BOUND STATES OF HOLES
IN AN ANTIFERROMAGNET

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The formation of bound states of holes in an antiferromagnetic spin-1/2 background is studied using numerical techniques applied to the $t - J$ Hamiltonian on clusters with up to 26 sites. An analysis of the binding energy as a function of cluster size suggests that a two hole bound state is formed for couplings larger than a “critical” value $J/t_c$. The symmetry of the bound state is $d_{x^2-y^2}$. We also observed that its “quasiparticle” weight $Z_{2h}$ (defined in the text), is finite for all values of the coupling $J/t$. Thus, in the region $J/t \geq J/t_c$ the bound state of two holes behaves like a quasiparticle with charge $Q = 2e$, spin $S = 0$, and $d_{x^2-y^2}$ internal symmetry. The relation with recent ideas that have suggested the possibility of d-wave pairing in the high temperature cuprate superconductors is briefly discussed.

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The study of high temperature superconductors continues attracting considerable attention. Recently, a novel theoretical scenario has been proposed (and supported by self-consistent calculations, [1]) where the symmetry of the superconducting condensate is $d_{x^2-y^2}$, instead of the more standard s-wave of the BCS theory. On the experimental side, the London penetration depth, $\lambda(T)$, has been measured [2] at low temperatures in $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$. A linear temperature dependence compatible with a d-wave superconducting state was observed. Angular resolved photoemission experiments in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ have found an anisotropic superconducting gap also compatible with $d_{x^2-y^2}$ superconductivity. [3] Before these recent developments, the presence of an attractive interaction in the $d_{x^2-y^2}$ channel appeared frequently in the theoretical analysis of holes in antiferromagnetic backgrounds. It has been shown that the interchange of magnons between carriers naturally leads to an attraction that is dominated by the d-wave channel. [4] Numerical studies have also consistently suggested that two holes on finite clusters form a bound state with $d_{x^2-y^2}$ symmetry in a staggered spin background. [5-8] However, it is not clear if these results are an artifact of the approximations made in their calculation. Since in the cuprates superconductivity appears in the presence of antiferromagnetic correlations, a connection between these results and real materials may exist, and thus it is important to understand if the above mentioned d-wave attraction indeed exists in realistic models of correlated electrons.

The purpose of this paper is to report on a detailed numerical study of the formation of hole bound states in an antiferromagnetic background represented by the $t-J$ model. A study of their properties is presented for several cluster sizes in the subspace of zero and two holes, which allow us to analyse finite size effects. Dynamical properties of the two holes bound state are discussed, including the “quasiparticle” weight, $Z_{2h}$, obtained by creating a pair of holes with the appropriate rotational and translational symmetry over a fluctuating spin-1/2 antiferromagnetic background. Our results for different cluster sizes confirm that two hole carriers on such a spin background tend to form a bound state in the d-wave spin-singlet channel for couplings $J/t$ larger than a critical (finite) value $J/t_c$. In this regime, individual holes are unstable towards pair formation, and the bound state behaves like a dressed quasiparticle with charge $Q=2e$, spin 0 and internal d-wave symmetry.
In addition, the present paper also addresses an important issue that has been highly controversial in the context of theories of strongly correlated electrons. Does the quasiparticle weight of holes injected in an antiferromagnetic background vanish? In other words, do holes behave like quasiparticles? While these questions can be experimentally settled by photoemission techniques in single crystals of cuprate superconductors, the analysis of the results is difficult due to the presence of a considerable background in the signal. Thus a definite answer has not been experimentally given. [9] In some theoretical approaches, like the RVB scenario, the dressed holes (“holons”) carry charge $e$ but zero spin, and the missing spin 1/2 is carried by a charge neutral excitation called spinon. [10] These ideas are supported by calculations in one dimensional models where the separation of spin and charge indeed takes place. In this toy model, the wave-function renormalization of one hole, $Z_{1h}$, vanishes in the bulk limit at the Fermi surface, and thus the Fermi liquid fixed point does not exist in one dimension (1D). [10] Although, there is no reason to assume that one and two dimensions are qualitatively similar, nevertheless it is important to explore this exotic scenario. The marginal Fermi liquid theory also interprets the photoemission results in terms of a vanishing $Z_{1h}$. [11] On the other hand, novel but more conservative ideas, like Schrieffer’s spin-bag approach, [12] predicts the reduction of $Z_{1h}$ due to the presence of strong correlations to values considerably smaller than those for a weakly interacting system, but remaining finite in the region of physical interest. [13] Such a reduction in $Z_{1h}$ affects the interpretation of the experimental data, but does not change the basic idea of the pairing theory where dressed quasiparticles form bound states at low temperatures due to the interchange of some suitable excitation. Thus far, numerical studies of $Z_{1h}$ have confirmed these ideas, namely that $Z_{1h}$ is small but finite in the interesting region of parameter space. [13] In particular, a recent finite size study on clusters of up to 26 sites has provided strong evidence in favor of this result. [14] However, due to the availability of only a discrete set of momenta, the currently available lattices larger than a $4 \times 4$ cluster do not allow the study of holes right at the Fermi surface [15]. Here, we address this problem by a study of the wave-function renormalization in the subspace of two holes, since in this case the ground state of two holes always belongs to the zero momentum subspace which is contained in
all clusters we have analyzed in the present paper. In agreement with the previous results obtained for one hole, in the present study we found that $Z_{2h}$ is finite for all values of the ratio $J/t$ different from zero. \[16\]

