vec{n}'}K(\vec{n},\vec{n}')\phi(\vec{n}'), \tag{2.3}$$

where

$$S(\vec{n})=\sum_{i=1}^{N}(n_i-n_{i+1})^2 \tag{2.4}$$

and

$$K(\vec{n},\vec{n}')=\sum_{i=1}^{N}[\delta(\vec{n},\vec{n}')+\tfrac{1}{2}\delta(\vec{n},\vec{n}'+\hat{e}_i)+\tfrac{1}{2}\delta(\vec{n},\vec{n}'-\hat{e}_i)], \tag{2.5}$$

where $\hat{e}_i$ is the N-component vector with jth component δ_{ij}.

To put the eigenvalue equation into a useful form, we define

$$\chi(\vec{n})=[Q^2+S(\vec{n})]\phi(\vec{n}); \tag{2.6}$$

this function satisfies the equation

$$\chi(\vec{n})=\lambda\sum_{\vec{n}'}K(\vec{n},\vec{n}')[Q^2+S(\vec{n}')]^{-1}\chi(\vec{n}'). \tag{2.7}$$

The GFMC method applies to an equation of this form. The method consists of simulation of a diffusion process with branching. The branching probability is proportional to $[Q^2+S(\vec{n}')]^{-1}$ and the diffusion is governed by $K(\vec{n},\vec{n}')$. We refer to $K(\vec{n},\vec{n}')$ as the Green's function, although in this problem it is *not* introduced as the inverse of an operator.

The GFMC method is most powerful when combined with an importance-sampling technique.[8] In very large systems this technique is necessary for obtaining accurate results. We implement importance sampling by introducing a trial wave function $\phi_T(\vec{n})$, which should be an approximation of the actual eigenfunction. Then we define the function $F(\vec{n})$ by

$$F(\vec{n})=\phi_T(\vec{n})\chi(\vec{n}). \tag{2.8}$$

This obeys the equation

$$F(\vec{n})=\lambda\sum_{\vec{n}'}\frac{\phi_T(\vec{n})}{\phi_T(\vec{n}')}K(\vec{n},\vec{n}')[Q^2+S(\vec{n}')]^{-1}F(\vec{n}'), \tag{2.9}$$

which is the equation to which we apply the GFMC diffusion process. Now the diffusion is governed by the biased Green's function $\phi_T(\vec{n})K(\vec{n},\vec{n}')/\phi_T(\vec{n}')$.

The GFMC method is based on iteration of Eq. (2.9). To iterate the equation we must take Q^2 to be the given quantity, and regard λ as the eigenvalue to be determined. Then iteration yields a sequence of functions $F^{(0)}(\vec{n})$, $F^{(1)}(\vec{n}),\ldots,F^{(r)}(\vec{n})$ defined by

$$F^{(r+1)}(\vec{n})=\lambda^{(r)}\sum_{\vec{n}'}\frac{\phi_T(\vec{n})}{\phi_T(\vec{n}')}K(\vec{n},\vec{n}')[Q^2+S(\vec{n}')]^{-1}\times F^{(r)}(\vec{n}'), \tag{2.10}$$

where the constant $\lambda^{(r)}$ may vary from one iteration to the next. It can be shown that $F^{(r)}(\vec{n})$ approaches the ground-state eigenfunction with energy $-Q^2$ as $r\to\infty$, independent of the initial function $F^{(0)}(\vec{n})$; and that the normalization obeys the relation

$$\lim_{r\to\infty}\frac{F^{(r+1)}(\vec{n})}{F^{(r)}(\vec{n})}=\frac{\lambda^{(r)}}{\lambda}, \tag{2.11}$$

where λ is the coupling constant for which the ground-state energy is $-Q^2$. Constant normalization of the function $F^{(r)}(\vec{n})$ (after convergence to the limit) requires $\lambda^{(r)}=\lambda$.

