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Green's-function Monte Carlo study of the t-J model

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We show how the Green's-function Monte Carlo method can be used to compute accurately the ground-state energy of the two-dimensional t-J model for lattices of large size. This is demonstrated for the case of a single hole, with the aid of suitable initial and guidance functions. Our transient estimates for the ground-state energy of the 4×4 lattice are in remarkable agreement with the exact values; we report results for lattices of significantly larger size than 4×4.

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Over the past few years, a considerable effort has been devoted to the study of the two-dimensional (2D) t-J model[1] with one or more holes, as it may capture the essential physics of the copper oxide superconductors. In the 2D t-J model the motion of holes is described by a simple nearest-neighbor hole-hopping term added to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (AFHM):

$$\hat{H} = -t \sum_{<ij>s} (\hat{a}^{\dagger}_{i,s}\hat{a}_{j,s} + \text{H.c.}) + J \sum_{<ij>} (\mathbf{s}_i \cdot \mathbf{s}_j - \tfrac{1}{4}\hat{n}_i\hat{n}_j) \ . \tag{1}$$

Here, $\hat{a}^{\dagger}_{i,s} = \hat{c}^{\dagger}_{i,s}(1 - \hat{n}_{i,-s})$, where $\hat{c}^{\dagger}_{i,s}$ creates an electron at lattice site i, with spin projection s in a given direction of the spin space, and $\hat{n}_i = \sum_s \hat{c}^{\dagger}_{i,s}\hat{c}_{i,s}$ is a number operator; $\hat{a}^{\dagger}_{i,s}$ creates an electron only on an empty site, thus avoiding double occupancy. We consider a square lattice of $N = L \times L$ sites with periodic boundary conditions. This Hamiltonian has been investigated with several analytical approaches, leading to important theoretical predictions.[2] Significant interest is directed toward numerical studies, not only to check the analytical results obtained with the different approximations, but also to gain quantitative information which may offer further insight. Exact diagonalization[3,4] has produced important results but is limited to lattices of small size (such as 4×4) by computer memory constraints; this renders the extrapolation to the infinite lattice problematic, due to the unavailability of calculations on lattices of significantly different sizes. Monte Carlo studies, which have relatively limited memory requirements and could therefore represent a viable alternative to extend the investigation to lattices of larger sizes, have so far proven ineffective because of the well-known "minus" sign problem, related to the fermionic character of the system.

The Green's-function Monte Carlo (GFMC) method[5] has been applied to several fermion problems including the Hubbard model,[6] using the so-called fixed-node approximation. In such an approach the "minus" sign problem is avoided by dividing the configuration space according to the sign of a simple Slater determinant. This is an approximation which assumes an *a priori* knowledge of the nodal surface of the ground-state wave function. The GFMC method has been successfully applied[7] to the no-hole case of the Hamiltonian (1), i.e., the spin-$\frac{1}{2}$ AFHM, where the "minus" sign difficulty can be removed by mapping the model onto a 2D Bose system. If mobile holes are present, as in the case of the t-J model, such transformation does not eliminate the "minus" sign complication. In this paper we show how the GFMC method, in conjunction with suitable trial and guidance functions, can be profitably used to accurately compute ground-state energy expectation values for the 2D t-J model on lattices of significantly larger sizes than the ones accessible to exact diagonalization. Despite the "minus" sign problem, our application of the GFMC method affords us to perform a transient estimation and obtain a significant improvement on the variational ground-state estimate yielded by our trial state. We carried out a GFMC calculation of the ground-state energy of a single hole, with the aid of a recently proposed variational ansatz,[8] used as a starting trial state. We report results for lattices of different sizes, up to 12×12. Our energy estimates for the 4×4 lattice coincide with the exact results, within statistical error bars, over the range $0 \leq t/J \leq 5$. We emphasize the importance of starting with a good variational state, in order to obtain as accurate as possible upper bounds on the exact ground-state energy. In addition, the GFMC method can be generally used to gauge the validity of a given variational ansatz.

