Spin bags in the doped $t-J$ model

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We present a nonperturbative method for deriving a quasiparticle description of the low-energy excitations in the $t-J$ model for strongly correlated electrons. Using the exact diagonalization technique we evaluated exactly the spectral functions of composite operators, which describe an electron or hole dressed by antiferromagnetic spin fluctuations as expected in the string or spin bag picture. For hole doping up to 1/8, use of the composite operators leads to a drastic simplification of the single particle spectral function: at half-filling it takes free-particle form, for the doped case it resembles a system of weakly interacting Fermions corresponding to the doped holes. We conclude that for all doping levels under study, the elementary electronic excitations next to the Fermi level are adequately described by the antiferromagnetic spin fluctuation picture.

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Despite great efforts the unusual properties of high-temperature superconductors remain a largely unresolved problem. There is general agreement that the electrons in these materials are strongly correlated, so that marked deviations from the single particle picture are to be expected. An important step in setting up a successful theory of both, their normal and superconducting state, therefore would be to find a description in terms of elementary excitations i.e. weakly or moderately interacting quasiparticles. We present an exact diagonalization study of the $t-J$ model which is specifically aimed at finding such a description.

We construct composite operators which reduce or increase the electron number by one and simultaneously rearrange the spins in the neighborhood of the newly created hole/electron so as to simulate the ‘cloud of spin defects’ surrounding the hole. For doping levels up to $1/8$, the spectral function of the composite operators then takes the form expected for weakly interacting Fermions, with a well defined ‘band’ right at the Fermi level. The $t-J$ model reads:

$$H = -t \sum_{<i,j>,\sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + H.c.) + J \sum_{<i,j>} [ \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} ].$$

The $\mathbf{S}_i$ are the electronic spin operators and the sum over $<i,j>$ stands for a summation over all pairs of nearest neighbors on a two dimensional square lattice. The operators $\hat{c}_{i,\sigma}^\dagger$ are expressed in terms of ordinary fermion operators as $\hat{c}_{i,\sigma}^\dagger (1 - n_{i,-\sigma})$. We present results for a $4 \times 4$ cluster of this model with $t/J=4$, similar results have been obtained also for different values of $t/J$.

A single hole in the half-filled band can be well described by the string [1–3] or spin bag [4] picture, where the hole is dressed by antiferromagnetic spin fluctuations. With this in mind, we make the following ansatz for a ‘spin bag operator’ ($N(j)$ denotes the nearest neighbors of $j$):

$$\tilde{c}_{k,\uparrow} = \frac{1}{\sqrt{N}} \sum_j \sum_{\lambda=0}^{\lambda_{\max}} e^{i\mathbf{k} \cdot \mathbf{R}_j} \alpha_\lambda(\mathbf{k}) A_{j,\lambda},$$

$$A_{j,0} = \hat{c}_{j,\uparrow},$$

$$A_{j,1} = \sum_{k \in N(j)} S_j^- \hat{c}_{k,\downarrow},$$

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When acting on the Néel state, the operator $A_{j,\lambda}$ creates all strings of length $\lambda$ which begin at site $j$, $\tilde{c}_{k,\sigma}$ reproduces a simple trial wave function for a single hole \[5\]. $A_{j,\lambda}$ also can be thought of as having been generated by $\lambda$-fold commutation of $\hat{c}_{j,\uparrow}$ with the kinetic energy, a procedure suggested by Dagotto and Schrieffer \[6\]. The parameters $\alpha_{\lambda}(k)$ are determined \[6\] from the requirement that the state $\tilde{c}_{k,\sigma} |\Psi_0^{(0h)}\rangle$ (where $|\Psi_0^{(0h)}\rangle$ denotes the half-filled ground state) has norm 1 and maximum overlap with the lowest totally symmetric single-hole eigenstate with momentum $k$, $|\Psi_0^{(1h)}(k)\rangle$. If we denote the Fourier transform of $A_{j,\nu}$ by $A_{k,\nu}$ and introduce

$$n_\nu = \langle \Psi_0^{(1h)}(k) | A_{k,\nu} | \Psi_0^{(0h)} \rangle,$$

$$A_{\mu,\nu} = n_{\mu}^* n_{\nu},$$

$$B_{\mu,\nu} = \langle \Psi_0^{(0h)} | A_{k,\mu}^\dagger A_{k,\nu} | \Psi_0^{(0h)} \rangle,$$