The GFMC algorithm for solving Eq. (2.9) is a simulation of a diffusion process with branching. At the rth step of the process we have an ensemble $\mathscr{E}_r$ of field configurations

$$\mathscr{E}_r=\{\vec{n}'_\sigma;\ \sigma=1,2,3,\ldots,N_r\};$$

let $P_r(\vec{n})$ denote the probability distribution of $\mathscr{E}_r$. The next ensemble $\mathscr{E}_{r+1}$ is obtained from $\mathscr{E}_r$ in two steps:

(i) Each $\vec{n}'_\sigma$ branches into k_σ new points, where k_σ is an integer picked by a random process such that the expected value of k_σ is

$$\lambda_0^{(r)}[Q^2+S(\vec{n}'_\sigma)]^{-1}\sum_{\vec{n}}\frac{\phi_T(\vec{n})K(\vec{n},\vec{n}'_\sigma)}{\phi_T(\vec{n}'_\sigma)}. \tag{2.12}$$

The possibility $k_\sigma=0$ is allowed. Here $\lambda_0^{(r)}$, which may be thought of as a guess of the value of λ, can vary from one iteration to the next.

(ii) Then each of the k_σ points is moved from $\vec{n}'_\sigma$ to a new configuration $\vec{n}$ chosen from the probability distribution

$$\frac{\phi_T(\vec{n})K(\vec{n},\vec{n}'_\sigma)/\phi_T(\vec{n}'_\sigma)}{\sum_{\vec{n}}\phi_T(\vec{n})K(\vec{n},\vec{n}'_\sigma)/\phi_T(\vec{n}'_\sigma)}. \tag{2.13}$$

Note that the form of $K(\vec{n},\vec{n}')$ implies that $\vec{n}$ differs from $\vec{n}'_\sigma$ by at most one unit.

The ensemble $\mathscr{E}_{r+1}$ is the result of processing all of the elements of $\mathscr{E}_r$ in this way. The probability distribution of $\mathscr{E}_{r+1}$ is

$$P_{r+1}(\vec{n})=\lambda_0^{(r)}\frac{N_r}{N_{r+1}}\sum_{\vec{n}'}\frac{\phi_T(\vec{n})}{\phi_T(\vec{n}')}K(\vec{n},\vec{n}')[Q^2+S(\vec{n}')]^{-1}$$

$$\times P_r(\vec{n}') . \tag{2.14}$$

That is, the evolution of $P_r(\vec{n})$ is the same as Eq. (2.10) with

$$\lambda_0^{(r)}\frac{N_r}{N_{r+1}}=\lambda^{(r)} . \tag{2.15}$$

Therefore, $P_r(\vec{n})$ approaches the eigenfunction $F(\vec{n})$ as $r\to\infty$. Also, since $P_r(\vec{n})$ and $P_{r+1}(\vec{n})$ have the same normalization, specifically $\sum_{\vec{n}}P_r(\vec{n})=1$ for all r, after a sufficient number of steps in the diffusion we shall have

$$\lambda_0^{(r)}\frac{N_r}{N_{r+1}}=\lambda . \tag{2.16}$$

This provides an estimate of the eigenvalue λ after each iteration. Note that $\lambda_0^{(r)}$ controls the size of the ensemble; in practice we readjust the value of $\lambda_0^{(r)}$ every few iterations so as to keep the ensemble size approximately constant. Thus the simulation yields an estimate of λ and a sequence of ensembles of $\vec{n}$-space configurations with probability distribution $F(\vec{n})$.

Use of the trial function ϕ_T is called importance sampling. The diffusion in the space of $\vec{n}$ configurations is controlled by the *biased* Green's function $\phi_T(\vec{n})K(\vec{n},\vec{n}')/\phi_T(\vec{n}')$. The factor $\phi_T(\vec{n})/\phi_T(\vec{n}')$ biases the diffusion in favor of moves $\vec{n}'\to\vec{n}$ in directions that increase $\phi_T(\vec{n})$. If ϕ_T is an approximation of the ground-state eigenfunction, then this bias accelerates the convergence to the ground state, and reduces fluctuations of the estimates of the eigenvalue λ.

