Two-hole d-wave binding in the physical region of the t-J model: A Green's-function Monte Carlo study

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We investigate numerically the ground state of two holes with $d_{x^2-y^2}$ symmetry in the two-dimensional t-J model, on lattices of significantly larger sizes than the ones studied so far. The Green's-function Monte Carlo method, in conjunction with suitable initial states and guidance functions, is used to estimate the ground-state energy of one and two holes, as well as to compute the two-hole distribution function. Our results show a significant decrease of the two-hole binding energy as the size of the lattice is increased from 4×4. A critical value $J_c\sim0.27t$ is found such that d-wave hole binding no longer occurs for $J<J_c$.

I. INTRODUCTION

The problem of two mobile holes in the two-dimensional (2D) t-J model[1] has elicited significant attention for its possible relevance to superconductivity in the cuprous oxides. The 2D t-J model attempts to describe mobile holes in a 2D quantum antiferromagnet by adding a simple nearest-neighbor hole-hopping term to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (AFHM):

$$\hat{H}=-t\sum_{\langle ij\rangle s}(\hat{a}_{is}^{\dagger}\hat{a}_{js}+\text{H.c.})+J\sum_{\langle ij\rangle}(\mathbf{s}_i\cdot\mathbf{s}_j-\tfrac{1}{4}\hat{n}_i\hat{n}_j)\ , \qquad (1)$$

where $\hat{a}_{is}^{\dagger}=\hat{c}_{is}^{\dagger}(1-\hat{n}_{i-s})$, $\hat{c}_{is}^{\dagger}$ being the creation operator for an electron with spin projection s at lattice site i, and where $\hat{n}_i=\sum_s\hat{c}_{is}^{\dagger}\hat{c}_{is}$ is a number operator; $\hat{a}_{is}^{\dagger}$ creates an electron only on an empty site, thus avoiding double occupancy. $\mathbf{s}_i$ is the spin operator associated with site i and is defined as $\mathbf{s}_i=\frac{1}{2}\sum_{\alpha\beta}\hat{c}_{i\alpha}^{\dagger}\boldsymbol{\sigma}_{\alpha\beta}\hat{c}_{i\beta}$, where $\boldsymbol{\sigma}$ is a vector of Pauli matrices. We consider a square lattice of $N=L\times L$ sites with periodic boundary conditions. Several analytical approaches have been employed to study the Hamiltonian (1), leading to important theoretical predictions mainly regarding the physics of a single hole.[2] Hole pairing has been investigated mostly numerically, both in the t-J model[3-4] and in the related strong-coupling limit of the Hubbard model,[5] by means of exact diagonalization on lattices of small size, such as 4×4. These studies have yielded some indications that the formation of a bound state of two holes may be energetically favorable within certain ranges of the parameters of the models. However, there are reasons to suspect that the relatively small size of the lattices studied may not afford a reliable prediction of the physics of the infinite system. Therefore the numerical investigation must be extended to lattices of significantly larger sizes than the ones accessible to exact diagonalization, which is limited by computer memory constraints. Monte Carlo techniques, with their relatively modest memory requirements, are a valid computational alternative; in particular, the Green's-function Monte Carlo (GFMC) method[6] has been successfully used to compute ground-state expectation values for the no-hole case of the Hamiltonian (1), i.e., the spin-$\frac{1}{2}$ AFHM.[7] This method consists of projecting out the ground state of a given Hamiltonian from a starting trial state by acting iteratively with a suitable projection operator. Its application to the t-J model in the case of mobile holes is complicated by the presence of the well-known "minus" sign problem, which affects Monte Carlo simulations of systems with fermionic character.[6] Because of increasingly larger statistical fluctuations, it is usually impossible to iterate the algorithm until convergence to the ground state is observed.

However, as we have recently shown for the case of a single hole,[8] such complications can be overcome if a sufficiently accurate initial trial state and a suitable guidance function are used. In that case, convergence to the ground state can be actually observed before the statistical fluctuations become too large and accurate ground-state estimates can be obtained by performing a transient estimation.

In this paper we extend our implementation of the GFMC method to carry out a numerical study of the ground state of two mobile holes in the Hamiltonian (1) on lattices of significantly larger sizes than the ones studied so far. We investigate the binding of two holes as a function of the parameter J/t of the model by computing the ground-state two-hole binding energy $\Delta=\delta E_2-2\delta E_1$, where $\delta E_M=E_M-E_0$, E_M being the ground-state energy of the Hamiltonian (1) with M holes. We gain further insight into the occurrence of binding by studying the ground-state two-hole distribution function.

Let us begin by reviewing what is known about the physics of the 2D t-J Hamiltonian in the presence of two holes. In the large-J/t limit, two holes in the ground state will reside on nearest-neighboring sites, as this configuration features the least number of broken antiferromagnetic bonds; this was observed in the static ($t=0$) limit by exact diagonalization on a 4×4 lattice.[9] As a result of the same mechanism, if more than two holes are present, they will aggregate in a single cluster (phase separation). Monte Carlo simulations for two and four holes in the static limit[10] and for relatively large values of J/t ($J/t>5$) (Ref. 11) have confirmed these intuitive predic-

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tions. It should be noted that in this limit the "sign" problem is not too important (it actually disappears at $t=0$). In the opposite limit ($J/t<1$), the higher hole mobility renders the situation much less clear; this limit is considered physically more realistic. It is argued by some authors[12] that phase separation will take place at *any* value of J/t; on the other hand, numerical results obtained by means of high-temperature expansion[13] and exact diagonalization[14] show evidence of hole binding and no phase separation at $J/t \leq 1$.

The results that we present in this paper for the ground state of two holes in the t-J model indicate that the magnitude of the two-hole binding energy Δ on an infinite lattice is considerably reduced from its value on a 4×4 lattice; for instance, at $J/t=0.4$, which is a value in the physical regime of the t-J model, we estimate Δ to be $\sim 0.1t$ in magnitude on an infinite lattice, as opposed to the value of $0.349t$ found on a 4×4 lattice. We find that the finite-size effects on Δ are mainly due to the single-hole energy δE_1, which shows a more pronounced dependence on the size of the lattice than the two-hole energy δE_2. Results for the two-hole distribution $C(r)$ give further indications of a weakened binding of the holes at $J/t<1$ as the lattice size is increased. Our results also indicate that a critical value J_c of the parameter J exists such that hole binding only takes place for $J \geq J_c$; we find $J_c \sim 0.27$ (with $t=1$).

