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Ground state of two holes in a quantum antiferromagnet: Green's function Monte Carlo study

Massimo Boninsegni [1] and Efstratios Manousakis

Department of Physics, Center for Materials Research and Technology, and Supercomputer Computations Research Institute, Florida State University, Tallahassee, FL 32306, USA

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We investigate numerically the ground state of two holes in the two-dimensional t–J model, by means of the Green function Monte Carlo method. A critical value of J, $J_c \sim 0.3t$, is found such that d-wave binding of holes only occurs for $J > J_c$.

One of the interesting models, that captures important aspects of the environment experienced by the system of electrons in the copper oxide superconductors, is the t–J model [1]. A number of theoretical approaches have been devoted to the solution and understanding of the implications of the model. In two or more space dimensions, however, it lacks exact solution as it presents a genuine quantum many-body problem of strongly interacting particles on the lattice [2]. The plethora of different results obtained by various approximations has created a certain degree of confusion as to what exactly happens, i.e., the nature of the phase diagram and the consequences of the model in general. A numerical approach might appear as an obvious alternative that could provide the solution of this model. Exact diagonalization studies of finite-size clusters [3] are limited to small-size lattices (a typical case is 4×4) and thus it is not possible to perform a reasonable extrapolation to infinite-size lattice. Furthermore, world-line or other Monte Carlo simulation methods are hindered by the fact that one needs to introduce many Hubbard–Stratonovich auxiliary fields due to the nature of the interactions in the model and in addition by difficulties arising from the fermion "minus" sign problem.

Recently, we proposed a stochastic method which, in principle, is exact and we successfully applied it to study the problem of a single-hole on large square lattices [4]. The general method is known in the many-body computational physics [5] as Green's function Monte Carlo (GFMC) method and it is a projection technique; the key point of the method is that one has to have a suitable starting and guidance functions from where the true ground state can be projected out within a relatively small number n of applications of a projection operator $\hat{G}$. If the starting state is not a good approximation to the true ground state many more operations of $\hat{G}$ would be required; thus, in a fermion Monte Carlo method where the signal to noise ratio decreases exponentially with n, the signal gets lost much before any sign of convergence is observed.

An important question is the existence of pairing in the t–J model in the physical region ($J/t < 1$). While it is believed that in the large J/t limit the holes tend to stay close to each other to minimize the damage to the antiferromagnetically coupled bonds, in the physical region the situation is much less clear. Exact diagonalization studies [3] suggest that there is binding of holes in a d-wave ground state in a wide part of the physical region (at least for $J/t > 0.2$). However, there are reasons to suspect that the rel-

[1] Present address: National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, Champaign, IL 61820, USA.

atively small size of the lattices studied by exact diagonalization may not afford a reliable prediction of the physics of the infinite system.

In this paper we apply the GFMC method to study the problem of binding of two holes in a d-wave state in large square lattices. We have tested our method by calculating the energy for one and two holes on a 4×4 lattice and they are in excellent agreement with the results of the exact diagonalization [3] for all values of J/t considered in this paper. When our calculation is extended to large lattices we find that the value of the binding energy Δ is significantly reduced; for example, we find that at $J/t=1$ the value of Δ is reduced by about 35% and at $J/t=0.4$ we obtain $\Delta/t\sim0.1$ which is about three times smaller than their corresponding value on the 4×4 lattice. We find that there is a finite value of $J=J_c\simeq0.28t$ below which there is no longer a two-hole bound state.

Let us start from the Hamiltonian of the t–J model in order to establish our notation,

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

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 a 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. The spin operator $\boldsymbol{s}_i$ is associated with site i and is defined as

$$\boldsymbol{s}_i=\tfrac{1}{2}\sum_{\alpha\beta}\hat{c}_{i\alpha}^{\dagger}\boldsymbol{\sigma}_{\alpha\beta}\hat{c}_{i\beta}\,,$$

where $\boldsymbol{\sigma}$ is a vector of Pauli matrices. We consider a square lattice of $N=L\times L$ sites with periodic boundary conditions.