Firstly, we briefly review the GFMC method and describe our Monte Carlo implementation. We wish to find the lowest eigenvalue E_0 of the Hamiltonian $\hat{H}$. The spectrum of $\hat{H}$ on a finite lattice is bounded; thus, we can use the projection operator $\hat{G} = E - \hat{H}$, with $E \geq E_{\max}$, $E_{\max}$ being the largest eigenvalue of $\hat{H}$. Starting from a suitable trial state $|\Psi_T>$ having nonzero overlap with the true ground state of $\hat{H}$, we form the succession of "mixed estimates" $E_0^{(n)}$, $n = 0, 1, 2, ...$, where

$$E_0^{(n)} = \frac{<\Psi_T|\hat{H}\,\hat{G}^n|\Psi_T>}{<\Psi_T|\hat{G}^n|\Psi_T>}. \tag{2}$$

On expanding $|\Psi_T>$ in eigenstates of $\hat{H}$ it can be eas-

ily shown that $E_0 \leq E_0^{(n+m)} \leq E_0^{(n)}$ for any n and m, and that $E_0^{(n)} \to E_0$ as $n \to \infty$. A Monte Carlo implementation of the above algorithm consists of a random walk performed by a set of $\mathcal{N}$ walkers through the configuration space; at each step n, the mixed estimate $E_0^{(n)}$ can be statistically evaluated. Let q stand for a given configuration of the system, specified by assigning the position of the holes and the value of the projection of the spin at all other lattice sites. Let $\Psi_G(q)$ be a real and positive "guidance" function, which contains some physical insight about the system under study and whose role is guiding the random walk toward the most favorable configurations (importance sampling), in order to reduce the statistical variance of the mixed estimates.[9] In order to assign each walker a starting point we create $\mathcal{N}$ configurations $\{q_1, q_2, ..., q_{\mathcal{N}}\}$ distributed according to $\Psi_G(q)|\Psi_T(q)|$. At the starting point each walker is assigned a phase factor $\phi_i = \Psi_T(q_i)/|\Psi_T(q_i)|$ and a weight $g_i = 1$. The action of the operator $\hat{G}$ on the state $|\Psi_T>$ is given the following stochastic interpretation: every walker is allowed to make a transition from the configuration q_i to the new configuration x_i with probability $w(q_i \to x_i) = \alpha(q_i)|G(q_i \to x_i)|[\Psi_G(x_i)/\Psi_G(q_i)]$, where $G(q_i \to x_i) =< x_i|\hat{G}|q_i >$ and $\alpha(q_i)$ is a normalization factor. This procedure will move each walker to a new point x_i in the configuration space and update its phase and weight as follows: the weight g_i is multiplied by $1/\alpha(q_i)$ and the phase ϕ_i is multiplied by the sign of $G(q_i \to x_i)$. It can be easily checked that a statistical estimate of $E_0^{(1)}$ is given by

$$E_0^{(1)} = \frac{\sum_i F(x_i)\ g_i\ \phi_i{}'\ E_L[\Psi_T(x_i)]}{\sum_i F(x_i)\ g_i\ \phi_i{}'}, \tag{3}$$

where $E_L[\Psi_T(x_i)] = [\hat{H}\Psi_T(x_i)/\Psi_T(x_i)]$ is the local energy and $F(x_i) = \Psi_T^*(x_i)/\Psi_G(x_i)$. By allowing for another transition of every walker and by updating again phases and weights, we can compute $E_0^{(2)}$, in the same way we computed $E_0^{(1)}$ [Eq. (3)], and so on. In order not to decrease the efficiency of the algorithm by carrying along walkers with negligible weight, a procedure called branching is usually implemented, which consists of making several copies of those walkers which have accumulated a relatively large weight and deleting those with small weight, in such a way that the size of the population (i.e., the total number of walkers) is kept roughly constant.

