Ground state of a triangular quantum antiferromagnet: Fixed-node Green-function Monte Carlo study

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(Received 17 July 1994)

A recently proposed "fixed-node" quantum Monte Carlo scheme for lattice Hamiltonians is adopted to study antiferromagnetic order of the Néel type in the ground state of the two-dimensional spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on the triangular lattice. Fixed-node Green-function Monte Carlo simulations, based on an antiferromagnetically correlated trial wave function, are performed on lattices of up to 324 sites. Extrapolation of the results to the thermodynamic limit indicates that an ordered ground state may exist with a sublattice magnetization of as much as $\sim 60\%$ of the classical value; an upper bound of $-0.5431 \pm 0.0001\ J$ is found for the ground-state energy per site.

I. INTRODUCTION

Quantum Monte Carlo (QMC) techniques have afforded considerable progress in the investigation of the ground state of low-dimensional quantum antiferromagnets. In particular, for the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (AFHM) on the square lattice, which has received a lot of attention in the context of high-T_c superconductivity,[1] QMC simulations at zero temperature have yielded accurate estimates of key quantities such as the energy, the sublattice magnetization, the magnetic susceptibility, and the spin-wave velocity.[2] These results have provided robust quantitative support to the hypothesis of an antiferromagnetically ordered ground state of the Néel type, in which quantum fluctuations reduce the sublattice magnetization to about 60% of its classical value.[1]

The situation is far less clear on two-dimensional (2D) lattices with geometries other than the square, such as the triangular and *kagomé* lattices. One of the theoretical aims motivating the study of the spin-$\frac{1}{2}$ AFHM on these lattices is determining whether frustration, caused by their particular geometries, may enhance the effect of quantum spin fluctuations to the point of causing the classical antiferromagnetic order to vanish, giving rise to a disordered, or, possibly, to a differently ordered ground state.

Due to the well-known *sign* problem, QMC methods have not yet been adopted to investigate Heisenberg antiferromagnets on nonsquare lattices. On the square lattice, the sign problem can be eliminated by means of a basis transformation that takes advantage of the bipartite character of the lattice;[2] however, there appears to be no analogous solution for nonbipartite, frustrated lattices such as the triangular or the *kagomé*.

In this paper the attention is focused on the spin-$\frac{1}{2}$ AFHM on the 2D triangular lattice (TAHFM); a number of analytical[3–8] and numerical[9–11] studies have attempted to shed light on the physics of this model, but the fundamental question of the existence of ground-state long-range order, of the Néel or other types, is yet to be answered definitively.

Numerical results have been obtained exclusively by means of the Lanczos algorithm.[12] Though it provides exact results, this technique is limited to lattices of relatively small size (to date, 36 sites at the most) by computer memory constraints. This renders the extrapolation of the estimates to the infinite lattice rather problematic; for example, the same Lanczos results have been interpreted by different authors as evidence both against[10] and in favor[11] of the existence of long-range order in the thermodynamic limit. Therefore, the extension of the numerical investigation to lattices of sufficiently large size, allowing an unambiguous extrapolation, is a necessary step.

To this aim, QMC techniques appear as the only realistic option, owing to the relatively favorable scaling of computer resources required versus the size of the system; however, something must be done to overcome, or at least alleviate, the sign problem.

Recently, a viable option has been made available by the introduction of a scheme,[13] consisting of an extension to lattice models of the well-known "fixed-node"[14] method, which effectively overcomes the sign problem in QMC simulations of continuum many-particle systems. Fixed-node QMC calculations have provided accurate results for a variety of fermion systems such as the one-component plasma,[14] the electronic cloud in atoms and molecules,[15] liquid ^{3}He (Ref. 16) and other systems plagued by the sign problem. As its continuum counterpart, the lattice fixed-node (LFN) scheme allows one to perform ground-state QMC simulations with no sign problem; the accuracy of the ground-state estimates depends on an input trial wave function for the system under study. A variational property exists for the fixed-node ground-state energy estimate, and this permits to gain insight by comparing the results of different calculations, based on wave functions describing alternative physical pictures.

In this work, the LFN scheme is adopted to perform a fixed-node Green-function Monte Carlo (FN-GFMC) study of the spin-$\frac{1}{2}$ AFHM on the 2D triangular lattice. Besides the physical motivation of exploring the yet elusive nature of the ground state of a frustrated quantum antiferromagnet, there is a methodological aspect to this work, namely assessing the effectiveness of the LFN scheme on a frustrated spin system for which no other QMC-based approach, such as a transient estimation,[16,17] is feasible, due to the severity of the sign problem. In a future publication, the application of this technique to a different type of frustrated quantum antiferromag-

0163-1829/95/52(21)/15304(8)/$06.00

net, namely the $J1/J2$ model on the square lattice, will be presented.[18]

The calculation described in this paper is based on a trial wave function incorporating antiferromagnetic 120° Néel spin ordering and including long-range antiferromagnetic spin-spin as well as three-spin correlations. This general type of wave function was originally proposed, in the context of the TAFHM, by Miyashita,[19] and successively generalized by Huse and Elser to include long-range spin-spin and three-spin correlations;[8] the wave function utilized in this work is essentially the one of Ref. 8, although with a slightly different long-range tail for the spin-spin correlation part.