the $\alpha$’s can be obtained by solution of the generalized eigenvalue problem $Ax = \lambda Bx$. We use $\lambda_{\text{max}} = 3$, so that the $\tilde{c}_{k,\sigma}$ effectively contain 3 free parameters. Having fixed the $\alpha$’s, we compute the spectral function

$$A_-(k, -\omega) = \sum_\nu |\langle \Psi_0^{(1h)} | \tilde{c}_{k,\sigma} | \Psi_0^{(0h)} \rangle|^2 \delta(\omega - (E_\nu^{(1h)} - E_0^{(0h)})),$$

via the standard Lanczos method. Here $|\Psi_0^{(nh)}\rangle$ denotes the $n$th eigenstate with $n$ holes and $E_\nu^{(nh)}$ the corresponding energy (in particular $\nu = 0$ implies the ground state). This spectral function is shown in Fig. \[\text{III}\] and compared to that of the ‘string-0 operator’ $\sqrt{2}\tilde{c}_{k,\sigma}$, which up to a factor 2 equals the usual photoemission spectrum. Despite the small number of adjustable parameters, use of the spin bag operators brings the spectral function to almost perfect free-particle form: the incoherent continua present in the bare electron spectra are removed, the spectral weight being concentrated essentially in one sharp peak with a well-defined next-nearest neighbor dispersion. This can be understood if one attributes the
incoherent continua to the retracable-path-type motion of the hole. Since the $A_{j,\mu}$ describe precisely the forward and backward hopping of the hole along a track of Néel ordered spins, this type of hole-motion is already ‘incorporated’ into the definition of the $\tilde{c}_{k,\sigma}$, so that their spectra emphasize the coherent hole motion. Some care is necessary: for momentum $(\pi, \pi)$ the lowest totally symmetric single-hole eigenstate has spin $\frac{3}{2}$, so that it can not be observed in the spectrum of the bare electron operator. On the other hand, since the $\tilde{c}_{k,\sigma}$ are not vector operators under spin rotations, it can be observed in their spectrum. Since this state fits very well into the next-nearest neighbor hopping dispersion relation expected for a single hole, we believe that the fact that it has spin $3/2$ in the $4 \times 4$ cluster is a finite size effect. We do not have any proof for that, so results for $(\pi, \pi)$ should be considered with care; however, none of the conclusions to be presented below depends crucially on the form of the spectra for this momentum.

So far, we have merely demonstrated the quality of the string picture at half-filling which may not be very surprising; a much more interesting question is, whether this description of the states next to the Fermi level remains valid upon doping. Exact diagonalization offers a very direct and natural way to check this issue, namely to evaluate the spectra of the $\tilde{c}_{k,\sigma}$ for a doped rather than the half-filled ground state. For the $\alpha_\lambda(k)$’s we thereby retain the values optimized at half-filling (it would be easy to recalculate the $\alpha$’s for the doped ground state but an important question is whether there is some continuity in the development of the electronic states at the Fermi level). We begin with the ground state with 8 up-spin electrons, 7 down-spin electrons and momentum $(\pi/2, \pi/2)$ i.e. the single hole ground state. In Fig. 2 (Fig. 3) the spectra of $\tilde{c}_{k,\uparrow}$ ($\tilde{c}_{k,\downarrow}$) are again compared to those of the respective string-0 operators, $\sqrt{2}\tilde{c}_{k,\uparrow}$ ($\sqrt{2}\tilde{c}_{k,\downarrow}$). Quite obviously, the $\tilde{c}_{k,\sigma}$ continue to ‘work’: there is the same elimination of the incoherent continua and enhancement of the peaks at the Fermi level as for half-filling. A novel feature is the broadening of these peaks, and it seems natural to ascribe it to the scattering of the added hole from the one already present in the system. Most important of all, however, the spectrum for $\tilde{c}_{k,\downarrow}$ shows an unambiguous ‘pocket’ at $(\pi/2, \pi/2)$, the momentum of the $\downarrow$-hole already present in the system: we clearly see the
Pauli principle working for the spin bags. This suggest weakly interacting spin-1/2 Fermions which correspond to the doped holes as the ‘effective theory’ for the low-lying states of the cluster with 2 holes.