The algorithm should be iterated to reach convergence, defined such that, for sufficiently large M, $E_0^{(M)} = E_0^{(M+1)} = \cdots = E_0^{(M+m)} = \cdots$ within statistical variance. However, when dealing with problems with fermionic character such as ours, the variance of $E_0^{(M)}$ increases exponentially with M. Thus, the computer time required to obtain the desired error bar on $E_0^{(M)}$ also increases exponentially with M. This is known as the "minus" sign problem,[9] which clearly makes it very difficult to compute $E_0^{(M)}$ for sufficiently large M until convergence is achieved. Therefore, an accurate initial trial state $|\Psi_T>$ is crucial in order to obtain a value of $E_0^{(M)}$ as close as possible to the exact ground-state energy with a relatively small number of iterations (each value of $E_0^{(n)}$ is strictly a ground-state energy upper bound, within statistical error bars). This approach is commonly referred to as a transient estimation. As we show below, the GFMC technique combined with the use of a variational ansatz which we devised for the problem of a hole in the t-J model permits to obtain very accurate ground-state energy estimates.

Next, we recall the variational ansatz we recently proposed[8] for a single quasihole excitation in the 2D t-J model, which we use in this work as starting trial state for our GFMC calculation. This ansatz can be expressed as follows:

$$|\Psi_T(\mathbf{k})> = \sum_c (-1)^{L(c)} \hat{F}(\mathbf{k})\ \exp\left(-\frac{1}{2}\sum_{i<j} u_{ij}\hat{s}_i^z\hat{s}_j^z\right)\ \hat{a}_{\mathbf{k}s}|c>, \tag{4}$$

where $|c>$ is a lattice spin configuration, specified by assigning the value of the projection of the spin in a given z direction of the spin space for each lattice site; the sum is restricted to lattice spin configurations with a value of the z component of the total spin, $S^z = 0$ and $L(c)$ is equal to the number of "down" spins in one of the two sublattices; $\hat{a}_{\mathbf{k},s} = 1/\sqrt{N}\sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}}\ \hat{a}_{\mathbf{R},s}$, where the sum runs over all lattice sites; the function u_{ij} is a spin-spin correlation function which depends on the distance between the two sites i and j. Finally,

$$\hat{F}(\mathbf{k}) = \left(1 + \sum_{\mathbf{a}} f_{\mathbf{a}}(\mathbf{k})\hat{\mathcal{P}}_{\mathbf{a}} + \sum_{\mathbf{a},\mathbf{a}'} f_{\mathbf{a}\mathbf{a}'}(\mathbf{k})\hat{\mathcal{P}}_{\mathbf{a}'}\hat{\mathcal{P}}_{\mathbf{a}}\right),$$

with $\mathbf{a} = \pm\hat{\mathbf{x}}, \pm\hat{\mathbf{y}}$ connecting two nearest-neighboring sites and $\hat{\mathcal{P}}_{\mathbf{a}} = \sum_{\mathbf{R},\sigma} \hat{a}^\dagger_{\mathbf{R},\sigma}\hat{a}_{\mathbf{R}+\mathbf{a},\sigma}$. $\hat{F}(\mathbf{k})$ is a spin-hole correlation operator. The variational parameters $f_{\mathbf{a}}(\mathbf{k})$, $f_{\mathbf{a}\mathbf{a}'}(\mathbf{k})$ have been determined in Ref. 8. The variational state (4) gives fairly good single-hole energy estimates in the range $0 \leq t/J \leq 5$ at $\mathbf{k} = (\pi/2, \pi/2)$.[8]

In our GFMC calculation we restricted ourselves to configurations with $s = -\frac{1}{2}$ and $\mathbf{k} = (\pi/2, \pi/2)$, i.e., the wave vector at which the hole band attains its minimum according to several calculations. We used the function $\Psi_G = \exp\left(-\frac{1}{2}\sum_{i<j} u_{ij}s_i^z s_j^z\right)$ as guidance function. The hole energy δE is computed by subtracting the ground-state energy of the no-hole case (spin-$\frac{1}{2}$ AFHM) from the total energy of the single-hole case. The ground-state energy for the no-hole case was also computed via GFMC, and our results for this case (which presents no sign problem) are in agreement with the ones given in Ref. 7. In Fig. 1 we show typical transient estimation results, for $t = 5J$ on a 4×4 lattice. The dashed line indicates the exact ground-state energy, from Ref. 4. To demonstrate the importance of the initial state we compare the results obtained using the following two different trial states, with the same population size: (a) the state Ψ^I (results are shown by squares in Fig. 1), given by Eq. (4) with