In the next section, we will briefly sketch the implementation of the GFMC method used in this paper (for a more detailed description, see Ref. 8); in Sec. III we will introduce the two-hole variational state which we use as the initial state in our GFMC simulation, whereas Sec. IV will be devoted to the discussion of our results.

II. THE METHOD

The GFMC method permits the calculation of the ground-state expectation value $\mathcal{O}$ of an observable $\hat{\mathcal{O}}$ as the limit of the sequence

$$\mathcal{O}^{(n)}=\frac{\langle \Psi_T|\hat{G}^n\hat{\mathcal{O}}\hat{G}^n|\Psi_T\rangle}{\langle \Psi_T|\hat{G}^{2n}|\Psi_T\rangle}, \tag{2}$$

as $n\to\infty$. Here $|\Psi_T\rangle$ is an initial state not orthogonal to the ground state $|\Psi_0\rangle$ and $\hat{G}$ is a suitable projection operator, whose role is enhancing the component of $|\Psi_T\rangle$ along $|\Psi_0\rangle$. If the spectrum of the Hamiltonian $\hat{H}$ of the system is bounded, as is the case of (1) on a finite lattice, a convenient choice for $\hat{G}$ is $\hat{G}=E-\hat{H}$ with $E\geq E_{\max}$, the largest eigenvalue of $\hat{H}$.[8] For the case of two holes in the t-J model, it is $E_{\max}=8t$, which corresponds to the maximum kinetic energy of two free holes in a ferromagnetic background.

A Monte Carlo implementation of this scheme consists of evaluating (2) as an average over the random walks of $\mathcal{N}$ independent "walkers" through configuration space. The walkers are initially assigned $\mathcal{N}$ starting points, corresponding to the $\mathcal{N}$ configurations $|c_1\rangle, |c_2\rangle, \ldots, |c_{\mathcal{N}}\rangle$ of the system. These configurations are stochastically drawn from the probability distribution $|\Psi_T(c)|\Psi_G(c)$, where $\Psi_T(c)$ is the wave function of the trial state $|\Psi_T\rangle$ and $\Psi_G(c)$ is a positive-definite "guidance" function, based upon some physical insight on the system and whose role is to guide the random walk toward the most important configurations.

The random walk of each walker consists of a succession of transitions to new configurations; a transition from a given configuration $|x\rangle$ to a new configuration $|x'\rangle$ is stochastically sampled from a probability distribution $w(x\to x')$ proportional to $|\langle x'|\hat{G}|x\rangle|\Psi_G(x')/\Psi_G(x)$. In order to obtain a statistical estimate of the quantity $\mathcal{O}^{(n)}$, each walker must be allowed to perform $2n$ transitions, since every transition corresponds to one operation of $\hat{G}$.

The quantity $\mathcal{O}^{(n)}$ must be computed for increasingly larger n until convergence is observed, within statistical error bars. In this paper we calculate the ground-state energy of a quantum antiferromagnet with mobile holes by following the same procedure explained in Ref. 8 for the single-hole calculation; we use a correlated two-hole variational state as the initial state $|\Psi_T\rangle$. We also compute the ground-state two-hole distribution function by means of a scheme known as "forward walking" (see Ref. 6). The difficulty, in the case of the t-J model and other fermionic problems, arises from the matrix elements $\langle x'|\hat{G}|x\rangle$ not being always positive. This results in what is known as the "minus" sign problem, i.e., in large statistical fluctuations of the quantity $\mathcal{O}^{(n)}$ as n increases, which clearly make it very difficult to perform a large number of iterations because of the increasing statistical uncertainty affecting the estimates. Therefore it is very important for the success of the method to have a sufficiently accurate initial state so that convergence to the ground state can be achieved within a relatively small number n of iterations, before the statistical fluctuations grow exceedingly. The algorithm can be also significantly enhanced by the use of a suitable guidance function, which by directing the random walk toward the most important configurations can prevent the statistical variance of the estimates from growing too rapidly, thereby improving the change of observing convergence.

III. TRIAL STATE FOR TWO HOLES

Our GFMC calculation for two holes is based upon an initial state which is a generalization of the "string"-based variational state used in Ref. 8 in the GFMC calculation for a single hole. Let us therefore recall the single-hole variational ansatz first (see also Ref. 17):

$$|\Psi_T(\mathbf{k})\rangle=\sum_{\mathbf{R}c} e^{-i\mathbf{k}\cdot\mathbf{R}}\hat{F}(\mathbf{k})\exp\left[-\frac{1}{2}\sum_{i<j}u_{ij}\hat{s}_i^z\hat{s}_j^z\right]\hat{a}_{\mathbf{R}s}|c\rangle\ , \tag{3}$$

where $\mathbf{k}$ is the hole momentum and where the sum runs over lattice sites $\mathbf{R}$ and over all lattice spin configurations $\{|c\rangle\}$, specified by assigning the value of the spin projection s^z at all lattice sites; the sum in (3) is restricted to configurations $|c\rangle$ with a value of the z component of the total spin $S^z=0$. The operator $\exp(-\frac{1}{2}\sum_{i<j}u_{ij}\hat{s}_i^z\hat{s}_j^z)$ is a background antiferromagnetic spin-spin correlation operator, and the function u_{ij} depends on the distance between the two sites i and j. Finally,