We thus push things further and proceed to the two-hole ground state. Having in mind the results obtained so far, we should model it as an interacting state of two spin bags with total momentum zero:

\[ |\tilde{\Psi}_0^{(2h)}\rangle = \sum_k \Delta(k) \tilde{c}_{k,\uparrow} \tilde{c}_{-k,\downarrow} |\Psi_0^{(0h)}\rangle. \tag{3} \]

Using the \( \tilde{c}_{k,\sigma} \) optimized at half-filling we consequently construct the states \( |\Phi(k)\rangle = \tilde{c}_{k,\uparrow} \tilde{c}_{-k,\downarrow} |\Psi_0^{(0h)}\rangle \) for all 16 allowed momenta in the cluster, evaluate the matrices \( h_{kk'} = \langle \Phi(k)|H|\Phi(k')\rangle \) and \( n_{kk'} = \langle \Phi(k)|\Phi(k')\rangle \) and solve the resulting eigenvalue problem to obtain \( \Delta(k) \). The estimate for the ground state energy obtained in this way is \(-8.21t\), to be compared with the exact value of \(-8.81t\), and we have \( \langle \tilde{\Psi}_0^{(2h)}|\Psi_0^{(2h)}\rangle = 0.67 \). Obviously the string ground state is not really an excellent approximation to the exact one, but it should be noted that it has been constructed from the half-filled groundstate, so that no relaxation of the ‘spin background’ (corresponding to the collapse of long range Néel order in the infinite system) is incorporated. On the other hand, the approximate ground state shares some basic features of the exact one, such as the correct \( d_{x^2-y^2}\)-symmetry \[\text{[3]}\]. In Tab. \[\text{[4]}\], the ‘spin bag momentum distribution’ \( \tilde{n}(k) = |\langle \Phi(k)|\tilde{\Psi}_0^{(2h)}\rangle|^2/\langle \Phi(k)|\Phi(k)\rangle \), is listed; due to the nonorthogonality of the \( |\Phi(k)\rangle \) there exists no simple sum rule for this quantity, so that its interpretation as ‘momentum distribution’ is strictly speaking questionable. However, it can give a rough idea of the distribution of the spin bags in momentum space, and obviously only \((\pi,0)\) and \((\pi,\pi/2)\) are appreciably occupied \[\text{[5]}\]. It is interesting to contrast \( \tilde{n}(k) \) with the ‘bare hole momentum distribution’ \( n_h(k) = \langle \tilde{c}_{k,\sigma} \tilde{c}_{-k,\sigma}^\dagger \rangle \) also given in Tab. \[\text{[4]}\] both for the approximate and exact two-hole ground state. Whereas the \( n_h(k) \) for the exact and approximate ground state agree reasonably well, there is no similarity with \( \tilde{n}(k) \): \( n_h(k) \) is roughly consistent with a free electron picture, \( \tilde{n}(k) \) would rather suggest that mainly \((\pi,0)\) is occupied by quasiparticles. This can be understood by recalling that the incoherent
retraceable path-type motion of the bare holes (which naturally contributes to $n_h(k)$) is already absorbed into the definition of the string operators, so that $\tilde{n}(k)$ measures predominantly the coherent hole motion.

Next, let us find an approximate annihilation operator for the dressed holes, i.e. an operator $\bar{c}^\dagger_{k,\sigma}$ so that this operator and $\tilde{c}_{k,\sigma}$ mutually undo the action of each other. Thereby the first guess, $\bar{c}^\dagger_{k,\sigma}=(\tilde{c}_{k,\sigma})^\dagger$ may not be expected to be reasonable because the ‘basis set’ $A_{j,\lambda}$ does not consist of operators which create electrons in orthogonal basis functions, i.e. $[A_{i,\mu}, (A_{j,\lambda})]^+ \neq \delta_{i,j}\delta_{\mu,\lambda}$. We thus introduce a shortcut: for $\bar{c}^\dagger_{k,\uparrow}$ we make the ansatz

$$\bar{c}^\dagger_{k,\uparrow} = \frac{1}{\sqrt{N}} \sum_j \sum_{\lambda=0}^{\lambda_{\text{max}}} e^{-ik\cdot R_j}\beta_\lambda(k)(A_j^{(\lambda)})^\dagger,$$

and construct the state $|\Psi^{(2h)}_c\rangle = [\bar{c}^\dagger_{k,\sigma}, \tilde{c}_{k,\sigma}]^+|\Psi^{(2h)}_0\rangle$.