The basic elements of the GFMC method and our application to the t–J model are described in ref. [4]. This method provides the ground state expectation value $\mathcal{O}$ of an observable $\hat{\mathcal{O}}$ from the sequence

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

in the limit $\mathcal{O}=\lim_{n\to\infty}\mathcal{O}^{(n)}$. Here $|\Psi_T\rangle$ is an initial state not orthogonal to the ground state $|\Psi_0\rangle$ and $\hat{G}$ a projection operator which projects out $|\Psi_0\rangle$ from $|\Psi_T\rangle$, namely $|\Psi_0\rangle\propto\lim_{n\to\infty}\hat{G}^n|\Psi_T\rangle$. 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 $E\geqslant E_{\max}$, the largest eigenvalue of $\hat{H}$. A Monte Carlo implementation of this scheme consists of evaluating (2) as an average over the random walks of $\mathcal{N}$ independent walkers through the configuration space. The quantity $\mathcal{O}^{(n)}$ must be computed for increasingly larger n until convergence is observed, within statistical error bars. We use a scheme known as "forward walking" (see ref. [5]) to compute the ground state two-hole distribution, whereas the ground state energy is evaluated as explained in ref. [4]. The difficulty, in the case of the t–J model and other fermionic problems, is that the matrix elements $\langle c|\hat{G}|c'\rangle$ are not all positive. This results in large statistical fluctuations of the quantity $\mathcal{O}^{(n)}$ as n increases; this is known as the "minus" sign problem [5]. Thus, it is very important for the success of the method to have a suitable initial and guidance functions to be able to find convergence at small n before the statistical fluctuations grow significantly.

Our calculation is based upon an initial state for two holes which is a generalization of the string-based variational state used in the single-hole calculation [4,6] and on the same guidance function used in the calculation for a single hole. We define the correlated two-hole state as follows,

$$|\Psi_T(\boldsymbol{Q})\rangle=\sum_{\boldsymbol{R},\boldsymbol{r},c}(-1)^{L(c)}\exp[-\mathrm{i}\boldsymbol{Q}\cdot(\boldsymbol{R}+\boldsymbol{r}/2)]$$

$$\times\hat{F}_{\boldsymbol{Q}}(\boldsymbol{r})\exp\Big(-\tfrac{1}{2}\sum_{i<j}u_{ij}\hat{s}_i^z\hat{s}_j^z\Big)g(\boldsymbol{r})a_{\boldsymbol{R}\uparrow}a_{\boldsymbol{R}+\boldsymbol{r}\downarrow}|c\rangle\,, \tag{3}$$

where the sum runs over all lattice sites $\boldsymbol{R}$ and over all lattice spin configurations $|c\rangle=|\{s_i^z\}\rangle$. $L(c)$ is equal to the number of "down" spins in one of the two sublattices. The operator

$$\exp\Big(-\tfrac{1}{2}\sum_{i<j}u_{ij}\hat{s}_i^z\hat{s}_j^z\Big)$$

is a spin–spin correlation operator and the function u_{ij} depends on the distance between the two sites i and j. Here $\boldsymbol{Q}$ is the total momentum of the state and $\boldsymbol{r}$ is the relative distance of the two holes. The "string" correlation operator,

$$\hat{F}_{\boldsymbol{Q}}(\boldsymbol{r})=1+\sum_{\boldsymbol{a}}f_{\boldsymbol{a}}(\boldsymbol{Q},\boldsymbol{r})\hat{\mathcal{P}}_{\boldsymbol{a}}+\sum_{\boldsymbol{a}\boldsymbol{a}'}f_{\boldsymbol{a}\boldsymbol{a}'}(\boldsymbol{Q},\boldsymbol{r})\hat{\mathcal{P}}_{\boldsymbol{a}'}\hat{\mathcal{P}}_{\boldsymbol{a}}\,, \tag{4}$$

with $\boldsymbol{a}=\pm\hat{\boldsymbol{x}}$, $\pm\hat{\boldsymbol{y}}$ connecting two nearest-neighboring (n.n.) sites and

$$\hat{\mathscr{P}}_{\boldsymbol{a}}=\sum_{\boldsymbol{R}s}\hat{a}^{\dagger}_{\boldsymbol{R}s}\hat{a}_{\boldsymbol{R}+\boldsymbol{a}s}\,,$$