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

with $\mathbf{a}=\pm\hat{\mathbf{x}},\pm\hat{\mathbf{y}}$ connecting two nearest-neighboring sites and $\hat{\mathcal{P}}_{\mathbf{a}}=\sum_{\mathbf{R}s}\hat{a}^{\dagger}_{\mathbf{R}s}\hat{a}_{\mathbf{R}+\mathbf{a}s}$. $\hat{F}(\mathbf{k})$ is a spin-hole correlation operator; $f_{\mathbf{a}}(\mathbf{k})$ and $f_{\mathbf{aa}'}(\mathbf{k})$ are variational parameters. This ansatz describe "strings" of spins displaced by one site along the path. In order to generalize the state (3) to the case of two holes, consider first a general, translationally invariant state of two holes with opposite spin projections in an antiferromagnetic spin background:

$$|\Psi_0(\mathbf{Q})\rangle=\sum_{c}\sum_{\mathbf{R},\mathbf{r}} e^{-i\mathbf{Q}\cdot(\mathbf{R}+\mathbf{r}/2)}\exp\left[-\tfrac{1}{2}\sum_{i<j} u_{ij}\hat{s}^z_i\hat{s}^z_j\right]\times g(\mathbf{r})a_{\mathbf{R}\uparrow}a_{\mathbf{R}+\mathbf{r}\downarrow}|c\rangle , \quad (4)$$

where $\mathbf{Q}$ is the total momentum of the state and $\mathbf{r}$ is the relative distance of the two holes. Analogously to the single-hole case, we introduce the "string" correlation operator

$$\hat{F}(\mathbf{Q},\mathbf{r})=1+\sum_{\mathbf{a}} f_{\mathbf{a}}(\mathbf{Q},\mathbf{r})\hat{\mathcal{P}}_{\mathbf{a}}+\sum_{\mathbf{aa}'} f_{\mathbf{aa}'}(\mathbf{Q},\mathbf{r})\hat{\mathcal{P}}_{\mathbf{a}'}\hat{\mathcal{P}}_{\mathbf{a}} , \quad (5)$$

where $f_{\mathbf{a}}(\mathbf{Q},\mathbf{r})$ and $f_{\mathbf{aa}'}(\mathbf{Q},\mathbf{r})$ are variational parameters. By acting on the state (4) with $\hat{F}(\mathbf{Q},\mathbf{r})$, we obtain our variational state for two holes:

$$|\Psi_T(\mathbf{Q})\rangle=\sum_{c}\sum_{\mathbf{R},\mathbf{r}} e^{-i\mathbf{Q}\cdot(\mathbf{R}+\mathbf{r}/2)}\hat{F}(\mathbf{Q},\mathbf{r})\times\exp\left[-\frac{1}{2}\sum_{i<j} u_{ij}\hat{s}^z_i\hat{s}^z_j\right]\times g(\mathbf{r})a_{\mathbf{R}\uparrow}a_{\mathbf{R}+\mathbf{r}\downarrow}|c\rangle . \quad (6)$$

The expectation value of the energy is minimized by taking $g(\mathbf{r})$ to be nonzero for nearest-neighbor distances only and with d-wave spatial symmetry, i.e., $g(\pm\hat{\mathbf{x}})=-g(\pm\hat{\mathbf{y}})$, corresponding to a singlet state of the two holes. With this choice of g, the variational parameters $f_{\mathbf{a}}(\mathbf{Q},\mathbf{r})$ and $f_{\mathbf{aa}'}(\mathbf{Q},\mathbf{r})$ can be computed approximately analytically by minimizing the energy expectation value with $u=0$. In our calculation we allowed for strings of length 1 only; i.e., we set $f_{\mathbf{aa}'}(\mathbf{Q},\mathbf{r})=0$. We found that allowing for strings of length 2 can improve the initial variational energy estimate, but has little effect on the convergence to the ground state; namely, the ground-state estimates are the same, within statistical error bars, with the ones obtained by including strings of length 1 only. We restricted our calculation to a state with $\mathbf{Q}=(0,0)$; in this case, it is $f_{\mathbf{a}}(\mathbf{Q},\mathbf{r})=f_0$, with f_0 real. This choice of variational state is consistent with exact diagonalization results according to which the lowest-energy state of two holes is a d-wave singlet with momentum $\mathbf{Q}=(0,0)$, although degeneracies exist which are attributed to peculiar geometrical properties of the lattice studied.[3]

As we did in the single-hole calculation, we used the function

$$\Psi_G=\exp\left[-\frac{1}{2}\sum_{i<j} u_{ij}s^z_i s^z_j\right] \quad (7)$$

as a guidance function. We compute the two-hole energy $\delta E_2=E_2=E_0$ by performing a transient estimation of the ground-state energy of (1) with two holes, E_2, from which we subtract the value of the ground-state energy E_0 of the no-hole case (corresponding to the spin-$\frac{1}{2}$ AFHM), also calculated by the GFMC method; note that in the no-hole case no "minus" sign problem arises, so that E_0 can be estimated rather straightforwardly and with remarkable accuracy (see Ref. 7).

IV. RESULTS AND DISCUSSION

Let $E_M^{(n)}$ be the estimate of the ground-state energy of (1) with M holes obtained at the nth GFMC iteration, and let E_M be the extrapolated value in the limit $n\to\infty$. In Fig. 1 the estimates $\delta E_2^{(n)}=E_2^{(n)}-E_0$ at different n, on a 4×4 lattice (open circles), are compared to the exact diagonalization results (dashed line) for $J/t=1$. At this relatively large value of J/t, it is possible to obtain sufficient evidence of convergence; upon averaging the data from the last three iterations shown, we estimate δE_2 on a 4×4 lattice to be $\delta E_2/t=0.43\pm0.01$, in agreement with the exact value of 0.42, which corresponds to the dashed line in Fig. 1. In Fig. 2 we show analogous results for δE_2 on an 8×8 lattice; convergence to the ground state can be observed, and if we average the values of the last two iterations we obtain $\delta E_2/t=0.27\pm0.02$. The dotted lines in Figs. 1 and 2 correspond to a fit of the data with the expression

$$E_2^{(n)}\approx E_2^{\infty}+\beta\exp(-\kappa n) , \quad (8)$$

using E_2^{∞}, β, and κ as fitting parameters. We find that E_2^{∞}, i.e., the extrapolated estimate of E_2, is the best determined of the three parameters. The extrapolated values for δE_2 for the two lattices are the same as the ones given above, within statistical error bars.