FN-GFMC simulations have been performed on lattices of several sizes, with up to 324 sites; extrapolation of the results to the thermodynamic limit yields an upper bound for the ground state energy per site ϵ of $-0.5431 \pm 0.0001\ J$, i.e., rather close to the most recent estimate obtained by extrapolating exact results on small clusters.[11] Results indicate that an ordered ground state may exist with a value of the sublattice magnetization as large as 62% of the classical value, the same value found for the square lattice. In order to consolidate this result, which would point to a considerable physical analogy between the ground states for the two lattices, other fixed-node calculations will have to be performed, using disordered, or differently ordered, trial states; to this aim, the results given in this paper should provide a useful reference.

The remainder of this paper is organized as follows: in the next section the model Hamiltonian of interest will be introduced, and the notation set; in Sec. III the Green-function Monte Carlo (GFMC) method and the lattice fixed-node procedure will be briefly outlined; in Sec. IV the variational wave function used in this work will be introduced; finally, in the last two sections the results and the conclusions will be presented.

II. THE MODEL

The spin-$\frac{1}{2}$ AFHM consists of the lattice Hamiltonian

$$\hat{\mathscr{H}} = J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j , \tag{1}$$

where the sum runs over all pairs of nearest-neighbor lattice sites and $\mathbf{s}_i$ is a spin-$\frac{1}{2}$ operator associated with site i. On a triangular lattice, the classical model orders antiferromagnetically,[20] with the spins arranged at 120° to one another in the three sublattices A, B, and C ($\sqrt{3}\times\sqrt{3}$ Néel ordering, Fig. 1); however, a disordered ground state was proposed for the quantum system, quite some time ago.[21]

In order to investigate the presence of an ordered ground state of a given type, an appropriate order parameter must be defined. For Néel-like antiferromagnetic order, it is the square of the sublattice magnetization vector $\mathbf{m}^\dagger$, defined as follows:

$$m^{\dagger 2} = \langle M_A^2 \rangle = \langle M_B^2 \rangle = \langle M_C^2 \rangle , \tag{2}$$

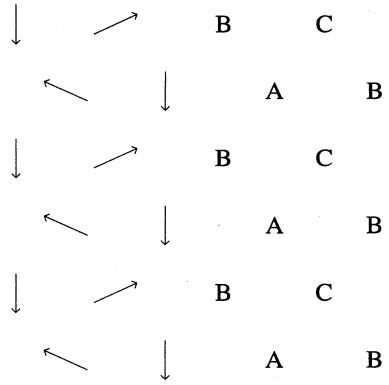

FIG. 1. Classical $\sqrt{3}\times\sqrt{3}$ Néel spin ordering on the triangular lattice.

where $\mathbf{M}_L = \Sigma_{i \epsilon L} \mathbf{s}_i$, is the magnetization of sublattice L, and $\langle \cdots \rangle$ indicates ground-state expectation value. It is a simple matter to show[1] that, if $N = 3P$ is the number of lattice sites, then

$$m^{\dagger 2} = P^2 \mathbf{s}_i \cdot \mathbf{s}_j + \mathscr{O}(P), \text{ as } r_{ij} \to \infty , \tag{3}$$

where r_{ij} is the distance between two sites i and j in the same sublattice. The order parameter $m^{\dagger 2}$ saturates to the value $(P/2)(P/2+1)$ in the classical Néel state. In the remainder of this paper, values of $m^{\dagger 2}$ and of $m^\dagger$, which is the magnitude of the sublattice magnetization vector, will be consistently given as fractions of their saturation values.

The theoretical problem is to determine whether or not the ground state of (1) on the 2D triangular lattice is characterized by a nonzero value of $m^\dagger$, i.e., if it features antiferromagnetic long-range order of the Néel type.

Analytical approaches such as linear spin-wave (LSW) analysis[3] and series expansion,[5] yielding similar and rather accurate results for the square lattice,[1] appear less conclusive and somewhat contradictory, particularly on the question of long-range order, when applied to the TAFHM. In fact, while LSW predicts a Néel-ordered ground state with a value of $m^\dagger$ around 0.48–0.50, series expansion predicts a value of $m^\dagger$ very close to zero.

In variational calculations, trial states incorporating antiferromagnetic long-range order[7,8] have been found to yield slightly lower ground-state energy estimates than other states based on different physical scenarios, such as the one of a spin liquid with chiral symmetry breaking.[4,6] In fact, the lowest variational estimate of the ground-state energy of the TAFHM in the thermodynamic limit[22] is given by the trial wave function optimized by Huse and Elser,[8] yielding a value of $m^\dagger$ equal to 0.68 in the thermodynamic limit. However, it is worth mentioning that variational calculations based on disordered trial states have been performed for rather small clusters, and it is not obvious how representative the results may be of the physics of the infinite lattice.

III. THE METHOD

QMC methods at zero temperature consist of projecting the ground state $|\Phi\rangle$, of a given Hamiltonian $\hat{\mathscr{H}}$, out of an

initial trial state $|\Psi\rangle$ not orthogonal to $|\Phi\rangle$, by repeated applications of a suitable projection operator $\hat{G}=G(\hat{\mathscr{H}})$. This operation can be mathematically expressed as a path integral over many-particle trajectories in configuration space, and represented by a stochastic process, which is in turn simulated on a computer by the random walks through the configuration space of a sample of independent "walkers."[23,24]

Different names have been used for this type of procedure: power method, projector Monte Carlo, Green-function Monte Carlo and others; in this paper, the name Green-function Monte Carlo (GFMC) will be used for definiteness, without implying any substantial methodological difference.