If $\tilde{c}_{k,\sigma}$ and $\bar{c}_{k,\sigma}$ indeed were adjoint fermionic creation and annihilation operators, the anticommutator on the right hand side would be 1 and consequently we determine the $\beta$’s from the requirement that $|\Psi^{(2h)}_c\rangle$ has norm 1 and maximum overlap with $|\Psi^{(2h)}_0\rangle$. The actual value of the overlap then also provides a measure for the quality of our ansatz and with $\lambda_{\text{max}} = 3$ we indeed find that for most $k$-points $|\langle \Psi^{(2h)}_c | \Psi^{(2h)}_0 \rangle|^2 \sim 1$ (see Tab. III), so that this way of obtaining an approximation to $\bar{c}^\dagger_{k,\sigma}$ appears quite reasonable. Using the $\bar{c}^\dagger_{k,\sigma}$ we now can also study the spin bag removal (electron addition) spectra in the two-hole ground state, defined as

$$A_+(k, \omega) = \sum_\nu |\langle \psi^{(1h)}_\nu | \bar{c}^\dagger_{k,\sigma} | \Psi^{(2h)}_0 \rangle|^2 \delta(\omega - (E^{(1h)}_\nu - E^{(2h)}_0)).$$

Thereby some care is necessary: in contrast to the ordinary electron operators, there exists no simple sum rule for the integrated weight of the spin bag addition and removal spectra. To facilitate the comparison with the usual single particle spectral function in the following all spectra are therefore normalized to unity.

Fig. IV then compares the spin bag spectral function and that of the ordinary electron operators. The spin bag creation (electron annihilation) spectra clearly show the simplification
already familiar from the previous calculations: the incoherent continua far from the Fermi energy are removed, the peaks near $E_f$ are markedly enhanced. We conclude that even for this level of doping, the $\tilde{c}_{k,\sigma}$ optimized at half-filling provide a good description of the electronic excitations closest to the Fermi energy, $E_f$. The degree of broadening of the spin-bag peaks is reminiscent of a Fermi liquid: there are sharp peaks close to $E_f$, diffuse peaks at lower energies. For the spin bag annihilation (electron creation) spectra use of the adjoint spin bag operators leads to an increase of spectral weight at $(\pi, 0)$ and a marked depletion at $(\pi, \pi)$. The resulting division of spectral weight between spin bag addition and removal spectra moreover is remarkably consistent with the ‘momentum distribution’ $\tilde{n}(k)$: spin bags can be annihilated predominantly at $k=(\pi, 0)$ and $k=(\pi, \pi/2)$, i.e. the momenta which were most probable in the variational ground state $|\tilde{\Psi}_0^{(2h)}\rangle$. All in all the doped cluster thus behaves very much like a system of weakly interacting ‘effective fermions’ corresponding to the doped holes.

In summary we have shown that for all doping levels studied the use of ‘spin bag operators’ leads to a drastic simplification of the spectral function. Since these operators describe the modification of the ‘spin background’ in the immediate neighborhood of the hole, we also expect that they are predominantly determined by the local spin correlations, which most probably are described adequately by the exact diagonalization. It thus seems reasonable to expect that a similar simplification of the spectral function occurs also in the infinite system. Our nonperturbative approach thus suggests a rather conventional ‘effective theory’, in which the electronic excitations right at the Fermi level are modelled by spin 1/2 Fermions corresponding to the doped holes (of course, like any other cluster calculation the present study cannot address the dependence of the quasiparticle lifetime on the distance in energy from the Fermi energy). The remarkable degree of continuity upon doping moreover shows that these quasiparticles are holes dressed by antiferromagnetic spin fluctuations in essentially the same way as a single hole moving in an antiferromagnet, a reasonably well understood problem [1–3,10,11]. The dressing of the holes with spin fluctuations leads to an interaction which favours a bound state with $d_{x^2-y^2}$ symmetry. Our exact results thus
clearly corroborate the basic assumptions of the antiferromagnetic spin fluctuation theory of high-temperature superconductivity [12,13]. Another important point is, that the absorption of the incoherent hole motion into the definition of the spin bag operators leads to an almost complete ‘decoupling’ of the quasiparticle spectral function and momentum distribution from that of the bare electrons. This suggests consequences for the interpretation of experiments: it seems plausible that measurements of transport properties [14,15] would rather probe the ‘quasiparticle properties’ and not resolve the internal structure of the spin bags. On the other hand, high-energy experiments like photoemission [16,17] should resolve the internal structure and reflect properties of the bare electrons. Discrepancies between the transport properties and the Fermi surface measured in photoemission [17] thus may be not surprising.

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FIGURES

FIG. 1. Spectral function of the spin bag operators (full line) and ordinary electron annihilation operator (dotted line) in the half-filled ground state of the 4×4 cluster.

FIG. 2. Spectral function $A_-(k, \omega)$ of the spin bag operators (full line) and ordinary electron annihilation operator (dotted line) in the single hole ground state (momentum $(\pi/2, \pi/2)$) of the 4×4 cluster. The spin of the newly created hole is antiparallel to that of the hole already present.