As we shall see below, our results indicate that the two-hole energy estimates at $J/t=0.4$ do not change significantly beyond 8×8; we expect this to be true at $J/t=1$ as well, since the holes are less mobile in this case and therefore finite-size effects will be even smaller than at $J/t=0.4$. Thus we did not devote our computational

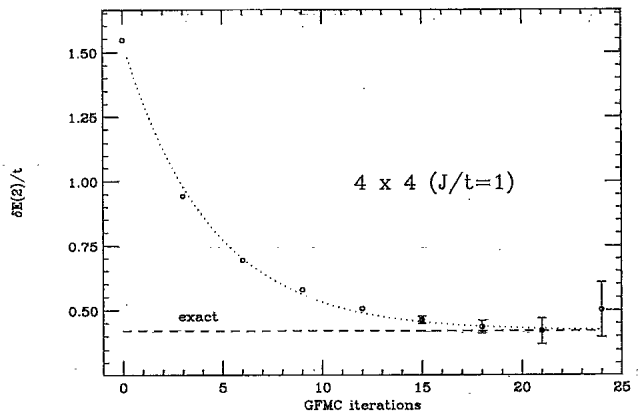

FIG. 1. Transient estimation of the two-hole ground-state energy δE_2 on 4×4 lattice at $J/t=1$. The dashed line refers to the exact value for the 4×4 lattice. The open circles refer to the estimates $\delta E_2^{(n)}=E_2^{(n)}-E_0$. The dotted lines have been obtained by fitting the data for $E_2^{(n)}$ with the expression $E_2^{\infty}+\beta\exp(-\kappa n)$.

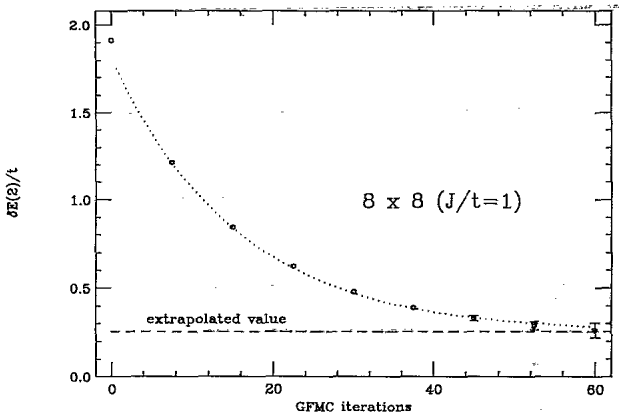

FIG. 2. Transient estimation of the two-hole ground-state energy δE_2 on an 8×8 lattice at $J/t=1$. The dashed line refers to the extrapolated value for the 8×8 lattice. The open circles refer to the estimates $\delta E_2^{(n)}=E_2^{(n)}-E_0$. The dotted lines have been obtained by fitting the data for $E_2^{(n)}$ with the expression $E_2^{\infty}+\beta\exp(-\kappa n)$.

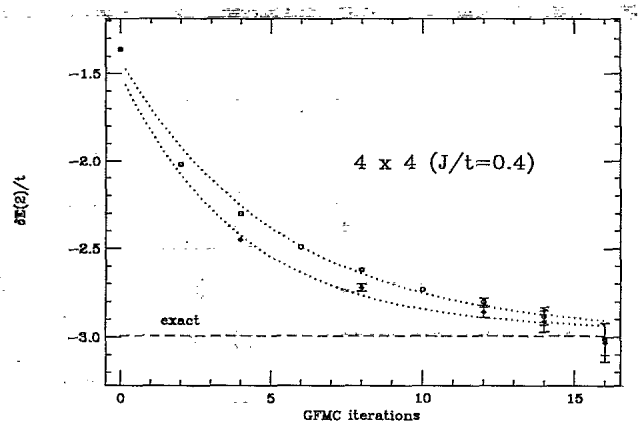

FIG. 3. Transient estimation of the two-hole ground-state energy δE_2 on a 4×4 lattice at $J/t=0.4$. The dashed line refers to the exact diagonalization result for the 4×4 lattice. The open circles refer to the estimates $\delta E_2^{(n)}$, and diamonds refer to the improved estimates $\delta\mathcal{E}^{(n)}$. The dotted lines have been obtained by fitting the data for $E_2^{(n)}$ and $\mathcal{E}^{(n)}$ with the expression $E_2^{\infty}+\beta\exp(-\kappa n)$.

resources to study lattices larger than 8×8 at $J/t=1$.

Because we are ultimately interested in a bound state of two holes, we consider the binding energy $\Delta=\delta E_2-2\delta E_1$, where $\delta E_1=E_1-E_0$ is the single-hole ground-state energy. We compute δE_1 in the same way as δE_2; we use the single-hole trial state (3) with momentum $\mathbf{k}=(\pi/2,\pi/2)$ (where the single-hole energy band attains its minimum) as the initial state; we allow for strings of length 1 and find values of δE_1 in agreement with the ones reported in Ref. 8. By using the estimates obtained above for δE_2, we obtain $\Delta/t=-0.90\pm0.03$ for the 4×4 lattice, in agreement with the exact value, and $\Delta/t=-0.59\pm0.03$ for the 8×8 lattice. Since we know that the single-hole energy estimates remain unchanged[8] beyond 8×8 in the range $0.2\le J/t\le5$, we conclude that the value of Δ/t found on an 8×8 lattice should be sufficiently close to the value in the infinite lattice limit and that binding occurs in this limit at $J/t=1$, with a binding energy of about $-0.6t$. A further indication of binding as well as of the limited finite-size effects affecting the calculation at this value of J/t comes from the very similar values found for the rms hole separation on the two lattices, namely, $R_{\rm rms}=1.40\pm0.02$ (in agreement with the exact result[4]) on a 4×4 lattice and $R_{\rm rms}=1.47\pm0.03$ on an 8×8 lattice, the lattice constant being set equal to 1.