The importance-sampling technique also provides a way to estimate expectation values of operators in the ground state, provided ϕ_T is a good approximation of the eigenfunction ϕ. If ϕ_T differs from ϕ by an amount of order ϵ, then to order ϵ^2 we have

$$\frac{\langle\phi\,|\,A\,|\,\phi\rangle}{\langle\phi\,|\,\phi\rangle}=2\frac{\langle\phi\,|\,A\,|\,\phi_T\rangle}{\langle\phi\,|\,\phi_T\rangle}-\frac{\langle\phi_T\,|\,A\,|\,\phi_T\rangle}{\langle\phi_T\,|\,\phi_T\rangle} . \tag{2.17}$$

The left-hand side is the desired expectation value of an operator A. The second term on the right-hand side is simply the expectation value in the trial state. The first term on the right-hand side, which is called the mixed expectation value, can be estimated as

$$\frac{\langle\phi\,|\,A\,|\,\phi_T\rangle}{\langle\phi\,|\,\phi_T\rangle}=\frac{\langle A(\vec{n})[Q^2+S(\vec{n})]^{-1}\rangle_{\text{ens}}}{\langle[Q^2+S(\vec{n})]^{-1}\rangle_{\text{ens}}} , \tag{2.18}$$

where $\langle\ \rangle_{\text{ens}}$ denotes the average of the enclosed quantity over the ensembles generated by the GFMC diffusion. Since Eq. (2.17) is only valid to order ϵ^2, this estimate is not trustworthy if $\langle A\rangle_T$ and $\langle A\rangle$ are very different.

The trial function ϕ_T is ordinarily obtained from a variational calculation. Thus the GFMC method can be thought of as an extension of the variational principle, that improves the accuracy of numerical estimates. The GFMC determination of the eigenvalue λ is in principle exact, even if ϕ_T is not a good approximation of ϕ; but that is only for a large enough ensemble, and in practice the calculations are not feasible if ϕ_T differs from ϕ too much. Expectation values computed from the mixed expectation value are valid to order $(\phi_T-\phi)^2$, so Eq. (2.17) gives the order-$(\phi_T-\phi)$ correction to the ordinary variational estimate. In addition, the GFMC approach can indicate whether a variational wave function is an accurate representation of the ground state by testing whether it works well as an importance-sampling function. It can be proven, for example, that fluctuations in the measurement of λ by Eq. (2.16) approach zero as the trial function approaches the exact eigenfunction.

In the next section we describe the two trial functions to be used for importance sampling in the GFMC calculations, and variational calculations which optimize the choice of these functions.

III. VARIATIONAL CALCULATIONS

We shall consider two trial wave functions to approximate the ground state of the XY model. The first is defined as a function in the space of $\vec{\theta}$ configurations as

$$\psi_1(\vec{\theta})=\prod_{i=1}^{N}u(\theta_i-\theta_{i+1}) ; \tag{3.1}$$

the energy $\langle\psi_1\,|\,H\,|\,\psi_1\rangle$ is to be minimized with respect to the choice of the function $u(\omega)$. It can be shown that the minimum energy is obtained if $u(\omega)$ is the ground-state eigenfunction of the Hamiltonian of a quantum pendulum,

$$h=-2\frac{\partial^2}{\partial\omega^2}+\lambda(1-\cos\omega) , \tag{3.2}$$

where $-\pi\le\omega\le\pi$. The resulting variational bound on the energy per spin is

$$-\frac{Q^2}{N}\le-2\lambda+e_0 , \tag{3.3}$$

where e_0 is the smallest eigenvalue of h. We shall present our results in terms of another energy E_0, rather than $-Q^2$, defined by

$$E_0=2\lambda N-Q^2 ; \tag{3.4}$$

note that E_0 is the ground-state energy of

$$-\sum_{i=1}^{N}\frac{\partial^2}{\partial\theta_i^{\,2}}+\lambda\sum_{i=1}^{N}[1-\cos(\theta_i-\theta_{i+1})] . \tag{3.5}$$

The variational estimate of E_0 based on ψ_1 is

$$\frac{E_0}{N}=e_0 . \tag{3.6}$$

The small- and large-λ limits of e_0 are

$$e_0 \simeq \lambda - \frac{\lambda^2}{4} + \frac{7\lambda^4}{256} + O(\lambda^6) \text{ as } \lambda \to 0 ,$$
$$e_0 \simeq \lambda^{1/2} - \tfrac{1}{8} + O(\lambda^{-1/2}) \text{ as } \lambda \to \infty . \quad (3.7)$$

For comparison these limits for E_0/N are easily shown to be

$$E_0/N \simeq \lambda - \frac{\lambda^2}{4} + \frac{5\lambda^4}{768} + O(\lambda^6) \text{ as } \lambda \to 0 ,$$
$$E_0/N \simeq \lambda^{1/2} d(N) - \tfrac{1}{8} d^2(N) + O(\lambda^{-1/2}) \text{ as } \lambda \to \infty , \quad (3.8)$$

where

$$d(N) = \frac{\sqrt{2}}{N} \left[1 - \cos\frac{\pi}{N} \right]^{-1} \sin\frac{\pi}{N} \quad (3.9)$$

for a chain of N spins with periodic boundary conditions; the value of $d(N)$ is approximately 0.90 for N greater than 10. Thus e_0 and E_0/N have the same small-λ limit, but e_0 is greater than E_0/N for large λ.