The $t-J$ model is defined by the Hamiltonian,

$$H = J \sum_{\langle ij \rangle} \langle S_i \cdot S_j \rangle - \frac{1}{4} \sum_{\langle ij \rangle} n_i n_j - t \sum_{\langle ij \rangle} \langle c_{i,s}^\dagger c_{j,s} + h.c. \rangle,$$

(0.1)

where $c_{i,s}^\dagger$ denote hole operators; $n_i = n_i,\uparrow + n_i,\downarrow$; and clusters of N sites with periodic boundary conditions are considered. The rest of the notation is standard. The calculations have been carried out on square clusters satisfying $N = n^2 + m^2$ (where $n, m$ are integers, and $N$ is the number of sites) with $N = 16, 18, 20$ and $26$ sites. These clusters are commonly studied to search for a smooth extrapolation of the results to the bulk limit. \[17\] The algorithm used was the standard Lanczos method, using translational symmetry to reduce the size of the (sparse) Hamiltonian matrix, as well as rotations in $\pi/2$ and spin inversion. For the $N = 26$ cluster the Hamiltonian block corresponding to the ground state (GS) symmetry sector ($B_1$) with the largest size has 4,229,236 states, which can be handled only by supercomputers like the Cray-2. \[18\]

Intuitively, it is clear that a bound state of two holes will be formed at large values of $J/t$. The reason is that each hole individually “breaks” four antiferromagnetic (AF) links, which costs an energy of the order of the exchange coupling. Two holes minimize the lost energy by sharing a common link, and thus reducing the number of broken AF links from eight to seven. When the coupling $J/t$ is reduced to more realistic values, this attraction may survive till some critical coupling is reached. A smooth behavior of the ground state energy of two holes (measured with respect to the zero hole energy) is observed both as a function of the coupling and of the cluster size, \[19\] suggesting that our results for the energy are close to the bulk limit. Having calculated the exact ground state by Lanczos methods, the symmetry of the two holes ground state can be easily analyzed. For all clusters studied here it has been found that the ground state belongs to the $B_1$ irreducible representation of the $C_4$ point group of the square lattice, which is equivalent to the d-wave symmetry. \[19\]

Note that, since the symmetry group of the clusters does not, in general, include reflections
we cannot exclude a partial mixing between $d_{x^2-y^2}$ and $d_{xy}$ symmetries (except for 16 and 18 sites).

In Fig. 1a, the average distance between the two holes, obtained from a study of hole-hole correlations in the exact ground state wave functions, is plotted as a function of $J/t$ for different cluster sizes. It is observed that for coupling $J/t = 0.5$ or larger, the results seem to have converged to a finite number, indicating the presence of hole binding. On the other hand, the results at $J/t = 0.2$ show that the average hole distance grows appreciably as the lattice size is increased, and thus binding may not occur in this regime. We believe that in the intermediate region a critical coupling exists where binding of holes starts.