We now turn to a more interesting and physically more relevant case, i.e., $J/t=0.4$. In Fig. 3 we show transient estimation results for δE_2 on a 4×4 lattice. The tendency of the succession of energy estimates to approach the exact value is clear, and if we average the values from the last two iterations, we obtain $\delta E_2/t=-2.94\pm0.03$, in good agreement with the exact value of -2.993. However, the rapid increasing of the error bar renders it much more difficult than in the single-hole case to determine the convergence value precisely. The problem is present on larger lattices as well, as shown in Fig. 4 for δE_2 (open circles) on an 8×8 lattice. The worsening of the sign problem passing from one to two holes is expected, particularly at $J/t<1$, as a larger hole concentration results in an increased rate of sign-changing transitions in the random walk; such transitions are responsible for the statistical fluctuations. Since the amount of information produced decreases dramatically with the number of iterations n, it is important to extract the maximum amount of information from the data generated at "early time," that is, at small n, when the size of the error bars is not too large.

A simple scheme[15] which effectively permits the acceleration of the convergence to the ground state with no additional computational cost consists of considering the expectation values

$$\mathcal{E}^{(n)}=\frac{\langle\chi_n|\hat{H}|\chi_n\rangle}{\langle\chi|\chi_n\rangle}, \tag{9}$$

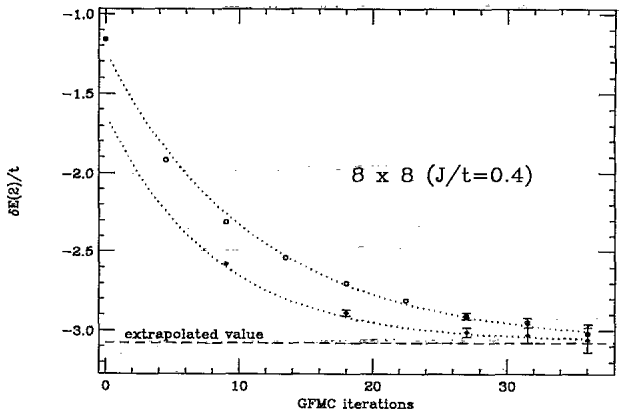

FIG. 4. Transient estimation of the two-hole ground-state energy δE_2 on an 8×8 lattice at $J/t=0.4$. The dashed line refers to the extrapolated value for the 8×8 lattice. The open circles refer to the estimates $\delta E_2^{(n)}$, and diamonds refer to the improved estimates $\delta\mathcal{E}^{(n)}$. The dotted lines have been obtained by fitting the data for $E_2^{(n)}$ and $\mathcal{E}^{(n)}$ with the expression $E_2^{\infty}+\beta\exp(-\kappa n)$.

where

$$|\chi_n\rangle=(1+\lambda_n\hat{G}^n)|\Psi_T\rangle\ , \tag{10}$$

λ_n being a variational parameter determined by minimizing the value of $\mathcal{E}^{(n)}$. $\mathcal{E}^{(n)}$ yields a better ground-state estimate than

$$E_2^{(n)}=\langle\Psi_T|\hat{G}^n\hat{H}\hat{G}^n|\Psi_T\rangle/\langle\Psi_T|\hat{G}^{2n}|\Psi_T\rangle\ ,$$

owing to the greater variational freedom of the state $|\chi_n\rangle$ compared to $\hat{G}^n|\Psi_T\rangle$. This Lanczos-type procedure can be applied to expectation values other than the energy, although the parameter λ_n has to be determined by minimizing the energy expectation value.

The improvement is particularly important at small n, when the difference between successive values of $E_2^{(n)}$ is larger; this is shown in Figs. 3 and 4, where we compare the values of $\delta\mathcal{E}^{(n)}=\mathcal{E}^{(n)}-E_0$ and $\delta E_2^{(n)}=E_2^{(n)}-E_0$ (circles). We can obtain extrapolated estimates for δE_2 by fitting the values for $E_2^{(n)}$ and $\mathcal{E}^{(n)}$ with the expression (8). The fits of the two sets of data yield the same extrapolated estimates, within statistical error bars. By using the single-hole energy values, we estimate the magnitude of the binding energy of the two-hole bound state in the infinite lattice to be greatly reduced from its value on a 4×4 lattice.

To illustrate this point more clearly, we plot in Fig. 5 the estimates of Δ/t obtained as the difference $\delta E_2^{(n)}-2\delta E_1^{(n)}$, at $J/t=0.4$ on an 8×8 lattice; the dotted line is obtained from the fitting curves for both $E_2^{(n)}$ and $E_1^{(n)}$. The solid line represents the exact value of the binding energy for a 4×4 lattice. Despite the size of the error bars, the results shown in Fig. 5 indicate rather clearly that the magnitude of the binding energy is considerably reduced, namely, from a value of $0.349t$ on a 4×4 lattice to about $0.1t$ on an 8×8 lattice.

Our results for the two-hole energy δE_2 at $J/t=0.4$ indicate that δE_2 does not change significantly in the infinite lattice from its value on the 8×8 lattice; thus, because the single-hole energy also remains unchanged beyond 8×8,[8] we estimate the binding energy Δ to be $(-0.12\pm0.04)t$ in the infinite lattice. The extrapolated estimates for δE_2, δE_1, and Δ for different values of J/t and on the various lattices studied are reported in Table I.

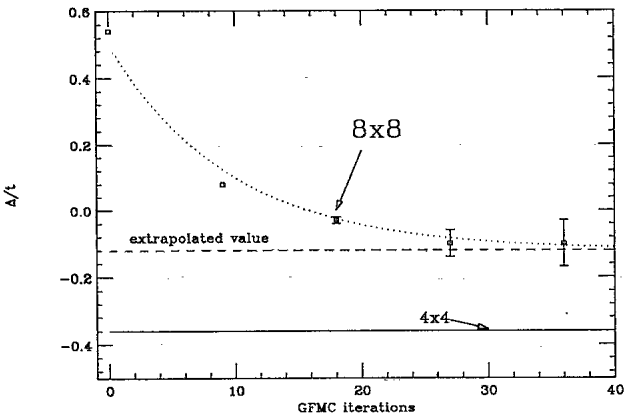

FIG. 5. Transient estimation of the two-hole binding energy Δ on a 8×8 lattice at $J/t=0.4$. The solid line refers to the exact value on a 4×4 lattice and the dashed line to the extrapolated value for the 8×8 lattice. The dotted line has been obtained from the corresponding fitting curves for E_2 and E_1.