This method and its application to lattice Hamiltonians have been thoroughly described in many other publications;[2,17] therefore, the details will not be reviewed here. Rather, the aim of this section will be to emphasize those elements that differentiate the lattice fixed-node GFMC method, which is used in this work, from standard GFMC.

Standard GFMC yields results which are, in principle, exact in the sense that no approximations are involved and the only errors are statistical; thus, they can be rendered arbitrarily small, given a sufficiently large statistical sample (i.e., CPU time). The main limitation to its applicability comes from the well-known *sign* problem,[25] which derives from the positivity requirement

$$w(c,c')=\langle c|\hat{G}|c'\rangle\frac{\Psi(c')}{\Psi(c)}>0 \tag{4}$$

for any two configuration vectors $|c\rangle$, $|c'\rangle$; $\Psi(c)$ is the wave function of the initial trial state. The reason for (4) is that in a scheme based on random walks, such as GFMC, $w(c,c')$ is interpreted as the *probability* for a walker to make a transition from the configuration $|c\rangle$ to the configuration $|c'\rangle$, along a random walk. For the typical projection operators used in GFMC simulations, (4) implies the following *negativity* requirement involving the Hamiltonian operator:

$$\langle c|\hat{\mathscr{H}}|c'\rangle\frac{\Psi(c')}{\Psi(c)}<0. \tag{5}$$

It is very difficult to fulfill (5) in general; for example, a fermion system must have a wave function that changes sign in different regions of the configuration space, and this normally prevents (5) from holding. Though, in principle, one can allow w to be negative, use its modulus as probability, and include the sign as an overall phase factor associated to the random walk, this leads to numerical instability, as physical averages are obtained as ratios of differences of exponentially large quantities. Therefore, in practice only a relatively limited number of operations of $\hat{G}$ can be performed before statistical errors grow exceedingly. Occasionally, it is possible to observe convergence of the estimates to their ground-state values in a small number of iterations, particularly if a sufficiently accurate trial wave function is known,[16,17] for a system for which the sign problem is not too severe; however, this is not a generally applicable procedure.

An effective scheme, enabling the application of GFMC to any Hamiltonian affected by the sign problem, is the one known as "fixed-node" or "restricted path-integral" method; originally developed for continuum systems, it has been recently extended to lattice models.

For a continuum many-particle Hamiltonian $\hat{\mathscr{H}}=\hat{\mathscr{H}}_0+\hat{V}$, where $\hat{\mathscr{H}}_0$ is a kinetic energy term and $\hat{V}$ a position-dependent, local interaction potential, the fixed-node approach consists of performing the random walk through the configuration space based on the transition probability

$$p(c,c')\propto\Theta\{w(c,c')\}, \tag{6}$$

where $\Theta(x)=1$ if $x>0$, 0 otherwise. This is equivalent to solving by GFMC the modified Hamiltonian $\hat{\mathscr{H}}_{\rm FN}=\hat{\mathscr{H}}+\hat{V}_{\rm FN}$ where $\hat{V}_{\rm FN}$ is an additional many-body potential:

$$\hat{V}_{\rm FN}(c)=\infty \text{ if } \Psi(c)=0,\ 0 \text{ otherwise.} \tag{7}$$

The effect of $\hat{V}_{\rm FN}$ is the confinement of the random walks to regions of the configuration space in which the trial wave function $\Psi(c)$ does not change sign.[14] By avoiding sign-changing transitions associated with negative values of $w(c,c')$, the fixed-node prescription eliminates the sign problem.

It can be shown[14,25] that the results of a fixed-node GFMC calculation are exact, i.e., the ground state of the effective Hamiltonian $\hat{\mathscr{H}}_{\rm FN}$ coincides with the ground state of the original Hamiltonian $\hat{\mathscr{H}}$, if the nodal surface of the trial wave function $\Psi(c)$ [i.e., the set of configurations c_n such that $\Psi(c_n)=0$] and the one of the true ground-state wave function $\Phi(c)$ of $\hat{\mathscr{H}}$ coincide, regardless of relative magnitudes and signs of the two functions where they differ from zero.

In general a complete knowledge of the nodal surface of $\Phi(c)$ is not available; in this case, FN-GFMC calculations based on the nodal surfaces of the trial wave function are only approximate. However, a variational property can be demostrated for the energy estimate $E_{\rm FN}$ obtained via FN-GFMC (i.e., the lowest eigenvalue of $\hat{\mathscr{H}}_{\rm FN}$) namely

$$E_{\rm FN}\geqslant E_0=\frac{\langle\Phi|\hat{\mathscr{H}}|\Phi\rangle}{\langle\Phi|\Phi\rangle}, \tag{8}$$

the equality holding if the nodal surfaces of $\Psi(c)$ and $\Phi(c)$ coincide. The usefulness of (8) lies in the possibility of gaining insight in a physical system by studying the dependence of the energy estimate on variations of the trial wave function.