In Fig. 1b the binding energy of two holes is presented. This quantity is defined as $\Delta_B = e_2 - 2e_1$, where $e_n = E_n - E_0$, and $E_n$ is the ground state energy of the $t - J$ model in the subspace of $n$ holes. The single GS energies $e_1$ have been calculated elsewhere on clusters up to 26 sites. If $\Delta_B < 0$ in the bulk limit, a bound state of two holes is formed. $\Delta_B$ is an intensive quantity and thus it is more severely affected by finite size effects than the (extensive) ground state energy. In addition, the energy of one hole enters in the definition of $\Delta_B$ and, as discussed before, this quantity carries an additional systematic error due to the absence of momentum $k = (\pi/2, \pi/2)$ in the discrete set of momenta of the clusters with $N = 18, 20$ and 26 sites, used in the present study. In spite of this problem, qualitative information can be obtained from Fig. 1b with some confidence. The “critical” coupling, $J/t|c$ where two holes reduce their energy by forming a bound state, slowly grows with increasing lattice size suggesting that it may converge to a finite value in the bulk limit. In Fig. 1b, recent Green Function Monte Carlo results on $8 \times 8$ clusters are also shown. With this approach, supplemented by the use of appropriate variational guiding states obtained from the analysis of smaller clusters, it has been possible to study couplings $J/t$ as small as 0.4. The dashed line in the figure shows an educated extrapolation suggesting that binding starts at $J/t|c \sim 0.3$, in qualitative agreement with our exact results on smaller lattices. Note also that calculations using a recently developed “truncation” method have provided evidence that the $t - J_z$ model, i.e. a model where transverse spin fluctuations are switched off, has also a finite critical coupling beyond which two holes form a bound state.
In this model, $J_z/t|_c \sim 0.18$, which is in qualitative agreement with our results for the $t-J$ model which suggest a larger critical coupling, since in the absence of spin fluctuations a stronger tendency to pairing would be expected. [23]

In Fig.2a, the wave-function renormalization $Z_{2h}$ is shown as a function of $1/N$ for several coupling constants. If two holes form a bound state then the analysis of $Z_{1h}$ becomes irrelevant, since isolated holes will become unstable towards pair formation. In other words, in simulations carried out in the grand canonical ensemble, where a chemical potential $\mu$ selects the fermionic density, the state of one hole is never stable in the region of pair formation. In such a regime the elementary charge carrier will be the two holes bound state, and thus it is necessary to analyze $Z_{2h}$, defined as,

$$Z_{2h} = \frac{\langle \psi_{gs}^2 \Delta^\dagger_\alpha | \psi_{gs}^0 \rangle}{\sqrt{\langle \psi_{gs}^0 | \Delta_\alpha \Delta_\alpha^\dagger | \psi_{gs}^0 \rangle}}, \quad (0.2)$$

where $|\psi_{gs}^{nh}\rangle$ is the ground state in the subspace of $n$-holes which can be obtained using exact diagonalization methods. The operator that destroys a pair of holes is defined as

$$\Delta_\alpha = \bar{c}_{i,\uparrow} (c_{i+\hat{x},\downarrow} \pm c_{i-\hat{x},\downarrow} \pm c_{i+\hat{y},\downarrow} \pm c_{i-\hat{y},\downarrow}),$$

where $\alpha = s$ corresponds to the (+) signs and defines an extended s-wave operator, while $\alpha = d$ corresponds to the (−) signs in the $\hat{y}$-direction, and defines a $d_{x^2−y^2}$ pair operator. $\hat{x}, \hat{y}$ are unit vectors along the axis, and the normalization is chosen such that $0 \leq Z_{2h} \leq 1$. The size dependence of $Z_{2h}$ shown in Fig.2a seems smooth and flat both in the large and small coupling regions suggesting that $Z_{2h}$ is nonzero in the bulk limit for all finite values of the coupling $J/t$. Fig.2b illustrates the coupling dependence of $Z_{2h}$. The results for different cluster sizes approximately follow a linear behavior, $Z_{2h} \sim J/t$, in the interval $0 \leq J/t \leq 1$. This result is in agreement with calculations carried out in the one hole sector that suggested $Z_{1h} \sim (J/t)^{1/2}$ (see ref. [24]).

