Anomalous spin and charge dynamics of the t-J model at low doping

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We present an exact diagonalization study of the dynamical spin and density correlation functions in small clusters of 2D t–J model for hole dopings \( \leq 25\% \). Both correlation functions show a remarkably regular, but very different scaling with both hole density \( \rho_h \) and parameters \( t \) and \( J \). The density correlation function is most consistent with that of condensed Bosons in a band of width \( \sim t \), the spin correlation function with that of fermions in a band of width \( \sim J \). We show that the familiar spin bag scenario explains these results in a natural way.

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The identification of a simple ‘effective theory’ for the doped Mott-Hubbard insulator which is capable of resolving the numerous anomalies of cuprate superconductors remains an intriguing problem. The simplest model which may be expected to contain the key features of these systems is the \( t–J \) model:

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

The \( \hat{S}_i \) are the electronic spin operators, \( \hat{c}_{i,\sigma}^\dagger = c_{i,\sigma}^\dagger (1 - n_{i,\sigma}) \) and the sum over \( <i,j> \) stands for a summation over all pairs of nearest neighbors.

For hole densities \( \rho_h > 0.3 \) the ground state of the model seems to represent a fairly conventional Fermi liquid with a particle-hole like spin and density excitation spectrum \([1,2]\). In this work we show that the situation is drastically different for \( \rho_h \leq 0.25 \): here the density excitations roughly resemble those of condensed Bosons with characteristic energy \( t \), the spin excitations still are consistent with Fermions, the characteristic energy, however, now is \( J \). We show that these results are naturally explained within the familiar spin bag \([3]\) or string \([4,5]\) scenario. For the standard 16 and 18-site clusters we used the Lanczos algorithm to compute the dynamical spin (SCF) and density (DCF) correlation functions:

\[
C_\alpha(q,\omega) = \frac{1}{\pi^3} \langle \Psi_0 | \hat{O}_\alpha(q) | \omega -(H-E_0) - i\epsilon \rangle \hat{O}_\alpha(q) | \Psi_0 \rangle.
\]

Here \( | \Psi_0 \rangle \) \( (E_0) \) denotes the ground state wave function (ground state energy), for the operator \( \hat{O}_\alpha(q) \) we choose the Fourier transform of either density operator \( (n_{i,\uparrow} + n_{i,\downarrow}) \) \( (\alpha = d) \) or spin operator \( (n_{i,\uparrow} - n_{i,\downarrow}) \) \( (\alpha = s) \). Fig. shows the DCF divided by the number of holes, \( n_h \), for \( n_h = 1, 2, 3, 4 \). Except for the \( \omega \rightarrow 0 \) parts at \( (\pi/2, 0) \) and \( (\pi/3, \pi/3) \) this is a universal function. Deviations are strongest for a single hole, but even there the characteristic shape is already present. Fig. thus first of all demonstrates a high degree of continuity over the entire range of dopings considered; quite obviously the essential physics is already realized for a single hole in an antiferromagnet. Next, the scaling of the spectra with hole concentration over their entire width is clearly inconsistent with particle-hole excitations in a Fermion system: at least the high-energy parts, where transitions from deep below to high above the Fermi energy \( E_F \) would contribute, should be unaffected by a change of particle density. Instead, the DCF could be modelled roughly by Bosons of density \( \rho_h \) which are condensed into the lowest state of the noninteracting band with the free electron dispersion \( \epsilon_q \); such a system would have a DCF of the form \( C_d(q,\omega) = \rho_h \cdot \delta(\omega - \epsilon_q) \). That the characteristic energy of the DCF indeed is \( t \) is seen in Fig. , which compares the DCF for different \( t/J \) and demonstrates that the positions of the dominant ‘peaks’ remain unaffected by a change of \( J \). Fig. also shows that the weight of the \( \omega \rightarrow 0 \) part decreases with \( t/J \), whereas the weight of the remainder other parts increases; together with the deviations in the scaling behaviour with \( n_h \) this suggests a two-component interpretation of the DCF.

We proceed to the SCF, shown in Fig. for \( n_h = 2, 3, 4 \). The spectra for 3 holes thereby are averaged over the 4 degenerate ground states (the 3 hole ground states have momentum \( (2\pi/3, 0) \) in the 18 and \( (\pi/2, \pi/2) \) in the 16-site clusters). With the exception of \( (\pi, \pi) \), the spectra are fairly independent of doping, changes occur mostly at the low-energy end of some of the spectra. Such a dependence on particle number is reminiscent of the particle-hole excitations in a Fermion system: the spectral weight of a given transition is expressed in terms of the Fermionic occupation numbers \( n_k \) as \( n_{k+q}(1 - n_k) \) and is affected only if either initial or final state cross the chemical potential. Here it should be noted that due to the coarse \( k \)-mesh of the 2D clusters (as well as the averaging process for 3 holes) one can not expect a well defined \( k_F \) which scales continuously with particle density. Instead a continuous increase of the hole occupation numbers \( n_k \) at the ‘Fermi momenta’ and hence a continuous increase/decrease of peak intensities will be realized. As for the energy scale Fig. shows the SCF for
Various $t/J$. When frequencies are measured in units of $J$, the peak positions obviously remain largely unaffected by a change of $t$, so that the characteristic energy of the SCF is $J$.