The main contribution to the significant size dependence found for Δ arises from the single-hole ground-state energy values. A possible explanation for the different size dependence of the results for one and two holes may come from a long-range effect of a single hole on the antiferromagnetic background; the addition of a second hole may result in an opposite contribution and therefore in a substantial cancellation of such an effect. As an example, consider the possible long-range planar distortion of the antiferromagnetic moment of the spin background caused by the motion of a single hole.[16] Far away from the hole, the distortion $\delta m^{\dagger}$ is proportional to $\mathbf{k}\cdot\mathbf{r}/r$, where $\mathbf{k}$ is the hole momentum; in a two-hole state with total momentum equal to zero, the distortions caused by the two holes have opposite signs and the net effect is a dipolarlike field decayings as $\sim1/r^3$ at large distances, as opposed to $\sim1/r$ for a single hole.

Further insight into the two-hole ground-state properties is provided by the calculation of the two-hole distribution function $C(r)$, defined as

$$C(r)=\frac{1}{N}\sum_{i<j}\langle\hat{h}_i\hat{h}_j\rangle\delta(|\mathbf{R}_j-\mathbf{R}_i|-r)\ , \tag{11}$$

where $\hat{h}_i=1-\hat{n}_i$ is the hole number operator associated with the ith site, which is positioned at $\mathbf{R}_i$. In Figs. 6 and 7, we show the results for $C(r)$ on a 4×4 and on an 8×8 lattice at $J/t=1$; different symbols refer to the values of $C(r)$ computed after different numbers of GFMC iterations. The dotted line refers to the data from the zeroth iteration, whereas the dashed line refers to the data from the last iteration performed. As we see, the holes are initially located at distances 1, $\sqrt{2}$, and 2 from one another;

TABLE I. Two-hole, single-hole, and binding energies estimated by the GFMC method on lattices of different size L at $J/t=1.0$, 0.7, and 0.4. The two-hole state has momentum $\mathbf{Q}=(0,0)$, whereas the single-hole state has momentum $\mathbf{k}=(\pi/2,\pi/2)$. Statistical errors (in parentheses) are on the last digits.

L	$\delta E_2/t$	$\delta E_1/t$	Δ/t
		$J/t=1.0$	
4	−0.42(01)	−0.66(01)	−0.90(03)
6	−0.30(03)		
8	−0.26(02)	−0.42(01)	−0.58(04)
12		−0.42(01)	
		$J/t=0.7$	
8	−1.31(02)	−0.50(01)	−0.31(03)
		$J/t=0.4$	
4	−2.98(02)	−1.32(01)	−0.32(03)
6	−3.07(03)		
8	−3.08(03)	−1.48(01)	−0.12(04)
10	−3.08(04)		
12		−1.48(01)	

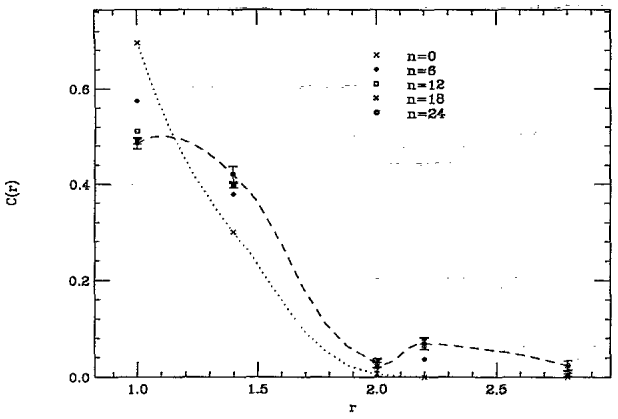

FIG. 6. Transient estimation of the two-hole distribution function on a 4×4 lattice at $J/t=1$. Different symbols refer to data from different GFMC iterations. The dotted lines refer to the data from the zeroth (variational) iteration and the dashed lines to the data from the last GFMC iteration.

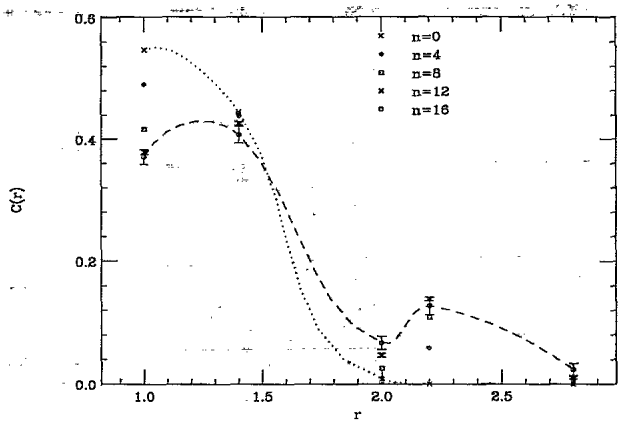

FIG. 8. Transient estimation of the two-hole distribution function on a 4×4 lattice at $J/t=0.4$. Different symbols refer to data from different GFMC iterations. The dotted lines refer to the data from the zeroth (variational) iteration and the dashed lines to the data from the last GFMC iteration.

that is, they are either located on nearest-neighboring or next-nearest-neighboring sites. As the algorithm is iterated, the weight is partially shifted to larger distances, but 1 and $\sqrt{2}$ remain largely dominant. Since the values of $C(r)$ change very little in the last three iterations sown for both lattices, we conclude that the values from the last iteration give a correct representation of the ground-state two-hole distribution. We compute the rms hole separation and obtain $R_{\rm rms}=1.40\pm0.2$ at the last iteration for the 4×4 lattice; this value is in agreement with the exact one.[4] On the 8×8 lattice, the rms separation is equal to $R_{\rm rms}=1.47\pm0.03$.