The trial function ψ_1 describes a disordered state of the spins. Specifically, the correlation between spins separated by a distance k is, for this wave function,

$$\langle \psi_1 \mid \cos(\theta_{i+k} - \theta_i) \mid \psi_1 \rangle = \left[\int_{-\pi}^{\pi} d\omega \, u^2(\omega) \cos\omega \right]^k \quad (3.10)$$

which decreases exponentially with k. We expect ψ_1 to be a good approximation of the eigenfunction for small λ, where the ground state is disordered in this way. But it can already be seen by comparing the limiting forms (3.7) and (3.8) that ψ_1 becomes less accurate as λ increases.

The second trial wave function is designed to be accurate in the large-λ limit; it turns out to be accurate at small λ as well. It is defined in the conjugate space of $\vec{n}$ configurations as

$$\phi_2(\vec{n}) = \exp\left[-\tfrac{1}{2}\alpha \sum_{j,j'} n_j \Delta_{jj'} n_{j'} \right] , \quad (3.11)$$

where α is the variational parameter, and

$$\Delta_{jj'} = \left[\frac{2}{\lambda} \right]^{1/2} \frac{2}{N} \sum_{q=1}^{N} \exp\left[\frac{2\pi i}{N} q(j-j') \right] \sin\frac{\pi q}{N} . \quad (3.12)$$

The motivation for this form is that with $\alpha = 1$ it duplicates the ground state of the spin-wave approximation of the model, which is known to be the eigenstate in the large-λ limit. The spin-wave approximation consists of replacing $1 - \cos(\Delta\theta)$ by $\frac{1}{2}(\Delta\theta)^2$ in the Hamiltonian, and extending the range of θ_i from $(-\pi, \pi)$ to $(-\infty, \infty)$. The resulting model is solvable since its Hamiltonian is quadratic; its ground state is ϕ_2 with $\alpha = 1$, but where the variables n_i take a continuum of values. We emphasize that the trial function ϕ_2 is not a naive harmonic approximation, because the n_i are restricted to integer values; this is necessary to preserve the periodicity of the wave function in $\vec{\theta}$ space.

We evaluate the expectation value $\langle \phi_2 \mid H \mid \phi_2 \rangle$ numerically, using the Metropolis Monte Carlo algorithm to generate a set of configurations $\{\vec{n}_1, \vec{n}_2, \vec{n}_3, \ldots, \vec{n}_k\}$ with probability distribution ϕ_2^2, and estimating the expectation value by the average of the operator over these configurations. This is done for many values of the variational parameter α. The resulting data on the energy as a function of α is then fit to a polynomial of sufficiently large degree to give a good fit. And finally we minimize the polynomial with respect to α.

Figure 1 is a graph of the value of α that minimizes the energy, as a function of the coupling constant λ. The error bars are calculated in a straightforward way from the standard errors in the polynomial coefficients found by the least-squares fit mentioned in the previous paragraph. The calculation is for a chain of 50 spins, with periodic boundary condition.

As anticipated, α approaches 1, the spin-wave value, at large λ. As λ decreases, α increases and so ϕ_2 becomes more sharply peaked at $\vec{n} = 0$, which implies a more disordered state in $\vec{\theta}$ space. There is a fairly dramatic variation of α for λ near 1. A similar variational calculation for the U(1) lattice gauge theory in three dimensions, discussed in Ref. 3, has a discontinuity in the value of α as a function of λ, indicating a phase transition in that model.

Figure 2 shows the variational bounds on E_0/N as a function of λ, for both trial functions ψ_1 and ϕ_2, along with the large- and small-λ limits given in Eq. (3.8). Clearly the trial function ϕ_2 derived from the spin-wave approximation is more accurate than the disordered function ψ_1 for $\lambda \gtrsim 1$; its energy approaches the correct large-λ limit, as it must by construction. The spin-wave function is also a good approximation at small λ, where its energy is only slightly larger than that of the disordered state. Both functions approach the correct small-λ limit.