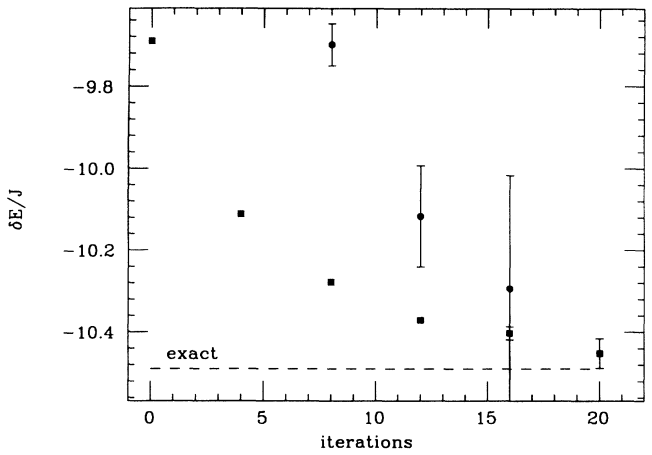

FIG. 1. Transient estimation of the hole energy for $t/J = 5$ on a 4×4 lattice, obtained with the states Ψ^I (squares) and Ψ^{II} (circles) as starting trial states. The dashed line refers to the exact diagonalization result. The hole state has wave vector $\mathbf{k} = (\pi/2, \pi/2)$.

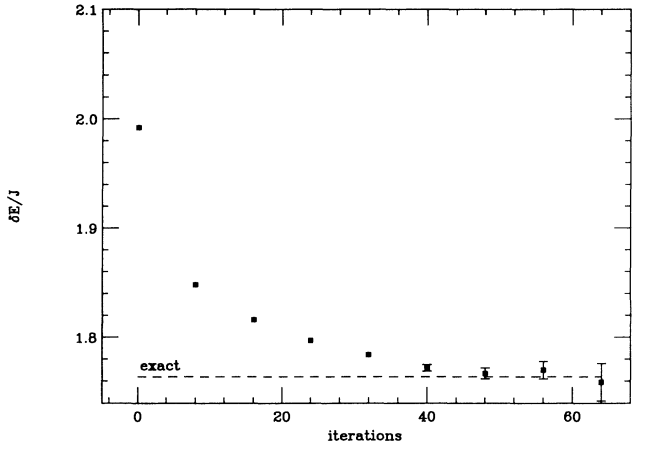

FIG. 2. Transient estimation of the hole energy for $t/J = 0.5$ on a 4×4 lattice. The hole state has wave vector $\mathbf{k} = (\pi/2, \pi/2)$. The dashed line refers to the exact diagonalization result.

the optimal variational parameters and (b) the state Ψ^{II} (results are shown by circles in Fig. 1), also given by Eq. (4) but with $f_{\mathbf{a}}(\mathbf{k})$, $f_{\mathbf{aa}'}(\mathbf{k}) = 0$, which corresponds to a state with no spin-hole correlations (both states retain spin-spin correlations). The exact ground-state energy is $-10.49J$, the variational energy estimate given by the trial state Ψ^I is $-9.691J$, the one given by the state Ψ^{II} is $2.565J$, i.e., Ψ^{II} is a poorer trial state. Ψ^I yields, for the same number of iterations, a much better ground-state energy estimate, although the algorithm permits us to obtain in both cases a remarkable improvement on the variational ground-state energy estimate (zeroth iteration); in addition, the size of the error bars is much smaller when the state Ψ^I is used. More quantitatively we can compare the error bar we obtained after 16 iterations in the two cases: we found $0.016J$ for Ψ^I and $0.124J$ for Ψ^{II}, which means that in order to obtain a comparable error bar when using the state Ψ^{II} we would roughly need 80 times as many walkers (and the energy estimate would still be worse than with Ψ^I); on the other hand, the computer time gain due to the simpler form of Ψ^{II} is only a factor of 6 or 7.