The lattice version of the fixed-node algorithm is also based on a restriction of the random walks through configuration space; unlike the continuum case, however, such a restriction cannot be simply enforced through the nodal surface of the trial wave function, because of the inherent difficulty of defining nodal boundaries on a lattice. Alternatively, this problem can be interpreted as due to the intrinsic nonlocality of lattice Hamiltonians; in fact, even in QMC calculations of continuum systems the fixed-node algorithm must be modified, if nonlocal interaction potentials are included.[26]

The analogy between the continuum and the lattice algorithms consists of the replacement of the original Hamiltonian with an effective one, for which no sign-changing

transition occurs. The LFN effective Hamiltonian is defined through its matrix elements between configuration vectors $|c\rangle, |c'\rangle$ as follows:

$$\langle c'|\hat{\mathscr{H}}_{\rm FN}|c\rangle = \langle c'|\hat{\mathscr{H}}|c\rangle, \text{ if } \langle c'|\hat{\mathscr{H}}|c\rangle \frac{\Psi(c')}{\Psi(c)} < 0,$$

$$\langle c'|\hat{\mathscr{H}}_{\rm FN}|c\rangle = 0 \quad \text{if } \langle c'|\hat{\mathscr{H}}|c\rangle \frac{\Psi(c')}{\Psi(c)} \geq 0,$$

$$\langle c|\hat{\mathscr{H}}_{\rm FN}|c\rangle = \langle c|\hat{\mathscr{H}}|c\rangle + \sum_{sf} \langle c'|\hat{\mathscr{H}}|c\rangle \frac{\Psi(c')}{\Psi(c)}, \tag{9}$$

where the sum Σ_{sf} is extended to all configurations $|c'\rangle$ connected to $|c\rangle$ by $\hat{\mathscr{H}}$ via a "sign-changing" transition, i.e., one for which $\langle c'|\hat{\mathscr{H}}|c\rangle\Psi(c')/\Psi(c) > 0$.

It is a simple matter to show that the effective Hamiltonian $\hat{\mathscr{H}}_{\rm FN}$, constructed from $\hat{\mathscr{H}}$ using a particular trial state $|\Psi\rangle$, fulfills the variational property (8), and that exact ground-state estimates for $\hat{\mathscr{H}}$ can be obtained using $\hat{\mathscr{H}}_{\rm FN}$ if the trial state $|\Psi\rangle$ satisfies the condition

$$\frac{\Psi(c)}{\Psi(c')} = \frac{\Phi(c)}{\Phi(c')} \tag{10}$$

for all pairs $|c\rangle$, $|c'\rangle$ for which $\langle c'|\hat{\mathscr{H}}|c\rangle\Psi(c')/\Psi(c) \geq 0$. Note also that $\hat{\mathscr{H}}_{\rm FN} \equiv \hat{\mathscr{H}}$ if $\hat{\mathscr{H}}$ is unaffected by the sign problem. The proof of all of the above is given in Ref. 13 and will not be repeated here.

As in the continuum fixed-node algorithm, the effective Hamiltonian used to overcome the sign problem explicitly contains the trial wave function $\Psi(c)$. In the LFN scheme, however, a more stringent condition must be fulfilled, with respect to the continuum case, in order to obtain exact results. In the continuum, the simple knowledge of the nodal surface of the true ground-state wave function $\Phi(c)$ guarantees the exactness of the method. On a lattice, on the other hand, a partial knowledge of the amplitude of the true ground-state wave function where it differs from zero is required, as expressed by condition (10).

IV. THE TRIAL WAVE FUNCTION

Consider a 2D triangular lattice with N sites, and specify a lattice spin configuration $|c\rangle$ by assigning the value of the spin projection along a chosen direction of the spin space, say z, at every lattice site, i.e., $|c\rangle \equiv |s_1^z s_2^z \ldots s_N^z\rangle$.

A generic trial state can be written as

$$|\Psi\rangle = \sum_c \Psi(c)|c\rangle, \tag{11}$$

where $\Psi(c)$ is the trial wave function.

In this work, a particular type of trial state is considered for the Hamiltonian (1) on the 2D triangular lattice, namely one that assumes the presence of underlying Neél-like antiferromagnetic long-range order (Fig. 1). A simple wave function describing this type of spin ordering is

$$\Psi(c) = \exp[i\Omega(c)]\exp\left\{-\frac{1}{2}\sum_{ij} u_{ij} s_i^z s_j^z\right\} \tag{12}$$

with

$$\Omega(c) = \frac{\pi}{3}[\mathscr{N}_\downarrow^C(c) - \mathscr{N}_\downarrow^A(c)], \tag{13}$$

where $\mathscr{N}_\downarrow^L(c)$ is the number of sites in the sublattice L for which $s^z = -1/2$ in the configuration $|c\rangle$ and u_{ij} is an antiferromagnetic spin-spin correlation function, which in general depends on the distance r_{ij} between sites i and j, and is aimed at describing quantum spin fluctuations around the classical Neél state. If u is set equal to zero, the wave function (12) describes the classical Néel state with $\mathbf{M}_B$ pointing in the x direction and with $\mathbf{M}_A$ and $\mathbf{M}_C$ lying in the xy plane of the spin space.

The same type of wave function affords a rather accurate quantitative description of the ground state of (1) on the square lattice, on optimizing the function u_{ij}.[1,27] In the context of the TAFHM, the state (12) was proposed by Miyashita,[19] who took the function u_{ij} to be equal to u for nearest-neighbor i,j and zero otherwise, and treated u as a variational parameter, obtaining a value for the ground-state energy per site of about $-0.507\ J$, to be compared with the value $-0.375\ J$ given by the simple Néel state, and for $m^\dagger$ of about 0.85.