Summarizing the numerical results one may say that both SCF and DCF scale with $n_0$ and $t/J$ in remarkably regular but completely different ways. Let us stress for clarity that the different doping dependence of the integrated weight with nonvanishing momentum transfer is trivial. By the $f$-sum rule the integrated spectral weight of both correlation functions equals the number of electrons, $n_e$.

For the DCF this value is almost exhausted by the $q=0$ spectrum, which contributes $n_e(n_e/N)$ (with $N$ the number of sites). For the SCF this contribution either vanishes or is a tiny $1/N$, so that the integrated spectral weight for finite $q$ is $\sim n_0$ for the SCF but $\sim n_h$ for the DCF. This argument, however does not explain e.g. the scaling with $n_h$ of the entire DCF spectra. This is not only inconsistent with the particle hole excitations in a Fermi liquid but also with the Luttinger liquid realized in the 1D model \[1\]. The low doping phase in 2D thus obviously exhibits qualitatively new physics.

To gain additional insight, Fig. compares the SCF for $t/J=2.5$ and $t=0$, i.e., mobile and static holes. For static holes there is a band of diffuse excitations, which roughly follow the characteristic spin wave dispersion; their diffuse nature is obviously due to the scattering from the holes, which in this case merely act as impurities. For mobile holes spin-wave excitations near $(\pi,\pi)$ seem to persist with reduced spectral weight and a wider gap at $(\pi,\pi)$; the qualitatively new feature are low energy peaks throughout the Brillouin zone which may naturally be associated with particle-hole transitions in the coherent band for mobile holes. This suggests a two-component interpretation for the SCF, namely low-energy particle-hole excitations plus spin-wave like excitations near $(\pi,\pi)$. This is also supported by the opposite $t/J$-dependence of these two components (Fig.): whereas the weight of the ‘spin wave’ parts decreases with increasing $t/J$, consistent with the more efficient degradation of antiferromagnetic correlations by more mobile holes) that of the particle-hole-excitations increases or remains unchanged.

Further information is obtained by studying the impact of $O_s$ and $O_d$ on the electronic momentum distribution (EMD) $n(k)$: $\langle \hat{c}_{\nu,k,\uparrow}^\dagger \hat{c}_{\nu,k,\downarrow} \rangle = \langle \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} \rangle$. To that end we compute first the ground state EMD, $n_0(k)$, and second the EMD $n_q(k)$ for the state $(1/n)O_d(q)|\text{GS}\rangle$ (where $n$ is chosen to normalize the state to 1). Table \[1\] shows the difference $\Delta_q(k)=n_q(k)-n_0(k)$ for $q=(\pi,\pi)$, as well as $n_{\text{shift}}(q)=\sum_k |\Delta_q(k)|$. The latter quantity may be interpreted as the number of electrons shifted in $k$-space, its value for free particles is 1. Table \[2\] reveals a clear difference between density and spin operator: whereas $O_d$ induces a substantial shift of electrons in $k$ space and always has $n_{\text{shift}}$ close to its free-particle value of 1, $O_s$ affects $n(k)$ to a much lesser degree. Via the kinetic energy sum rule

$$E_{\text{kin}} = 2 \sum_k \epsilon_k n(k),$$

(with $\epsilon_k = -2t(\cos(k_x) + \cos(k_y))$), this result on one hand immediately explains the different energy scales of SCF and DCF: $O_d$ substantially changes $E_{\text{kin}}\sim t$, $O_s$ leaves it essentially unchanged. On the other hand, this only complicates the puzzle about the doping dependence of the DCF: quite obviously the electrons react to the density operator as if they were free particles, hence one naturally would expect a Fermion-like particle-hole spectrum for the DCF, in contrast to the numerical result.

We now want to show that all results obtained so far can be resolved in a simple and natural way if one adopts the familiar string or spin bag picture. Thereby we consider holes moving in (and hence coupled to) a ‘background’ of antiferromagnetically correlated spins. Our key assumption is that the spin background carries excitations which are independent of the hole system, so that their momentum is not ‘visible’ in the EMD (compare Table \[3\]) and hence does not increase the kinetic energy. Natural candidates are the remnants of the short-wavelength spin waves, as would be suggested by Fig.. We next assume that the relevant hole states are described by operators of the type

$$\hat{c}_{\nu,k,\uparrow} = \alpha_{\nu}(k)\hat{c}_{\nu,k,\uparrow} + \sum_{k'\sigma,\sigma'} \beta_{\sigma,\sigma'}(k,k')\hat{c}_{k',\sigma}S_{k-k'}^{\sigma}$$