In Table I we report results for the hole energy δE, computed by transient estimation on lattices of sizes 4×4, 8×8, and 12×12, using the state (4) as trial state; we also indicate the number of iterations needed to reach convergence. In this work we assumed convergence to be achieved when the value of the mixed estimate does not change for at least five iterations, within statistical error bars. At low values of t/J evidence of convergence can be shown over a larger interval, as in the cases shown in Figs. 2 and 3, which refer to calculations on a 4×4 and on an 8×8 lattice, at $t/J = 0.5$. At larger values of t/J, however, the statistical variance rapidly increases with the number of iterations; a substantially larger amount of CPU time is therefore needed to obtain the same evidence of convergence we found at low values of t/J.

On comparing the GFMC results for the 4×4 lattice with exact diagonalization results (from Ref. 4, second column of Table I) we find excellent agreement in the entire range $0 \leq t/J \leq 5$. The results for lattices of size $L > 4$ can give an indication of the finite-size effects affecting the calculation on lattices of small size.

As the lattice size is increased, the difference between the variational estimate of the total energy of the single-hole case, given by the trial state (4), and the exact single-hole ground-state total energy increases as NJ, due to the approximate way in which the state (4) accounts for the background antiferromagnetic energy, i.e., the dominant contribution to the total energy for large N. Therefore, a larger number of iterations is necessary to achieve convergence on a lattice of larger size, for the same value of t/J, with a consequent rapid increase in the computer time required.

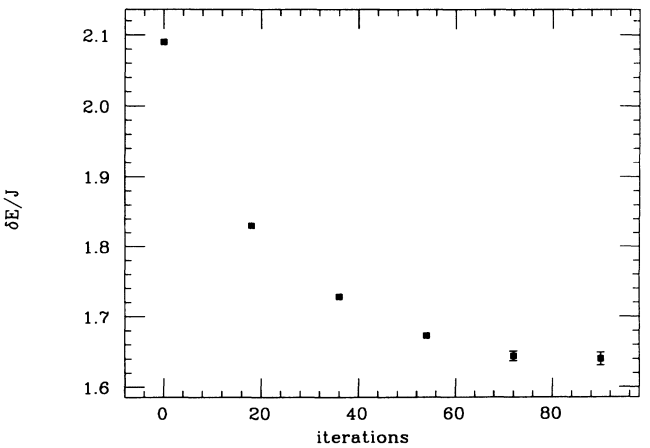

FIG. 3. Transient estimation of the hole energy for $t/J = 0.5$ on an 8×8 lattice. The hole state has wave vector $\mathbf{k} = (\pi/2, \pi/2)$.

TABLE I. Hole energy at various values of t/J, computed by GFMC on lattices of different sizes. The hole state has wave vector $\mathbf{k} = (\pi/2, \pi/2)$. For the 4×4 lattice exact diagonalization results are given for comparison. Results are expressed in units of J. For each lattice, the number on the left indicates the iterations required to obtain the GFMC estimate on the right. Statistical errors (in parentheses) are on the last two digits.

t/J	4×4 (exact)	4×4		8×8		12×12	
0.20	2.235	48	2.241(05)	150	2.129(07)	300	2.125(15)
0.50	1.765	48	1.767(05)	90	1.640(09)	200	1.599(22)
1.00	0.655	34	0.662(10)	96	0.417(16)	200	0.419(33)
2.50	−3.305	26	−3.288(18)	80	−3.678(32)	160	−3.676(42)
5.00	−10.49	20	−10.456(36)	24	−10.783(12)	72	−10.838(56)

In conclusion, the combination of variational and Green's-function Monte Carlo methods can be an effective way to extend the numerical investigation on the t-J model to systems of significantly larger sizes than the ones accessible to exact diagonalization, as our results for the ground-state energy of a single hole show. Our interest is now toward investigating the pairing between holes within the 2D t-J model, with the approach outlined in this paper.

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