where $f_{\boldsymbol{a}}(\boldsymbol{Q},\boldsymbol{r}), f_{\boldsymbol{a}\boldsymbol{a}'}(\boldsymbol{Q},\boldsymbol{r})$ are variational parameters. This operator generates "strings" of spins displaced by one site along the hole path. The energy expectation value is minimized by taking $g(\boldsymbol{r})$ to be nonzero for only n.n. and with d-wave spatial symmetry, i.e. $g(\pm\hat{\boldsymbol{x}})=-g(\pm\hat{\boldsymbol{y}})$, which corresponds to a singlet state of the two holes. With this choice of g the variational parameters $f_{\boldsymbol{a}}$, $f_{\boldsymbol{a}\boldsymbol{a}'}$ can be computed approximately analytically by minimizing the energy expectation value and taking $u=0$, as in the single-hole case [6]. In our calculation we allowed for strings of length one only, i.e. we set $f_{\boldsymbol{a}\boldsymbol{a}'}(\boldsymbol{Q},\boldsymbol{r})=0$. We found that allowing for strings of length two can improve the initial variational energy but has little effect on the convergence to the true ground state. We restricted our calculations to $\boldsymbol{Q}=(0,0)$ and in this case $f_{\boldsymbol{a}}(\boldsymbol{Q},\boldsymbol{r})=f_0$, with f_0 real. As we did in the single-hole calculation, we used as guidance function

$$\Psi_{\mathrm{G}}=\exp\left(-\tfrac{1}{2}\sum_{i<j}u_{ij}s^z_i s^z_j\right).$$

Let us call $E^{\{n\}}_M$ the transient estimate for the ground state energy of the system with M holes at the nth iteration which corresponds to the mixed estimate [4] after $2n$ iterations and E_M the extrapolated value as $n\to\infty$. In fig. 1 the transient estimation for $\delta E^{\{n\}}_2=E^{\{n\}}_2-E_0$ on a 4×4 lattice (open circles) is compared to the results of the exact diagonalization (dashed line) for $J/t=1$. Notice that it is possible to obtain sufficient evidence of convergence; upon averaging the data from the last three iterations shown we obtain an estimate of $\delta E_2/t=0.43\pm0.01$ on a 4×4 lattice in agreement with the exact value of 0.42. This gives a value for $\Delta/t\equiv\delta E_2/t-2\delta E_1/t=-0.90\pm0.03$, using the single hole energy $\delta E_1=E_1-E_0$ calculated in ref. [4] for $\boldsymbol{k}=(\frac{1}{2}\pi,\frac{1}{2}\pi)$. In fig. 2 we present results for Δ on an 8×8 lattice also for $J/t=1$. If we average the values of the last two iterations shown in fig. 2 we obtain $\Delta/t=-0.59\pm0.03$ about 30% smaller than the value calculated on the 4×4 lattice. As we shall see below, our results show that the two-hole energy estimates on a 10×10 lattice are indistinguishable within our error bars from those obtained on the 8×8 lattice. A similar conclusion was drawn in ref. [4] for the single-hole energy estimates which remained also unchanged beyond 8×8 in the range $J/t\geqslant0.2$.

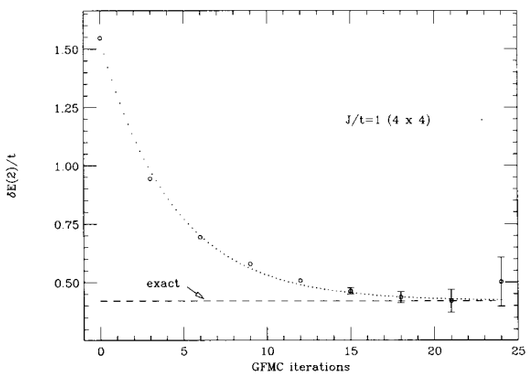

Fig. 1. Transient estimation of the two-hole ground state energy δE_2 on a 4×4 lattice at $J/t=1.0$. The dashed line refers to the exact diagonalization result [3].

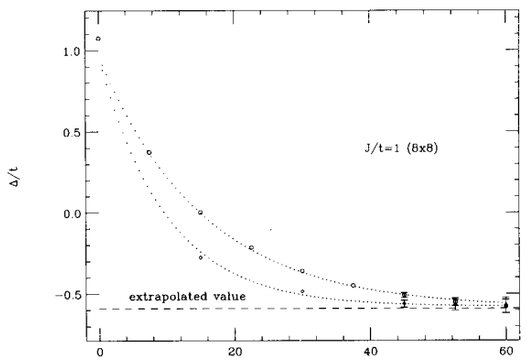

Fig. 2. Transient estimation of the binding energy Δ/t on an 8×8 lattice at $J/t=1.0$ obtained from $E^{\{n\}}_2$ (open circles), and $\mathscr{E}^{\{n\}}_2$ (diamonds). The dashed line refers to the $n\to\infty$ extrapolated value.

