ON THE INTERNAL STRUCTURE OF THE SINGLET
\( d_{x^2-y^2} \) HOLE PAIR IN AN ANTIFERROMAGNET

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Exact diagonalizations of two dimensional small t–J clusters reveal dominant hole-hole correlations at distance \( \sqrt{2} \) (ie between holes on next nearest neighbor sites). A new form of singlet \( d_{x^2-y^2} \) pair operator is proposed to account for the spatial extension of the two hole-bound pair beyond nearest neighbor sites.

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Some time ago it has been proposed that the exchange of spin fluctuations could lead to superconductivity in the singlet $d_{x^2-y^2}$ channel [1]. Such mechanisms were recently discussed in connection with the new copper oxide superconductors. Occurrence of d-wave pairing in strongly correlated models have been further supported by quantum Monte Carlo calculations [2], weak coupling approaches [3] and recent finite size scaling analysis [4]. The issue of pairing between holes moving in an antiferromagnetic fluctuating background is of central importance in the field of high-$T_c$ superconductivity. Theoretical predictions [5] for NMR in a d-wave superconductor seem to be consistent with the measured data [6]. Also consistent with d-wave pairing let us briefly mention recent microwave experiments [7] showing a linear temperature behavior of the penetration depth and recent photoemission data [8] revealing nodes in the gap function.

In standard notations the t–J Hamiltonian on a two dimensional (2D) reads

$$H = J \sum_{i,\bar{\epsilon}} (\vec{S}_i \cdot \vec{S}_{i+\bar{\epsilon}} - \frac{1}{4} n_i n_{i+\bar{\epsilon}}) - t \sum_{i,\bar{\epsilon},\sigma} (c^\dagger_{i,\sigma} c_{i+\bar{\epsilon},\sigma} + h.c.),$$  

(0.1)

where $\vec{S}_i$ and $c_{i,\sigma}$ stand for the localized spins and the itinerant holes respectively.

Numerical calculations of the binding energy between two holes on $4 \times 4$ [3–12], $\sqrt{18} \times \sqrt{18}$ [13], $\sqrt{20} \times \sqrt{20}$ [14] and $\sqrt{26} \times \sqrt{26}$ [4] square clusters suggested that binding occurs for realistic values of the antiferromagnetic exchange interaction ($0.3 < J/t < 0.6$) [15]. The bound state is found to be a spin singlet with $d_{x^2-y^2}$ internal symmetry. As revealed by a quasiparticle pole in the dynamical pair correlation function [17,4] the bound pair exhibits a coherent motion characteristic of a unique (bosonic) particle of charge $+2e$ which leads to flux quantization with a periodicity in flux of $\Phi_0/2$ [16].

The hole-hole correlations $C(R)$ in the two hole-ground state (GS) of the $\sqrt{26} \times \sqrt{26}$ cluster are shown in Fig. 1 in good agreement with previous data on the $4 \times 4$ cluster [4,12] and with approximate results on the same cluster obtained from a restricted Hilbert space analysis [18]. Over a broad region, $0.2 < J/t < 0.9$, the correlation at distance $\sqrt{2}$ dominates. Strong correlations are also found at distance 1 (i.e. for holes sitting on nearest neighbor sites) which become in turn dominant for large $J/t$ (unphysical). If the two holes do form a bound state, as it is suggested by a finite size scaling analysis [4], we expect the
correlation $C(R)$ at small distance $R$ as well as the mean-hole separation $[1]$ to remain finite in the thermodynamic limit.