The wave function (12) was later revisited by Huse and Elser,[8] who improved considerably the ground-state energy estimate by (a) allowing u to be a long-range function of the distance r between two lattice sites, and (b) including three-spin correlations through the following modification of the phase factor $\Omega(c)$ in (12):

$$\Omega(c) \rightarrow \Omega'(c) = \Omega(c) + F \sum_{i<j<k} \gamma_{ijk} s_i^z s_j^z s_k^z, \tag{14}$$

where F is a variational parameter, the sum includes all triplets of lattice sites i,j,k, and $\gamma_{ijk} = \pm 1$ if $r_{ij} = 1$, $r_{jk} = 1$ and $r_{ik} = \sqrt{3}$, zero otherwise. The sign of γ_{ijk} is determined by assuming that the modified wave function retain all the rotational and translational properties of the wave function (12), i.e., of the classical Néel state. As a result, γ_{ijk} does not change sign under rigid translations or rotations in real space by an angle $2\pi/3$ of the triplet ijk, but changes sign under rotations of $\pi/3$ or π. Upon choosing a particular triplet in which, say, i and k belong to sublattice A and j to sublattice B, and setting $\gamma_{ijk} = 1$ for such a triplet, the sign of γ_{ijk} for all other triplets for which it is nonzero follow.[8]

By taking $u(r) = K/r^\sigma$ and using K,σ as variational parameters, Huse and Elser obtained an estimate of the ground-state energy per site, in the thermodynamic limit, of $-0.5364\ J$, and of the sublattice magnetization of about 0.68, with $K \sim 0.625$, $\sigma \sim 1.8$ and $F \sim 0.3125$.

The wave function $\Psi(c)$ utilized in this work has the functional form (12), with $\Omega'(c)$ given by (14), but with a different long-range tail for the function $u(r)$, with respect to the wave function used in Ref. 8. The reason is that a variational state characterized by a wave function of the type (12) assumes antiferromagnetic long-range order of the Néel type for the ground state, and the function u describes quantum fluctuations around the classical Néel state; if these are assumed to be in the form of long-wavelength spin-wave excitations, then they can be shown[3,10] to feature a linear disper-

sion relation $\omega(k)$, which translates into a long-range tail for the function $u(r) \sim 1/r$ in two dimensions.[1,27]

Thus, in this work the function $u(r)$ was taken to be equal to K for $r=1$, to K' for $r=\sqrt{3}$ and to K''/r for $r>\sqrt{3}$, with K, K', and K'' variational parameters. This modification of the long-range tail of u is not expected to improve significantly the ground state energy estimate, with respect to the results of Ref. 8 as the energy is known not to be too sensitive to the tail of u; however, it can affect other quantities such as spin-spin correlations. Also, in this work $\Psi(c)$ was taken to be zero for all spin configurations for which $S^z=\Sigma_i s_i^z \neq 0$, i.e., the calculation was restricted to the subspace with $S^z=0$; this is allowed since S^z is a good quantum number, and was found to improve slightly the variational energy estimate. It can be shown that, with this choice, the trial state still features antiferromagnetic order of the Néel type in the xy plane of the spin space, but the sublattice magnetization no longer has a well-defined direction.

Optimal values for the variational parameters were found by minimizing the variance of the ground-state energy estimate obtained on performing variational calculations with the wave function Ψ, using the Metropolis Monte Carlo method. These optimal values are $K=0.58$, $K'=0.2$, and $K''=0.35$; for the variational parameter F, associated with the three-spin correlation term in $\Omega'(c)$, the same optimal value proposed in Ref. 8 was found, namely $F=0.3125$. The optimal values were found on a 36-site lattice, and were found not to change on larger lattices, within the statistical errors of the variational calculation.

It should be noted that the trial state described by the wave function (12) is not a spin singlet on any finite lattice with an even number of sites; although there is no proof that the ground state of (1) on nonbipartite lattices is a singlet, this is the case for the finite clusters which have been diagonalized exactly.[11] However, a symmetry-breaking ground state is possible in the thermodynamic limit; therefore, the wave function (12) can be expected to yield increasingly accurate results as the thermodynamic limit is approached.

V. RESULTS OF THE FN-GFMC CALCULATION

Using the wave function $\Psi(c)$ described in the previous section, a fixed-node Green-function Monte Carlo study of the ground state of the spin-$\frac{1}{2}$ AFHM was performed, on triangular lattices of several sizes, with periodic boundary conditions. As mentioned at the end of the previous section, variational calculations were also performed, using the Metropolis Monte Carlo method.

In principle, the introduction of the modified phase factor $\Omega'(c)$ renders the wave function $\Psi(c)$ complex; although complex wave functions can be utilized in GFMC-type calculations,[28] in this work the real part of Ψ was actually used, as the quantities of interest here do not require retaining the complex character of Ψ.

Apart from the fixed-node prescription, the details of the GFMC calculation are not different from standard GFMC simulations of quantum Heisenberg Antiferromagnets.[2] A rather large (over 50 000) ensemble of walkers was utilized, in order to reduce the bias due to the control of the population size. A sufficient number of operations of $\hat{G}$ was performed, until estimates were observed to stabilize around the ground-state value; then, roughly ten times as many operations of $\hat{G}$ were performed to achieve the desired statistical accuracy.

TABLE I. Ground-state energy per site, in units of J, computed with a variational and a FN-GFMC calculation, both based on the trial wave function Ψ, introduced in Sec. IV. Statistical errors, in parentheses, are the last digit. The column "exact" reports the results of Ref. 11.