The two trial functions ψ_1 and ϕ_2 are analogs of the trial functions that we used in U(1)-lattice-gauge-theory calculations.[3] The analog of ψ_1 is a product of single-plaquette functions, and the analog of ϕ_2 derives from the free-field harmonic approximation of the U(1) gauge theory.

In the next section we describe the results of GFMC calculations that use these two trial functions for importance sampling.

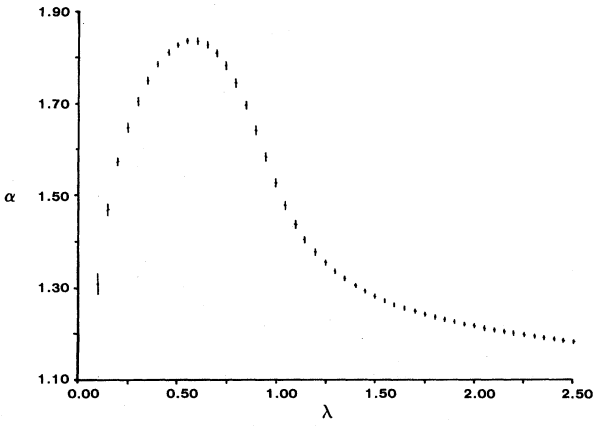

FIG. 1. Variational parameter α vs coupling constant λ.

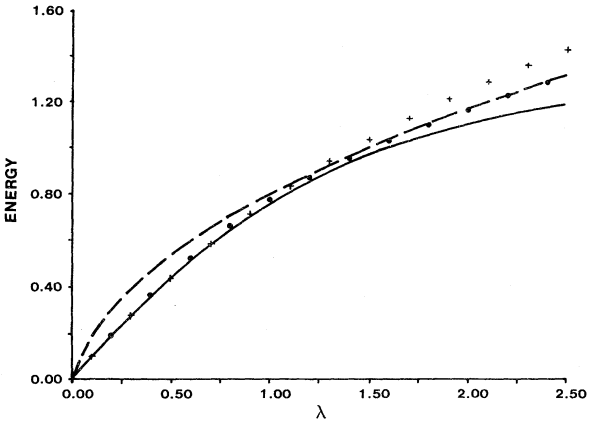

FIG. 2. Variational estimates of the ground-state energy per spin vs coupling constant λ. The solid and dashed curves are perturbation expansions for small and large λ, respectively. The crosses (+) and circles (○) are variational estimates with trial wave functions ψ_1 and ϕ_2, respectively. Error bars are much smaller than the size of the points.

IV. MONTE CARLO RESULTS

Figure 3 is a graph of E_0/N, the ground-state energy per spin of the Hamiltonian (3.5), as a function of the coupling parameter λ, from Green's-function Monte Carlo calculations with importance functions ψ_1 and ϕ_2. The curves are the variational bounds obtained in Sec. III, and the points are the GFMC results. The GFMC calculations used an ensemble of approximately 100 configurations; this ensemble size changes with each iteration. The results in Fig. 3 are averages over 800 iterations. Each GFMC point required approximately 90 sec of computation time on a CDC Cyber 750 computer at Michigan State University.

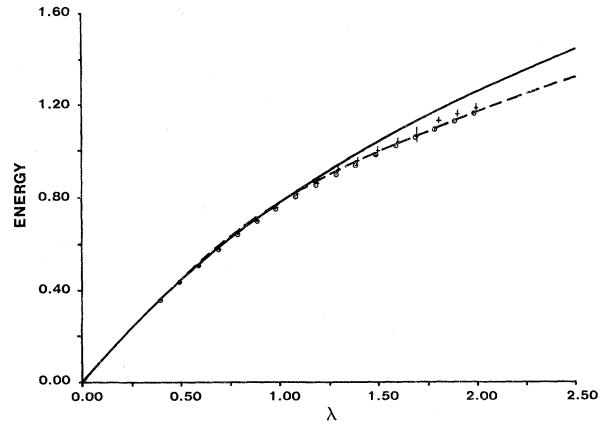

FIG. 3. Monte Carlo estimates of the ground-state energy per spin vs coupling constant λ. The solid and dashed curves are variational estimates with trial wave functions ψ_1 and ϕ_2, respectively. The crosses (+) and circles (○) are Monte Carlo results with importance functions ψ_1 and ϕ_2, respectively.