A simple scheme [7] which accelerates the speed of convergence to the ground state at no additional computational cost consists of considering the expectation values $\mathscr{E}^{\{n\}}_2$ of the Hamiltonian with the state $|\chi_n\rangle=(1+\lambda_n\hat{G}^n|\Psi_{\mathrm{T}}\rangle$, λ_n being a variational parameter determined by minimizing the value of $\mathscr{E}^{\{n\}}_2$. $\mathscr{E}^{\{n\}}_2$ yields a better ground state estimate than $E^{\{n\}}_2$, owing to the greater variational freedom of the state $|\chi_n\rangle$ compared to $\hat{G}^n|\Psi_{\mathrm{T}}\rangle$. 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. 2, 3, where we compare the values of $\delta\mathscr{E}_2^{\{n\}} = \mathscr{E}_2^{\{n\}} - E_0$ (diamonds) and $\delta E_2^{\{n\}}$ (circles).

The dotted lines in figs. 1–3 correspond to a fit using the expression: $E_2^{\{n\}} \approx E_2 + \beta \exp(-\kappa n)$, using E_2, β and κ as fitting parameters. This expression can be derived from eq. (2) as $n \to \infty$, where κ is proportional to the energy gap between the ground state and the first excited state of the system. We find that E_2 is the best determined of the three parameters. We obtained the same extrapolated estimates, within statistical errors, for E_2 by fitting both the data for $E_2^{\{n\}}$ and $\mathscr{E}_2^{\{n\}}$ with this expression. These estimates are reported in the first column of table 1.

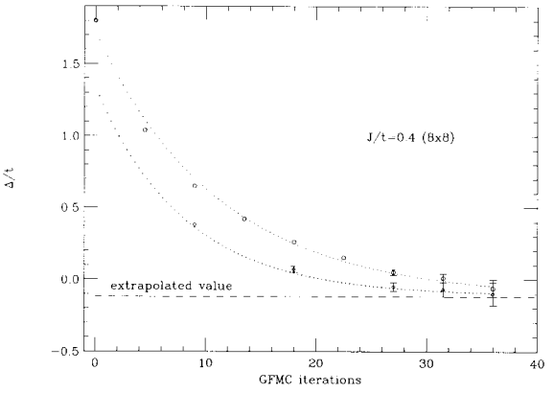

Fig. 3. The same as in fig. 2 for $J/t = 0.4$.

Table 1
Two-hole, single-hole and binding energies estimated by GFMC on lattices of size L, for $J/t = 1.0$, 0.7, and 0.4. The statistical errors (in parentheses) correspond to the last two digits.

J/t	L	$\delta E_2/t$	$\delta E_1/t$	Δ/t
1	4	−0.42(01)	−0.66(01)	−0.90(03)
	6	−0.30(02)	-	-
	8	−0.26(02)	−0.42(01)	−0.58(04)
	12	-	−0.42(01)	-
0.7	8	−1.34(03)	−0.50(01)	−0.34(04)
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)	-

We now turn to a value of J/t ($J/t = 0.4$) closer to the physical region. For $J/t = 0.4$, on a 4×4 lattice and in $n \sim 20$ iterations we obtain $\delta E_2/t = -2.94 \pm 0.03$, in good agreement with the value -2.993 from the exact diagonalization [3]. In fig. 3 we show our results for Δ on an 8×8 lattice obtained from E_2 (open circles) and from $\mathscr{E}_2$ (diamonds) both giving an extrapolated value for $\Delta/t = 0.12 \pm 0.04$. Our extrapolated value for δE_2 for the 10×10 lattice (see table 1), indicates that its value for the infinite lattice is not significantly different from that for the 8×8 lattice. Despite the size of the error bars, these results indicate rather clearly that the magnitude of the binding energy is considerably reduced, namely from a value of $0.349t$ on the 4×4 lattice to about $0.1t$ on the 8×8 lattice.