N	Variational	FN-GFMC	Exact
36	-0.5449(1)	-0.5513(2)	-0.5604
144	-0.5382(1)	-0.5441(1)	
324	-0.5376(1)	-0.5434(1)	
Extrapolated	-0.5373(1)	-0.5431(1)	-0.5445

The projection operator used is $\hat{G}=E-\hat{\mathscr{H}}_{\mathrm{FN}}$, where E is a constant which must be $\geq E_M$, the largest eigenvalue of $\hat{\mathscr{H}}_{\mathrm{FN}}$. While determining the largest eigenvalue $\mathscr{E}_M$ of $\hat{\mathscr{H}}$ is trivial, $\hat{\mathscr{H}}_{\mathrm{FN}}$ explicitly contains the trial wave function Ψ; thus, its largest eigenvalue depends on the largest value that $|\Psi(c)/\Psi(c')|$ can assume for a pair of configurations c and c' connected by a sign-changing transition (Sec. III), and is not easily determined. A signature of the fact that the selected value of E is not sufficiently large is the occasional occurrence, along the random walks, of configurations for which the diagonal matrix elements of $\hat{G}$ are negative, whereas it should be always positive if $E \geq E_M$.

A practical solution to this problem is to repeat the calculation for a few, increasing values of E, and study the dependence of the results on the value chosen; for E sufficiently large, the results of the calculations become independent of E, and no configuration featuring a negative diagonal matrix element of $\hat{G}$ is ever encountered. In this work, this was found to be the case upon choosing $E \geq 10J+\mathscr{E}_M$. Naturally, if a different trial wave function is used, a different value of E will be needed too, in general.

In Table I the results for the ground-state energy per site ϵ, obtained in the different calculations and for the various lattices, are reported. For comparison purposes, the Lanczos result is also reported for the only lattice size considered in this work (36 sites) for which it is available. The last row of Table I reports the results of the extrapolation of the estimates to the thermodynamic limit; for FN-GFMC data, this was carried out by assuming the functional scaling form for the energy per site $\epsilon(N)=\epsilon_\infty+\alpha N^{-3/2}$, from LSW analysis;[3,10] this is consistent with the form adopted for the trial wave function. These results are also shown in Fig. 2.

The variational estimate in the thermodynamic limit is $-0.5373\pm0.0001\ J$, only slightly below that of Ref. 8, i.e., $-0.5364\ J$; this was expected, as explained in Sec. IV; the extrapolated FN-GFMC estimate for the same quantity is $-0.5431\pm0.0001\ J$.

On the 36-site lattice, the FN-GFMC result does not compare particularly well with the exact result; the FN-GFMC algorithm can recover about 40% of the energy that is missing at the variational level, and this might appear somewhat disappointing, if compared with 70–90% that can often be recovered in fixed-node calculations for continuum systems,[14–16] even with a relatively simple choice of nodal

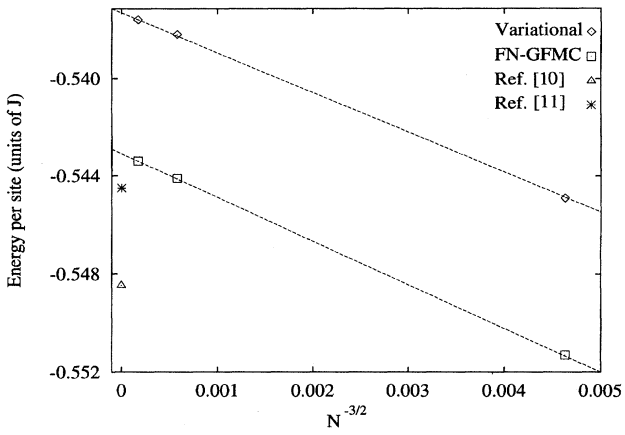

FIG. 2. Variational (diamonds) and FN-GFMC (squares) estimates of the ground-state energy per site for (1) on the $2d$ triangular lattice. Dashed lines represent extrapolations of the results to the infinite lattice limit. The triangle and the star refer to extrapolations to the thermodynamic limit of the exact diagonalization results of Refs. 10 and 11.

surface for the trial wave function.

As explained in Sec. III, in order to obtain exact results, within the LFN scheme, a considerably more detailed knowledge is required of the true ground-state wave function $\Phi(c)$, with respect to the continuum case,[13] in which the trial wave function enters in the effective Hamiltonian only through its nodal surface. For example, for a one-dimensional continuum many-body Hamiltonian, for which the locations of the nodes of $\Phi(c)$ are known (i.e., the coincidence points), the FN-GFMC scheme will yield exact results, in principle, no matter how poor the trial wave function. On the other hand, for a one-dimensional lattice Hamiltonian, the knowledge of the sign of $\Phi(c)$ everywhere is not sufficient to ensure that exact results will be obtained.

Due to this somewhat stricter requirement, it is to be expected that the LFN scheme may not yield, in general, the same quantitative improvements on the variational estimate that its continuum counterpart often affords. In fact, the LFN method may only produce a very small improvement on the variational energy estimate, if the wave function used is poor.

To illustrate this point more quantitatively, consider the results of a separate FN-GFMC calculation performed in this work, for the 36-site lattice, using the wave function (12) in the simple form proposed by Miyashita, i.e., without the three-spin term and with no long-range tail in the function u. The variational energy estimate obtained was -0.5182 ± 0.0001 J, and the FN-GFMC algorithm lowered it to -0.5240 ± 0.0001 J, only recovering 14% of the missing energy.