To complete our study, let us consider the spectral decomposition of the pairing operator that can be carried out using standard techniques. It is defined as,

$$P(\omega) = \sum_n |\langle \psi_n^{2h} | \Delta^\dagger_\alpha | \psi_{gs}^0 \rangle|^2 \delta(\omega - (E_n^{2h} - E_{gs}^{0h})) \quad (0.3)$$

where the notation is standard. The pair spectral functions shown in Fig. 3 illustrate some of the conclusions of this paper. The calculations shown in the figure correspond to a $\sqrt{20} \times \sqrt{20}$ cluster at $J/t = 0.3$ and two different symmetry operators, namely $d_{x^2−y^2}$ and
extended-s wave. The difference between the two is clear. While the spectral decomposition of the d-wave operator shows a clear sharp peak at the bottom of the spectrum with an intensity given by the $Z_{2h}$ presented in Fig.2, the decomposition for the s-wave shows no appreciable spectral weight at low frequencies. The fact that Fig. 3 reproduces most of the qualitative features found on smaller systems [7] gives credibility to small cluster calculations. The study of the size dependence of the d-wave pairing spectral function discussed before [16] shows that, with increasing system size, (i) the low energy QP peak survives, and (ii) the higher energy peaks eventually merge into a continuous background.

Lastly we discuss the nature of the pairing in momentum space. The form of the d-wave pair operator in $k$-space, $\Delta^d_\alpha = \sum_k (\cos k_x - \cos k_y) c^\dagger_{k,\uparrow} c^{-\dagger}_{-k,\downarrow}$, suggests that the pairing occurs predominantly between two holes at momenta ($\pi, 0$) (or $(0, \pi)$) in agreement with the calculation of the single hole spectral function in one hole-doped clusters [25].

Summarizing, in this paper we have presented a complete study of the behavior of two holes injected on a spin-1/2 antiferromagnetic background. In agreement with previous numerical studies carried out by the authors, we observed the tendency towards the formation of bound states for couplings larger that some finite critical value $J/t_{ic}$. The bound state in that region has $d_{x^2-y^2}$ symmetry, spin zero and carries a nonzero overlap with the state obtained by applying a local pair creation operator over the ground state of zero hole. Such a behavior, signalled by a nonzero $Z_{2h}$, favors the interpretation of the two holes bound state as a quasiparticle of charge $2e$ and spin zero, which would be the actual carriers of charge under an applied electric field. The analysis of the spectral decomposition of the pairing operator illustrates a dramatic difference between the favored d-wave bound state and an extended s-wave state. These quasiparticles are natural candidates to Bose condensate at low temperatures into a superconducting d-wave ground state in the $t-J$ model, similar to that recently found by two of us (E.D. and J.R.) away from half-filling. [8] Such a condensate may become a realization of the recently proposed new theoretical ideas [1] to explain the behavior of the actual high-Tc cuprate superconductors.

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[19] We assume here that the fermionic statistics is associated to the holes. Alternatively, if a convention is used where each spin is considered as an electron with its fermionic statistics, then additional work is necessary to arrive to the symmetry of the ground state. Actually, for clusters of size \( N = M \times M \), the half filled GS of the Hubbard or Heisenberg model is, in the fermion representation, s-wave when \( M/2 \) is even and d-wave when \( M/2 \) is odd. See A. Moreo and E. Dagotto, Phys. Rev. B 41, 9488 (1990).
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FIGURE CAPTIONS

Figure 1a
Average hole-hole distance in the ground state as a function of the coupling constant for the four clusters studied in this paper. Open triangles denote results for a cluster of 16 sites, open squares for 18 sites, full triangles for 20 sites, and full squares for 26 sites.

Figure 1b
Binding energy, $\Delta_B$, of two holes in the $t-J$ model as defined in the text. Open triangles denote results for a cluster of 16 sites, open squares for 18 sites, full triangles for 20 sites, and full squares for 26 sites. The points with the error bars joined by a dashed line are Green’s Function Monte Carlo results taken from Ref. [21].

Figure 2a
The wave-function renormalization, $Z_{2h}$ (defined in the text), as a function of the inverse of the number of sites $N$ for several values of the coupling $J/t$ between 5 and 0.1.

Figure 2b
The wave-function renormalization, $Z_{2h}$ (defined in the text), as a function of the coupling $J/t$. Open triangles denote results for a cluster of 16 sites, open squares for 18 sites, full triangles for 20 sites, and full squares for 26 sites.

Figure 3
The dynamical response of the pairing operator defined in the text obtained on a $\sqrt{20} \times \sqrt{20}$ cluster, and at $J/t = 0.3$. In (a) the pairing operator used has d-wave symmetry, while in (b) it corresponds to extended s-wave.