The results shown are for a chain of 50 spins with periodic boundary condition. As λ varies from 0 to ∞ the energy interpolates between the small-λ asymptotic behavior described well by the disordered wave function ψ_1 and the harmonic spin-wave behavior described by ϕ_2. The crossover from one form to the other occurs for $\lambda \sim 1$.

The two Monte Carlo estimates are almost equal, and are consistent with the variational bounds. However, there is a tendency for the GFMC estimate obtained with the disordered function ψ_1 to lie higher in energy than that obtained with ϕ_2 in the region $\lambda \gtrsim 1$. Furthermore, the former estimates have greater uncertainty, as indicated by the error bars, than the latter, for which the error bars are much smaller than the size of the point plotted. These error bars come only from the fluctuation associated with stochastic sampling. These two tendencies are not unexpected; they reflect the fact that ψ_1 is not a good approximation of the ground state for $\lambda \gtrsim 1$, where the spins are more correlated than in ψ_1.

It is interesting to compare these results to the analogous calculations for the U(1) lattice gauge theory in 3 and 2 spatial dimensions. In the three-dimensional model, the Monte Carlo results obtained using the disordered wave function for importance sampling are definitely different than those obtained with the harmonic wave function, in the region of large λ; in fact the former results are inconsistent with the variational bound provided by the harmonic wave function. We interpret this as evidence of the phase transition of the three-dimensional U(1) gauge theory: the disordered state is metastable with respect to the GFMC diffusion process. In contrast, the Monte Carlo results are the same for the two importance functions in the two-dimensional model; this is consistent with the fact that there is no phase transition in the two-dimensional model.

Our XY model results show evidence of the Kosterlitz-Thouless phase transition, in that the disordered function does not provide effective importance sampling for $\lambda \gtrsim 1$. The disordered state is not metastable, as it is in the three-dimensional U(1) gauge theory, but the energy estimate obtained with the disordered importance function is slightly larger, and has larger fluctuations, than that obtained with the spin-wave function in this region. The difference between the XY model and the U(1) gauge model is explained by the fact that the Kosterlitz-Thouless phase transition is an infinite-order transition, while the gauge-model transition is a second-order transition.

The Kosterlitz-Thouless renormalization-group calculation predicts that the phase transition of the XY model occurs at $\lambda = 1.02$; this point is discussed briefly in the Appendix. That value is perfectly consistent with the interpretation of our results given above. For $\lambda \leq 1.02$ the ground state is disordered so ψ_1 acts as an effective importance function; but for $\lambda > 1.02$ the spin directions are more correlated than in ψ_1 so this function gives weaker importance sampling.

Figures 4(a) and 4(b) show Monte Carlo estimates of the correlation function of neighboring spins

$$\mathscr{C} = \langle 1 - \cos(\theta_i - \theta_{i+1}) \rangle \ . \tag{4.1}$$