As mentioned at the end of the previous section, the symmetry-breaking trial wave function utilized in this work is expected to afford an increasingly accurate description as the thermodynamic limit is approached, i.e., on relatively large lattices. An important indication that this is the case comes from the fact that the extrapolated FN-GFMC value in the thermodynamic limit compares quite well with the one obtained in Ref. 11 by extrapolating results of exactly diagonalizable clusters (star in Fig. 2). Exact results were also extrapolated to a different, somewhat lower value, in another work[10] (triangle in Fig. 2), but even if that value were taken as reference point, the above conclusion on the wave function would still hold.

TABLE II. Ground-state expectation values of the order parameter $m^{\dagger 2}$ computed with variational and FN-GFMC calculations based on the trial wave function Ψ, introduced in Sec. IV. Statistical errors, in parentheses, are the last digit.

N	Variational	FN-GFMC
36	0.1480(2)	0.1458(2)
144	0.1276(2)	0.1204(2)
324	0.1244(3)	0.1144(3)

It should also be noted that within the statistical errors of this calculation, the FN-GFMC ground-state estimate on the 36-site lattice is below the exact energy of the first excited state,[11] which is -0.5500 J, which indicates that the trial wave function is not orthogonal to the true ground state.

To conclude on this point, note that another estimate of ϵ may be obtained in the thermodynamic limit by applying a "rigid" shift $\delta\epsilon$ to all the FN-GFMC estimates, with $\delta\epsilon$ given by the difference between the FN-GFMC and the exact result on the 36-site lattice. This yields an estimate of about -0.5522 J, which is presumably a lower bound on the true value, since, as mentioned above, the difference between FN-GFMC and exact results is expected to narrow down, in the thermodynamic limit. The two values -0.5431 J and -0.5522 J bracket the two estimates from Refs. 10 and 11.

The antiferromagnetic order parameter $m^{\dagger 2}$ was determined by taking advantage of (3), i.e., by calculating the ground-state expectation value $\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle$ for two sites i and j belonging to the same sublattice and spaced apart by the largest distance r_{ij}.

Because the quantity $\mathbf{s}_i \cdot \mathbf{s}_j$ is not diagonal in the representation $\{|c\rangle\}$, the commonly adopted "extrapolated" GFMC estimator was utilized, as opposed to the potentially exact one based on "forward walking";[29] though inherently biased, the extrapolated estimator is often rather reliable, particularly if a sufficiently accurate trial wave function is used,[2,25] so that the difference between the value computed with the trial wave function and the exact one is small.

In Table II variational and extrapolated FN-GFMC results are reported for the order parameter $m^{\dagger 2}$; in Fig. 3, FN-GFMC results are shown, together with their extrapolation to the infinite lattice limit performed by assuming the functional scaling form $m^{\dagger 2}(N) = m_{\infty}^{\dagger 2} + \beta N^{-1/2}$.

Extrapolation of the FN-GFMC results for $m^{\dagger 2}$ yields a ground-state estimate equal to 0.098 ± 0.002 in the thermodynamic limit, i.e., a value for $m^{\dagger} \sim 0.62$. This value is the same as the one found in GFMC calculations for the spin-$\frac{1}{2}$ AFHM on the square lattice. While it is certainly possible that the value of $m^{\dagger}$ might be overestimated in this calculation, due to the particular wave function utilized in the FN-GFMC algorithm and the use of the extrapolated GFMC estimator, it seems reasonable to conclude that these results are consistent with a nonzero value of $m^{\dagger}$ in the thermodynamic limit.

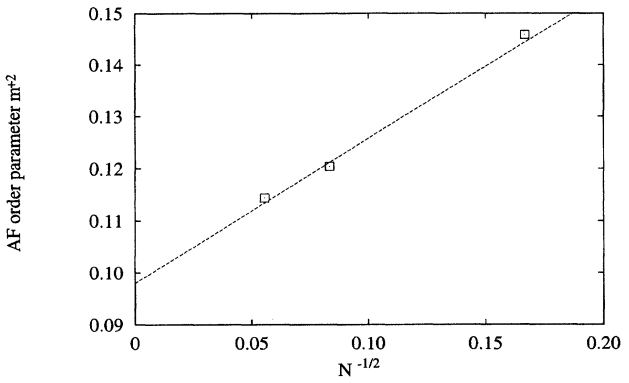

FIG. 3. FN-GFMC estimates of the order parameter $m^{\dagger 2}$ in the ground state of (1) on the $2d$ triangular lattice. The dashed line represents the extrapolation of the results to the infinite lattice limit.

VI. CONCLUSIONS

In this work, a scheme[13] to perform QMC simulations at zero temperature of lattice Hamiltonians, overcoming the *sign* problem and yielding variational energy estimates, was adopted to study antiferromagnetic order of the Néel type in the ground state on the spin-$\frac{1}{2}$ AFHM on the 2D triangular lattice.

The calculation described in this work was based on a trial wave function assuming the existence of Néel order in the ground state; an upper bound of $-0.5431 \pm 0.0002\ J$ was obtained for the ground-state energy per site, for the infinite lattice, presently the lowest variational estimate for the model under study, in good quantitative agreement with the most recent extrapolation to the thermodynamic limit of exact results on small lattices.[11] As for the existence of Néel order in the ground state, the results of this calculation are consistent with an antiferromagnetically ordered ground state, with a value of the sublattice magnetization as large as about 62% of the classical value. Although this result probably overestimates the value of $m^{\dagger}$, due to the particular trial wave function used, which appears in the projection operator used in the FN-GFMC calculation, it certainly points to the existence of low-lying antiferromagnetically ordered states, in interesting analogy with the physics of the same model on the square lattice.