Our purpose here is to define a proper pair operator which properly accounts for the internal structure of the pair, with strong density-density correlations at distance 1 and $\sqrt{2}$. A generalized form of a pair operator can be defined as

$$\Delta = \sum_R \frac{\langle \Psi_0^{N-2} | \Delta_R | \Psi_0^N \rangle}{\langle \Psi_0^N | \Delta_R^\dagger \Delta_R | \Psi_0^N \rangle} \Delta_R,$$  

where $\Psi_0^N$ and $\Psi_0^{N-2}$ are the Néel and two hole GS respectively on the N site cluster and $\Delta_R$ creates a pair of holes on two sites at a distance $R$. The sum can be restricted to a small set of lattice distances determined by the actual size of the pair. Fig. 1 suggests that, in practice, it is sufficient to include $R = 1$ and $R = \sqrt{2}$. The prefactors in (0.2) [19] are chosen in order to maximize the quasiparticle (QP) weight of the pair [20,4],

$$Z_{2h} = \frac{|\langle \Psi_0^{N-2} | \Delta | \Psi_0^N \rangle|^2}{\langle \Psi_0^N | \Delta^\dagger \Delta | \Psi_0^N \rangle} = \sum_R \frac{|\langle \Psi_0^{N-2} | \Delta_R | \Psi_0^N \rangle|^2}{\langle \Psi_0^N | \Delta_R^\dagger \Delta_R | \Psi_0^N \rangle}.$$  

From Eq. (0.3) it is clear that the QP weight increases with the number of pair operator $\Delta_R$ included in the sum. Hence adding a contribution at $R = \sqrt{2}$ could significantly increase the weights $Z_{2h}$ calculated in Ref. [4] with the conventional $d_{x^2-y^2}$ BCS spin singlet operator for nearest neighbor sites $\Delta_1 = \sum_i c_{i,\uparrow}(c_{i+\hat{x},\downarrow} + c_{i-\hat{x},\downarrow} - c_{i+\hat{y},\downarrow} - c_{i-\hat{y},\downarrow})$.

Unlike for $R=1$, the pair operator at separation $\hat{x} + \hat{y}$ can not be written in a simple BCS form because of the $d_{x^2-y^2}$ character of the GS wavefunction. Indeed, simple symmetry arguments imply that the pair operator must be odd under reflections with respect to the $x = \pm y$ directions. Let us define $\Delta_{\sqrt{2}}$ as

$$\Delta_{\sqrt{2}} = \sum_i \{(\vec{S}_{i+\hat{y}} - \vec{S}_{i+\hat{x}}) \cdot \vec{T}_{i,i+\hat{x}+\hat{y}} - (\vec{S}_{i-\hat{x}} - \vec{S}_{i+\hat{y}}) \cdot \vec{T}_{i,i-\hat{x}+\hat{y}}\},$$

where $\vec{T}_{i,j} = \frac{1}{\tau} c_{i,\sigma}(\sigma_i \vec{\sigma})_{\sigma\sigma'} c_{j,\sigma'}$ is the regular spin triplet pair operator [21]. This expression is very similar to the pair function proposed by Balatsky and Bonca [22] for the 1D t–J model in the context of odd-gap pairing. However, we stress that (0.4) is, as far as symmetry properties are concerned, entirely similar to $\Delta_1$ (spin singlet, $d_{x^2-y^2}$ spatial symmetry) as schematically depicted in Fig. 2 whereas the odd-gap singlet operator of [22] is odd under space inversion, $r \rightarrow -r$ (p-wave character).
In summary, the hole-hole density correlation function calculated exactly on a $\sqrt{26} \times \sqrt{26}$ cluster shows further evidence in favor of a two hole $d_{x^2-y^2}$ bound state in the fluctuating antiferromagnetic background. In order to include the strong tendency of the holes to stay together across the diagonal of a plaquette a new form of pair operator is introduced which couples the hole pair to the neighboring spins. Although its form is very similar to pair field operators introduced in the context of odd-gap pairing its symmetry properties are identical to the symmetry properties of the conventional BCS pair operator at distance 1.

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REFERENCES

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[1] F.J. Ohkawa and H. Fukuyama, J. Phys. Soc. Jpn. 53, 4344 (1984); J.E. Hirsch and D.J. Scalapino, Phys. Rev. Lett. 56, 2732 (1986); K. Miyake, S. Schmitt-Rink and C.M. Varma, Phys. Rev. B 34, 6554 (1986); D.J. Scalapino, E. Loh and J.E. Hirsch, Phys. Rev. B 35, 6694 (1987).