Figures 8 and 9 show the same calculation for the two lattices at $J/t=0.4$. Here, as the algorithm is iterated, the weight is significantly redistributed to the larger distances, and little evidence of convergence can be found. The value of $R_{\rm rms}$ obtained from the last iteration on the 4×4 lattice is $R_{\rm rms}=1.53\pm0.03$, lower than the exact one. We attribute this difference to the need of iterating the GFMC algorithm longer in order to recover fully the large-distance features of the function $C(r)$. The fact that the same number of iteration yields better evidence of convergence for the energy than for the two-hole distribution can be explained as being from the energy not being very sensitive to the form of $C(r)$ at large distances. From the results for $C(r)$ on an 8×8 lattice, we can see that there is an evident tendency of the two holes to "spread" at distances larger than the ones at which they are positioned in the initial state and larger than the ones available on a 4×4 lattice. This is consistent with the decrease in the binding energy found as the lattice size is increased and is a further indication of important finite-size effects affecting the calculation on a 4×4 lattice. We estimated the rms hole separation $R_{\rm rms}$ by fitting the values of $R_{\rm rms}^{(n)}$ obtained at different GFMC iterations with an exponential. On a 4×4 lattice, we find $R_{\rm rms}=1.61\pm0.04$, in agreement with the exact value within error bars. On lattices of larger size, the asymp-

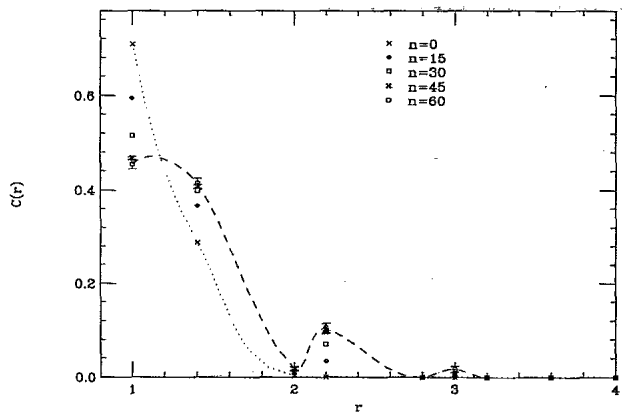

FIG. 7. Transient estimation of the two-hole distribution function on an 8×8 lattice at $J/t=1$. Different symbols refer to data from different GFMC iterations. The dotted lines refer to the data from the zeroth (variational) iteration and the dashed lines to the data from the last GFMC iteration.

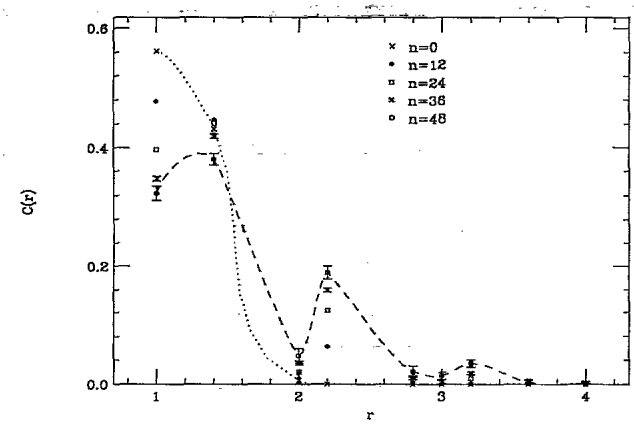

FIG. 9. Transient estimation of the two-hole distribution function on an 8×8 lattice at $J/t=0.4$. Different symbols refer to data from different GFMC iterations. The dotted lines refer to the data from the zeroth (variational) iteration and the dashed lines to the data from the last GFMC iteration.

totic value of $R_{\rm rms}$ given by the fit is significantly larger than the one from our last iteration, which indicates the need for a larger number of iterations. For instance, on a 10×10 lattice, $R_{\rm rms}^{\infty}=2.07\pm0.04$, whereas the estimate from the last (48th) iteration is only equal to 1.71 ± 0.03. From the fit we estimate the number of iterations needed to reach convergence to be of the order of 200 on the 10×10 lattice, whereas we could only perform 60 iterations because of the rapid increase of the size of the error bars. The extrapolated value of $R_{\rm rms}$ is 2.07 ± 0.04 on both the 8×8 and 10×10 lattices.

The rapid decrease of Δ with increasing t/J for an infinite lattice is in marked contrast with the results on a 4×4 lattice, where Δ seems to vary mildly with t/J (in fact, $\Delta\sim-0.8J$ for $0\le t/J\le5$.[4] Our results suggest that hole binding will no longer occur for J less than a critical value $J_c<0.4t$; such a critical value is known to exist in two dimensions for a d-wave bound state in the continuum case.[18] We can estimate the value of J_c by fitting the data in Table I by means of an extrapolation formula; it should be noted that in region $J<0.4t$ the binding energy is very small and our GFMC calculation cannot resolve the energy difference $\delta E_2-2\delta E_1$ with sufficient accuracy. We can obtain an extrapolation formula by modeling the complicated many-body problem of two mobile holes in a quantum antiferromagnet with a simple effective Hamiltonian describing the motion of two interacting quasiparticles in a square lattice with N sites and periodic boundary conditions:

$$\hat{H}_{\rm eff}=\sum_{i,j<i,\sigma} t'(\mathbf{R}_i,\mathbf{R}_j)(\hat{b}_{i\sigma}^{\dagger}\hat{b}_{j\sigma}+\text{H.c.}) + \sum_{i,j<i} J'(\mathbf{R}_i,\mathbf{R}_j)\hat{n}_i\hat{n}_j \ , \tag{12}$$

where $\hat{b}^{\dagger}$ is a "dressed" quasiparticle creation operator and $\hat{n}$ is a number operator; the sum runs over all pairs of lattice sites, as well as over all spin projections σ; $\mathbf{R}_i$ is the position vector of the ith site. The quasiparticles move in a band $E(\mathbf{k})$, which is assumed to have a minimum at $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$. We assume that the effective interaction $J'(\mathbf{R}_i,\mathbf{R}_j)$ is attractive and short ranged, i.e., $J'(\mathbf{R}_i,\mathbf{R}_j)=-J'$ for nearest neighbors and zero otherwise; the effective Hamiltonian (12) neglects effects of quantum spin fluctuations. The eigenvalue problem can be solved exactly (see also Ref. 19); if we seek a solution corresponding to a state with zero total momentum and with the spatial symmetry of a d wave, we find the following condition for the existence of a solution:

$$1=-2J'(I_{xx}-I_{xy}) \ , \tag{13}$$

which determines the ground-state energy E. We have introduced the quantities

$$I_{xx}=\frac{1}{N}\sum_{\mathbf{k}}\frac{\cos^2(k_x)}{E-2E(\mathbf{k})} \ , \qquad I_{xy}=\frac{1}{N}\sum_{k}\frac{\cos(k_x)\cos(k_y)}{E-2E(\mathbf{k})} \ , \tag{14}$$

and we have used $E(\mathbf{k})=E(-\mathbf{k})$. In the vicinity of $\mathbf{k}_{\rm min}=(\pi/2,\pi/2)$, where $E(\mathbf{k})$ attains its minimum, we can set $E(\mathbf{k})\approx E_{\rm min}+t_1'q_1^2+t_2'q_2^2$, where $\mathbf{q}=\mathbf{k}-\mathbf{k}_{\rm min}$ and q_1 and q_2 are the components of $\mathbf{q}$ along the high-symmetry direction $(0,0)\rightarrow(\pi,\pi)$ and $(0,\pi)\rightarrow(\pi,0)$, respectively. We introduce the binding energy $\Delta'=E-2E_{\rm min}$; in the limit where Δ' is small, it is straightforward to check that, upon neglecting terms of order Δ'^2 and higher, (13) can be expressed as

$$\frac{1}{J'}=\frac{1}{J_c'}[1-\gamma'\Delta'\ln(\Delta'/\varepsilon')] \ , \tag{15}$$

where we have introduced the constants J_c', γ', and ε'. We have expressed all energy scales in units of t_1', since $t_1'\gg t_2'$ for a single hole in the 2D t-J model,[2] and neglected terms of order Δ'^2 and higher (a linear term in Δ' has been conveniently absorbed in the cutoff energy scale ε' in the logarithm). If we assume that the function $t/J\equiv f(\Delta/t)$ for the problem of two holes in the 2D t-J model will have an expansion analogous to (17) around $\Delta/t=0$ (i.e., around $J=J_c$), we write

$$\frac{1}{J}=\frac{1}{J_c}\left[1-\gamma\frac{\Delta}{t}\ln(\Delta/\varepsilon)\right] \ , \tag{16}$$

where we have omitted terms of order $(\Delta/t)^2$ and $(\Delta/t)\ln(\Delta/\varepsilon)^2$. A simple fit of our extrapolated values of Δ (Table I) yields $J_c\sim0.27t$.

The main conclusion that can be drawn from the results of the GFMC calculation for two holes outlined in this paper is that since $\Delta(J/t<0.4)<0.1t$, the actual value of J/t in the copper-oxide superconductors (taking $t\sim0.5$ eV) cannot be much different than $J/t=0.4$ if this model is relevant for their superconductivity. There is an open question, namely, what happens if a finite fraction of holes is introduced on the infinite square lattice? The existence of a two-hole bound state is known to be related to the occurrence of a many-body pairing instability, to the extent that the system can be approximated by a continuum system where holes interact via a two-body potential.[18] Another possibility is that phase separation may take place for some range[13,14] or at any value of J/t.[12]

ACKNOWLEDGMENTS

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[1] P. W. Anderson, Science **235**, 1196 (1987); F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[2] S. A. Trugman, Phys. Rev. B **37**, 1597 (1988); C. Kane, P. Lee, and N. Read, *ibid.* **39**, 6880 (1989); Z. Liu and E. Manousakis, *ibid.* **44**, 2414 (1991).

[3]Y. Hasegawa and D. Poilblanc, Phys. Rev. B **40**, 9035 (1989); E. Dagotto, J. Riera, and A. P. Young, *ibid.* **42**, 2347 (1990).
[4]T. Barnes, A. E. Jacobs, M. D. Kovarik, and W. G. Macready, Phys. Rev. B **45**, 256 (1992).
[5]E. Kaxiras and E. Manousakis, Phys. Rev. B **38**, 866 (1988); J. Riera and A. P. Yound, *ibid.* **39**, 9697 (1989).
[6]M. H. Kalos, Phys. Rev. **128**, 1791 (1962); D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer-Verlag, Berlin, 1979), S. A. Chin, J. W. Negele, and S. E. Koonin, Ann. Phys. (N.Y.) **157**, 140 (1984).
[7]J. Carlson, Phys. Rev. B **40**, 846 (1989); N. Trivedi and D. M. Ceperley, *ibid.* **41**, 4552 (1990).
[8]M. Boninsegni and E. Manousakis, Phys. Rev. B **46**, 560 (1992).
[9]N. Bulut, D. Hone, D. J. Scalapino, and E. Y. Loh, Phys. Rev. Lett. **62**, 2192 (1989).
[10]T. Barnes and M. D. Kovarik, Phys. Rev. B **42**, 6159 (1990).
[11]M. Boninsegni and E. Manousakis (unpublished).
[12]V. Emery, S. Kivelson, and H. Lin, Phys. Rev. Lett. **64**, 475 (1990).
[13]M. Luchini, M. Ogata, W. Putikka, and T. M. Rice, Physica C **185**, 141 (1991).
[14]E. Dagotto, A. Moreo, F. Ortolani, D. Poiblanc, and J. Riera, Phys. Rev. B **45**, 10 741 (1992).
[15]M. Caffarel, F. X. Gadea, and D. M. Ceperley, Europhys. Lett. **16**, 249 (1991).
[16]B. Shraiman and E. Siggia, Phys. Rev. Lett. **61**, 467 (1988); M. Boninsegni and E. Manousakis, Phys. Rev. B **43**, 10 353 (1991).
[17]M. Boninsegni and E. Manousakis, Phys. Rev. B **45**, 4877 (1992).
[18]M. Randeria, J.-M. Duan, and L.-Y. Shieh, Phys. Rev. Lett. **62**, 981 (1989); Phys. Rev. B **41**, 327 (1990).
[19]Y.-L. Wang, E. Manousakis, and C. D. Wentworth, Phys. Lett. A **140**, 200 (1989).