In order to make further progress toward establishing whether the ground state is ordered, a necessary step will be to perform other FN-GFMC calculations based on different wave functions, such as resonating-valence bond describing disordered spin liquids[4,6] or differently ordered states[7] and compare the results with those presented in this paper.

The lattice fixed-node QMC method, recently introduced, is effective in allowing QMC simulations of Hamiltonians affected by the sign problem. As its continuum analog, it always permits one to improve the variational energy estimate given by an initial trial wave function; such an improvement depends considerably on the accuracy of the input variational ansatz, probably more so than in the continuum, at least according to the results found in this work; future calculations, based on this method, for different lattice Hamiltonians, will provide further clarifications on this point. In any case, it appears rather likely that the LFN algorithm will prove a very valuable tool in the investigation of the physics of frustrated antiferromagnets.

ACKNOWLEDGMENTS

This work was supported by the Office of Naval Research under Contract No. N00014-J-92-1320 and by the National Center for Supercomputing Applications (NCSA). Calculations were performed on the HP-Convex Exemplar at NCSA. The author wishes to acknowledge useful discussions with D. M. Ceperley, D. A. Huse, G. Ortiz, and K. J. Runge.

[1] For a comprehensive review of this subject, see E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

[2] J. Carlson, Phys. Rev. B **40**, 846 (1989); N. Trivedi and D. M. Ceperley, *ibid.* **40**, 2747 (1989); K. J. Runge, *ibid.* **45**, 7229 (1992); **45**, 12 292 (1992).

[3] S. J. Miyake, Progr. Theor. Phys. **74**, 468 (1985); J. Phys. Soc. Jpn. **61**, 983 (1992).

[4] V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2905 (1987); T. Jolicoeur and J. C. Le Guillou, Phys. Rev. B **40**, 2727 (1989).

[5] R. P. Singh and D. A. Huse, Phys. Rev. Lett. **68**, 1766 (1992).

[6] K. Yang, L. K. Warman, and S. M. Girvin, Phys. Rev. Lett. **70**, 2641 (1993).

[7] P. Sindzingre, P. Lecheminant, and C. Lhuillier, Phys. Rev. B **50**, 3108 (1994).

[8] D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).

[9] H. Nishimori and H. Nakanishi, J. Phys. Soc. Jpn. **57**, 626 (1988); **58**, 2607 (1989); **58**, 3433 (1989).

[10] P. W. Leung and K. J. Runge, Phys. Rev. B **47**, 5861 (1993).

[11] B. Bernu, P. Lecheminant, C. Lhuillier, and L. Pierre, Phys. Rev. B **50**, 10 048 (1994).

[12] J. K. Cullum and R. A. Willoughby, *Lanczos Algorithms for Large Symmetric Eigenvalue Computations* (Birkauser, Boston, 1985).

[13] D. F. B. ten Haaf, H. J. M. van Bemmel, J. M. J. van Leeuwen, W. van Saarloos, and D. M. Ceperley, Phys. Rev. B **51**, 13 039 (1995).

[14] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980).

[15] P. J. Reynolds, D. M. Ceperley, B. J. Alder, and W. A. Lester, J. Chem. Phys. **77**, 5593 (1982); D. M. Ceperley and B. J. Alder, *ibid.* **81**, 5583 (1984).

[16] R. Panoff and J. Carlson, Phys. Rev. Lett. **62**, 1130 (1989).

[17] M. Boninsegni and E. Manousakis, Phys. Rev. B **46**, 560 (1992); M. Boninsegni, Phys. Lett. A **188**, 330 (1994).

[18] M. Boninsegni (unpublished).

[19] S. Miyashita, J. Phys. Soc. Jpn. **53**, 44 (1984).

[20] J. Villain, J. Phys. (Paris) **38**, 385 (1977).

[21] P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973); P. Fazekas and P. W. Anderson, Philos. Mag. **30**, 423 (1974).

[22] In a recent publication (Ref. 7), a resonating-valence-bond-type wave function was proposed, yielding very accurate variational results on small clusters (up to 48 sites), as well as some evi-

dence of antiferromagnetic long-range order; however, no extrapolation of the results to the thermodynamic limit was attempted.

[23] N. Metropolis and S. A. Ulam, J. Am. Stat. Assoc. **44**, 247 (1949).

[24] M. H. Kalos, Phys. Rev. **128**, 1791 (1962).

[25] See, for instance, M. H. Kalos, *Monte Carlo Methods in Quantum Problems*, Vol. 125 of NATO Advanced Study Institute Series C, edited by M. H. Kalos (Reidel, Dordrecht, 1982).

[26] L. Mitas, E. L. Shirley, and D. M. Ceperley, J. Chem. Phys. **95**, 3467 (1991).

[27] E. Manousakis, Phys. Rev. B **40**, 4904 (1989); Z. Liu and E. Manousakis, *ibid.* **40**, 11 437 (1989).

[28] G. Ortiz, D. M. Ceperley, and R. M. Martin, Phys. Rev. Lett. **71**, 2777 (1993).

[29] See, for instance, K. J. Runge and R. Runge, in *Quantum Simulations of Condensed Matter Phenomena*, edited by J. Doll and J. E. Gubernatis (World Scientific, Singapore, 1989).