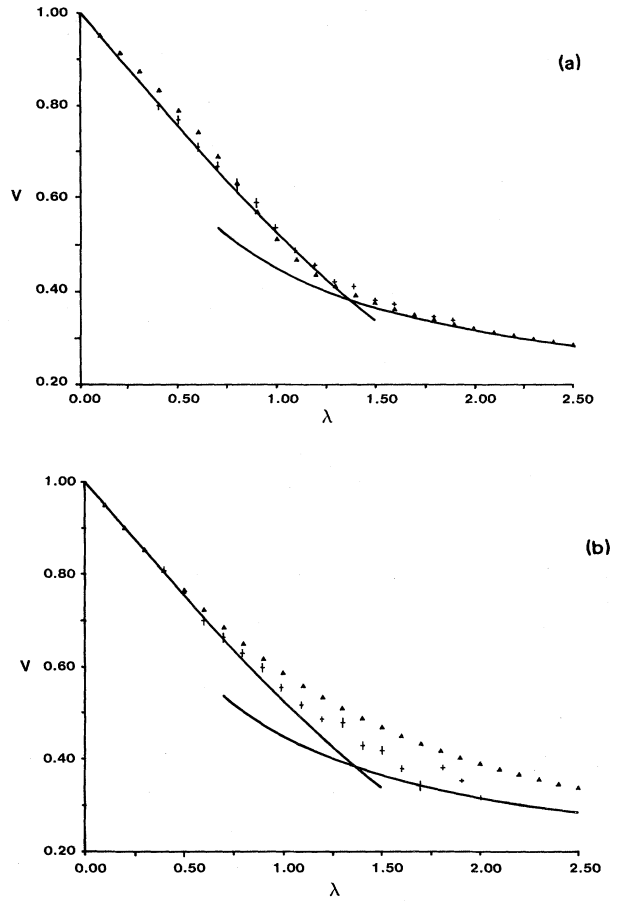

FIG. 4. The expectation value of $1-\cos(\theta_i-\theta_{i+1})$ vs coupling constant λ. The curves are perturbation expansions. The triangles ($\triangle$) are simple expectation values in the variational wave functions, and the crosses ($+$) are Monte Carlo estimates of the mixed expectation value, Eq. (2.17). The trial functions are ϕ_2 for (a) and ψ_1 for (b).

Note that $\mathscr{V}$ is related to the energy E_0 by

$$\mathscr{V}=\frac{1}{N}\frac{dE_0}{d\lambda} . \tag{4.2}$$

The Monte Carlo points in Figs. 4(a) and 4(b) are obtained from the mixed expectation value, i.e., Eq. (2.17), for the importance functions ϕ_2 and ψ_1, respectively. The curves on these graphs are from small- and large-λ perturbation theory. Here there are marked differences between the Monte Carlo results. In particular, the GFMC estimates of $\mathscr{V}$ obtained with the disordered importance function have large uncertainty and differ significantly from the ordinary expectation value in ψ_1, in the region $\lambda \gtrsim 1$. Again, this is precisely what we expect from calculations with an importance function that does not approximate the ground-state eigenfunction. It is interesting to note that the GFMC and variational estimates of $\mathscr{V}$ obtained with the spin-wave function ϕ_2 are almost equal for all λ, suggesting that ϕ_2 is quite a good representation of the eigenfunction.

V. SUMMARY

In this paper we describe results of an application of the Green's-function Monte Carlo method to the Hamiltonian XY model. These calculations are parallel to calculations described in an earlier paper for the compact U(1) lattice gauge theory in 2 and 3 spatial dimensions.

In these models an important issue is the existence and nature of a phase transition separating a disordered phase and a phase in which the model is accurately described by its harmonic approximation. We find that the GFMC results give a good indication of such a phase transition. In particular, we can judge whether a wave function resembles the ground-state eigenfunction by its performance in reducing fluctuations when used in the importance-sampling procedure. In our calculations the disordered trial function performs poorly for values of the coupling constant for which the harmonic wave function approximates the ground state. For the three-dimensional compact U(1) gauge theory the inadequacy of the disordered trial function is obvious: it yields energy estimates that are greater than the variational bound provided by the harmonic wave function, at least for the ensemble size that we use in the GFMC diffusion. For the XY model this inadequacy is more subtle, but can be seen in the large fluctuations of energy estimates.

The GFMC method offers a second way to judge whether a trial function represents a good approximation of the ground state, based on the mixed expectation value, i.e., Eq. (2.17). If ϕ_T approximates ϕ then the mixed expectation value of an operator A is nearly equal to the expectation value of A in ϕ_T; if these two quantities are quite different, then ϕ_T cannot be a good approximation of ϕ. Thus, for example, the increasing difference between the two estimates of $\mathscr{V}$ as λ increases beyond 1 in Fig. 4(b), is another indication that the disordered wave function does not resemble the eigenfunction for $\lambda \gtrsim 1$.

The Monte Carlo results imply by these considerations that the ground state of the XY model changes from a disordered state to a state better described by a harmonic wave function for $\lambda \cong 1$. This value is in agreement with the Kosterlitz-Thouless renormalization-group analysis, which predicts a phase transition at $\lambda = 1.02$.