[2] N. E. Bickers, D. J. Scalapino, R. T. Scalettar, Int. J. Mod. Phys. B 1, 687 (1987); N. E. Bickers, D. J. Scalapino, S. R. White, Phys. Rev. Lett. 62, 961 (1989).

[3] T. Moriya, Y. Takahashi, K. Ueda, Physica C 185, 114 (1991); P. Monthoux, A. V. Balatsky, D. Pines, Phys. Rev. Lett. 67, 3448 (1991).

[4] D. Poilblanc, E. Riera, and E. Dagotto, submitted to Phys. Rev. Lett.; D. Poilblanc, Phys. Rev. B 47 (june 1993).

[5] N. Bulut and D. Scalapino, Phys. Rev. Lett. 68, 706 (1992); P. Monthoux and D. Pines, Phys. Rev. B 47, 6069 (1993).

[6] M. Takigawa, P. C. Hammel, R. H. Heffner, Z. Fisk, Phys. Rev. B 39, 7371 (1989); S. E. Barrett et al. Phys. Rev. Lett. 66, 108 (1991).

[7] W. N. Hardy, D. A. Bonn, D. C. Morgan, R. Liang, K. Zhang, submitted to Phys. Rev. Lett.

[8] Z.-X. Shen et al. Phys. Rev. Lett. 70, 1553 (1993).

[9] E. Kaxiras and E. Manousakis, Phys. Rev. B38, 566 (1988).

[10] J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B39, 7074 (1989).

[11] J. Riera, Phys. Rev. B40, 833 (1989).

[12] Y. Hasegawa and D. Poilblanc, Phys. Rev. B40, 9035 (1989).

[13] J. Riera, Phys. Rev. B43, 3681 (1991).
[14] T. Itoh, M. Arai, and T. Fujiwara, Phys. Rev. B 42, 4834 (1990); H. Fehske, V. Waas, H. Röder and H. Büttner, Phys. Rev. B 44, 8473 (1991).

[15] For larger J/t values phase separation may occur. See e.g. V. J. Emery, S. A. Kivelson and H. Q. Lin, Phys. Rev. Lett. 64, 475 (1990).

[16] D. Poilblanc, Phys. Rev. B 44, 9562 (1991).

[17] E. Dagotto, J. Riera and A. P. Young, Phys. Rev. B 42, 2347 (1990).

[18] P. Prelovšek and X. Zotos, Phys. Rev. B, in press.

[19] For a standard BCS pairing operator the normalization factor \( \langle \Psi_N^0 | \Delta_R^{\dagger} \Delta_R | \Psi_N^0 \rangle \) is simply equal to the spin-spin correlation \( \langle \Psi_N^0 | (1/4 - \vec{S}_i \cdot \vec{S}_{i+r}) | \Psi_N^0 \rangle \) (where \( r \) is such that \( R = | r | \)).

[20] E. Dagotto and J. R. Schrieffer, Phys. Rev. B 43, 8705 (1991).

[21] \( \vec{S}_k \cdot \vec{T}_{ij} \) is a scalar in spin space and can easily be expressed as \( S_k^Z (c_{i,\uparrow} c_{j,\downarrow} + c_{j,\uparrow} c_{i,\downarrow}) - S_k^+ c_{i,\uparrow} c_{j,\uparrow} - S_k^- c_{i,\downarrow} c_{j,\downarrow} \).

[22] A. V. Balatsky and E. Abrahams, Phys. Rev. B 45, 13125 (1992); A. V. Balatsky and J. Bonča, preprint.
FIGURE CAPTIONS

Figure 1
Hole density correlations for 2 holes on a $\sqrt{26} \times \sqrt{26}$ cluster. The symbols corresponding to the various hole-hole separations are shown on the plot.

Figure 2
Schematic picture of the d-wave pair operator $\Delta_{\sqrt{2}}$ around a lattice site $i$. The arrows correspond to the triplet pair operators (oriented) and the signs $\pm$ in parenthesis correspond to the phase factors of the spin operators in $(04)$. 