The main contribution to the significant finite-size effects found for $\Delta = \delta E_2 - 2\delta E_1$ at both values of J/t arises from δE_1. This is consistent with the expectation that the addition of a second hole partly repairs the long-range part of the distortion of the antiferromagnetic order caused by a single hole. Consider, for example, the long-range planar distortion of the antiferromagnetic moment of the spin background $\delta m^{\dagger} \sim \boldsymbol{k}\cdot\hat{\boldsymbol{r}}/r$, caused by the motion of a single hole [2,6] of momentum $\boldsymbol{k}$. In a two-hole state with total momentum equal to zero the distortions caused by the two holes have opposite signs.

We have computed the two-hole distribution function and the r.m.s. hole separation distance $R_{\text{r.m.s.}}^{(n)}$. We have extrapolated $R_{\text{r.m.s.}}^{(n)}$ to the $n \to \infty$ limit by fitting the values obtained at different GFMC iterations with an exponential. We find $R_{\text{r.m.s.}} = 1.41 \pm 0.02$ for $J/t = 1$ in agreement with the one from exact diagonalization [3] for the 4×4 lattice and $R_{\text{r.m.s.}} = 1.47 \pm 0.03$ on the 8×8 lattice. At $J/t = 0.4$ and on a 4×4 lattice we find $R_{\text{r.m.s.}} = 1.61 \pm 0.04$, in agreement with the exact value within error bars and $R_{\text{r.m.s.}} = 2.07 \pm 0.04$ on both 8×8 and 10×10 lattices. The distribution function and further details of the calculation will be given elsewhere [8].

Our results suggest that in the infinite lattice limit, Δ decreases rapidly with decreasing J/t in contrast with the results on the 4×4 lattice where Δ seems to vary mildly with J/t. In small lattices (4×4) the results of our calculation (the same as those obtained by exact diagonalization), show that in a wide region of J/t ($0.2 < J/t < \infty$), $\Delta \sim -0.8J$ (which is the $t = 0$

value of Δ). For a d-wave bound state there is always a threshold value of $J=J_c$ below which there is no two-hole binding [9]. In order to find an expression to extrapolate our data and estimate J_c we assumed that the hole–hole interaction is short-ranged and we modeled the problem of two holes in a quantum antiferromagnet by a simple problem of two quasiparticles moving in the square lattice in a band $E(\boldsymbol{k})$ and feeling a n.n. attraction of the order of J'. This problem can be solved exactly, up to a two-dimensional integral, for a singlet d-wave ground state using the method of ref. [10]. In the limit of small binding energy Δ and with an $E(\boldsymbol{k})$ having a minimum at $\boldsymbol{q}_0=(\frac{1}{2}\pi, \frac{1}{2}\pi)$ and

$$E(\boldsymbol{k}\to\boldsymbol{q}_0)=E_0+t'_1q_1^2+t'_2q_2^2,$$

where q_1 and q_2 are deviations of $\boldsymbol{k}$ from $\boldsymbol{q}_0$ along the directions $(0, 0)\to(\pi, \pi)$ and $(0, \pi)\to(\pi, 0)$ respectively, we obtain [8]

$$\frac{1}{J'}=\frac{1}{J'_c}\left[1-\gamma'\Delta'\ln(\Delta'/\epsilon')\right].$$

Here all energy scales are in units of t'_1 and there is a term linear in Δ' which has been conveniently absorbed in the cutoff energy scale ϵ' in the logarithm and the higher order terms in Δ' have been omitted. Assuming that the function $t/J\equiv f(\Delta/t)$ has a similar expansion around $\Delta/t=0$ (i.e., t/J around t/J_c) we obtain

$$\frac{t}{J}=\frac{t}{J_c}\left(1-\frac{\gamma\Delta}{t\ln(\Delta/\epsilon)}\right),$$

where we have omitted terms of order $(\Delta/t)^2$ and $[(\Delta/t)\ln(\Delta/\epsilon)]^2$. A simple fit to our extrapolated $(L\to\infty)$ values of Δ for $J/t=0.4$, 0.7 and 1.0 (table 1) gives $J_c\simeq 0.28t$.

Since $\Delta(J/t<0.4)<0.1t$, our calculation suggests that the actual value of J/t in the copper oxide superconductors (taking $t\sim 0.5$ 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 in the infinite square lattice. The existence of a two-hole bound state is a necessary condition for a many-hole pairing instability to occur, to the extent that the system can be approximated by a continuum system where holes interact via a two-body potential [9]. Another possibility is that phase separation may take place for some range [11] or at any value of J/t [12].

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