APPENDIX

The connection between the Hamiltonian (2.1) and the partition function (1.1) of the classical XY model derives from the Feynman path integral of the quantum problem. The path integral for the Hamiltonian H is, with imaginary time,

$$Z=\int d\theta_i(t)e^{-A} , \tag{A1}$$

where $d\theta_i(t)$ denotes integration over paths in the space of $\vec{\theta}$ configurations, and A is the imaginary-time action

$$A=\int dt \sum_i \left[\frac{1}{4}\left[\frac{d\theta_i}{dt}\right]^2+\lambda[1-\cos(\theta_{i+1}-\theta_i)]\right] . \tag{A2}$$

We now consider a discrete approximation of the time coordinate; let t take the values

$$t_j = aj, \quad j = 0,1,2,3,\ldots \tag{A3}$$

with interval a to be specified later. If a is small compared to the time over which $\theta_i(t)$ varies then we may replace the integral over t by a sum over j, and the time derivative by a difference; i.e.,

$$\int dt \to a \sum_j ,$$
$$\frac{d\theta_i}{dt} \to \frac{1}{a}[\theta(i,j+1)-\theta(i,j)] , \tag{A4}$$

where $\theta(i,j)=\theta_i(t_j)$. Again for small a, we may assume that $\theta(i,j+1)-\theta(i,j)$ is small and approximate

$$[\theta(i,j+1)-\theta(i,j)]^2 \simeq 2\{1-\cos[\theta(i,j+1)-\theta(i,j)]\} . \tag{A5}$$

With these substitutions the action becomes

$$A = \sum_{i,j} \left\{ \frac{1}{2a}\{1-\cos[\theta(i,j+1)-\theta(i,j)]\} + a\lambda\{1-\cos[\theta(i+1,j)-\theta(i,j)]\} \right\} . \tag{A6}$$

At this point we let the interval a be $(1/2\lambda)^{1/2}$; then

$$A = \left[\frac{\lambda}{2}\right]^{1/2} \sum_{i,j} \{2-\cos[\theta(i,j+1)-\theta(i,j)] - \cos[\theta(i+1,j)-\theta(i,j)]\} . \tag{A7}$$

The lattice "path integral" over $\theta(i,j)$ is precisely the partition function (1.1) for classical statistical mechanics of the XY model, where the direction of the spin at (i,j) is defined by the angle $\theta(i,j)$, and the inverse temperature is

$$\beta = \left[\frac{\lambda}{2}\right]^{1/2} . \tag{A8}$$

This derivation of the connection between the one-dimensional quantum problem and the two-dimensional classical statistical mechanics problem is the inverse of the usual derivation,[7] which starts from the partition function and derives the Hamiltonian H as the transfer matrix in the limit that one of the dimensions becomes continuous.

The Kosterlitz-Thouless phase transition occurs at inverse temperature $\beta = 2.24/\pi$, according to a renormalization-group calculation.[4] Therefore, by Eq. (A8) the critical value of λ is 1.02. This value is perfectly consistent with the results of the GFMC calculations described in Sec. IV.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under Grant No. PHY81-01520, and by a grant from Control Data Corporation.

[1]M. H. Kalos, Phys. Rev. 128, 1791 (1962); Phys. Rev. A 2, 250 (1970); M. H. Kalos, D. Levesque, and L. Verlet, *ibid.* 9, 2178 (1974).

[2]D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics,* Topics in Current Physics, Vol. 7, edited by K. Binder (Springer, New York, 1979). This reference is a comprehensive review of the Green's-function Monte Carlo method.

[3]D. W. Heys and D. R. Stump, Phys. Rev. D 28, 2067 (1983).

[4]J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973); J. M. Kosterlitz, *ibid.* 7, 1046 (1974).

[5]A. M. Polyakov, Phys. Lett. 59B, 79 (1977); Nucl. Phys. B120, 429 (1977); T. Banks, R. Myerson, and J. Kogut, *ibid.* B129, 493 (1977); D. R. Stump, Phys. Rev. D 23, 972 (1981).

[6]J. Tobochnik and G. V. Chester, Phys. Rev. B 20, 3761 (1979).

[7]E. Fradkin and L. Susskind, Phys. Rev. D 17, 2637 (1978); J. Kogut, Rev. Mod. Phys. 51, 659 (1979).

[8]The importance-sampling procedure that we use is similar to that described in the paper by Kalos, Levesque, and Verlet (Ref. 1). See also Ref. 2.