FIG. 3. Spectral function $A_-(k, \omega)$ of the spin bag operators (full line) and ordinary electron annihilation operator (dotted line) in the single hole ground state (momentum $(\pi/2, \pi/2)$) of the 4×4 cluster. The spin of the newly created hole is parallel to that of the hole already present.

FIG. 4. Spectral function $A_-(k, \omega) + A_+(k, \omega)$ of the spin bag operators (full line) and ordinary electron operators (dotted line) in the two hole ground state of the 4×4 cluster. The Fermi energy is marked by a thin line and the frequency region $\omega<E_F$ ($\omega>E_F$) corresponds to the annihilation (creation) of an electron.
TABLES

TABLE I. ‘Quasiparticle momentum distribution’ \( \tilde{n}(k) \) in the approximate two-hole ground state and bare hole distribution function \( n_h(k) \) for the approximate (A) and exact (E) two-hole ground state.

| \( k \)         | (0, 0) | (\( \frac{\pi}{2} \), 0) | (\( \pi \), 0) | (\( \frac{\pi}{2} \), \( \frac{\pi}{2} \)) | (\( \pi \), \( \frac{\pi}{2} \)) | (\( \pi \), \( \pi \)) |
|-----------------|--------|--------------------------|----------------|---------------------------------|-------------------------|----------------|
| \( \tilde{n}(k) \) | 0.0000 | 0.0586                   | 0.7649         | 0.0000                          | 0.2269                  | 0.0000         |
| \( n_h(k), A \)  | 0.0164 | 0.0237                   | 0.2538         | 0.0658                          | 0.2212                  | 0.2239         |
| \( n_h(k), E \)  | 0.0069 | 0.0319                   | 0.1752         | 0.0660                          | 0.2529                  | 0.2675         |

TABLE II. The quantity \( |\langle \Psi_0^{(2h)} | \Psi_c^{(2h)} \rangle|^2 \) for all momenta in the 4 \times 4-cluster.

| \( k \)         | (0, 0) | (\( \frac{\pi}{2} \), 0) | (\( \pi \), 0) | (\( \frac{\pi}{2} \), \( \frac{\pi}{2} \)) | (\( \frac{\pi}{2} \), \( \pi \)) | (\( \pi \), \( \pi \)) |
|-----------------|--------|--------------------------|----------------|---------------------------------|-------------------------|----------------|
| \( n(k) \)      | 0.9846 | 0.9702                   | 0.9497         | 0.9445                          | 0.9455                  | 0.7921         |
REFERENCES

[1] B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. 60, 740 (1988).

[2] S. A. Trugman, Phys. Rev. B 37, 1597 (1988).

[3] J. Inoue and S. Maekawa, J. Phys. Soc. Jpn. 59, 2110 (1990).

[4] J. R. Schrieffer, X. G. Wen, S. C. Zhang, Phys. Rev. B 39, 11663 (1989).

[5] R. Eder and K. W. Becker, Z. Phys. B 78, 219 (1990).

[6] E. Dagotto and J. R. Schrieffer, Phys. Rev. B 43, 8705 (1990).

[7] W. Brinkman and T. M. Rice, Phys. Rev. B 2, 1324 (1970).

[8] D. Poilblanc and E. Dagotto, Phys. Rev. B 42, 4861 (1990).

[9] R. Eder and K. W. Becker, Phys. Rev. B 44, 6982 (1991).

[10] S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. 60, 2793 (1989).

[11] C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B 39, 6880 (1989).

[12] T. Moriya, Y. Takahashi, and K. Ueda, J. Phys. Soc. Jpn. 49, 2905 (1990).

[13] P. Monthoux, A. Balatsky, and D. Pines, Phys. Rev. Lett. 67, 3448 (1991).

[14] S. A. Trugman, Phys. Rev. Lett. 65, 500 (1990).

[15] H. Takagi et al. Phys. Rev. Lett. 69, 2975 (1992).

[16] C. G. Olson et al., Science 245, 731 (1989);

[17] D. M. King et al. Phys. Rev. Lett. 70, 3159 (1992).
Fig. 1

\[ A(k, \omega) \]

\( A(\pi, \pi) \)

\( A(\pi/2, \pi/2) \)

\( A(\pi/2, 0) \)

\( A(\pi,ur) \)

\( A(0,0) \)
Fig. 3

$A(k,\omega)$

$(0,0)$

$(\pi/2,0)$

$(\pi/2,\pi/2)$

$(\pi,0)$

$(\pi,\pi)$

$(\pi,\pi/2)$
$A(k, \omega)$