$$+ \sum_{k',q,\sigma,\sigma',\sigma''} \gamma_{\sigma,\sigma',\sigma''}(k,k',q)\hat{c}_{k',\sigma}S_{q}^{\sigma}S_{k-k'-q}^{\sigma''} + \ldots,$$

where $S_q^{\sigma}$ denotes the electronic spin operator. Equation \[3\] describes a hole which has transferred a part of its momentum to a variable number of spin excitations; it has many degrees of freedom (as reflected by the many parameters $\alpha, \beta, \gamma \ldots$) so that there will be a large number of bands, which presumably form the extended incoherent continua present in the single particle spectral function \[3\]. The bands are labelled by the index $\nu$, $\nu=0$ denotes the ‘quasiparticle band’ \[4\] split off from the bottom of the continuum. For this quasiparticle band the validity of the spin bag description has been verified previously by explicit numerical check \[3\]. The driving force behind the momentum transfer to spin excitations is gain in kinetic energy: scattering a hole e.g. from $\nu=(\pi/2,\pi/2)$ to $\nu'=(\pi,\pi)$ and transferring the excess momentum to a spin excitation reduces the kinetic energy $\sim t$, but requires only exchange energy $\sim J/t$.

We can conclude that in the low lying spin bag states the bare hole predominantly occupies momenta near $(\pi,\pi)$: via \[4\] the depletion of $n(k)$ on these momenta lowers the kinetic energy most efficiently. This is corroborated by the numerical result \[4\] that the addition of e.g. a
single hole with total momentum $(\pi/2, \pi/2)$ reduces $n(k)$ strongest near $(\pi, \pi)$. A rough estimate for the degree of admixture of spin excitations is the quasiparticle weight $Z$: the simplest estimate would be $Z=|a_0(k_F)|^2$; $Z \approx 0.3$ thus suggest a rather strong admixture of spin fluctuations.

We now assume that in the $n_h$ hole-ground state the holes occupy the $n_h$ lowest states of the $\nu=0$ band, i.e. rigid-band filling of the quasiparticle band; this is consistent with numerical results [13]. Since the dispersion of the $\nu=0$ band strictly scales with $J$ [1], we may conclude from (1) that the distribution of the bare holes in $k$-space is essentially the same for all $\nu=0$ states. In other words, the coefficients $\beta, \gamma$ in (2) depend strongly on the ‘bare hole’ momentum $k'$ but only weakly on the total momentum $k$. We can conclude that when $n_h$ holes are filled into the $\nu=0$ band, the hole occupation of e.g. $(\pi, \pi)$ should be $n_h$ times that for a single hole; that this indeed is the case is shown in Table I which gives the hole occupation, $\bar{n}_h(k)=(1/2) \sum (c_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}^\dagger)$, for momenta near $(\pi, \pi)$ in the ground state with different $n_h$.

With this picture of the ground state in mind, we can distinguish two types of excitations: there can be ‘particle-hole excitations’ within the $\nu=0$ band or an excitation of the ‘internal degrees of freedom’ of a spin bag, where the final state has $\nu' \neq 0$. An important point is that $O_s$ and $O_d$ transfer momentum to a spin bag in a very different way: $O_s$ changes the momentum of the bag by adding (or removing) a spin excitation, whereas $O_d$ can transfer its momentum only to the bare hole itself. $O_s$ consequently does not change the distribution of holes in $k$-space appreciably whereas $O_d$ necessarily must do so (see Table I). Hence, $O_s$ is essentially limited to transitions within the $\nu=0$ band, so that its spectrum is Fermionic and scales with the quasiparticle bandwidth $J$. On the other hand, $O_d$ induces transitions from the $\nu=0$ band to ‘bands’ in the continuum, with an excitation energy $\sim t$ which usually far exceeds the bandwidth $\sim J$. Then, particle-hole transitions of Fermions between bands of width $W$, which are separated in energy by $E \gg W$, will give the contribution $C(\omega) \approx \rho_f \delta(\omega - E)$, to the correlation function, where $\rho_f$ is the density of Fermions in the lower (partially occupied) band. This immediately explains the apparently Bosonic doping dependence of the DCF, which thus originates from the possibility to excite high-energy degrees of freedom of the structured spin bag quasiparticles. Only for small momentum transfer the increase in kinetic energy is small, so that $O_d$ also can generate particle-hole transitions in the $\nu=0$ band, where restrictions due to the Pauli principle apply, hence the deviations from the scaling of the DCF with $n_h$ in the low energy region. The spin bag scenario thus provides a natural explanation for the unusual scaling behaviour of the different correlation functions; it is supported by detailed consistency with a substantial body of numerical evidence. For completeness we note that slave-boson mean-field theories [14] describe the ground state of the $t-J$ model as a product of condensed Bosons in a band of width $\sim 8t$ and Fermions in a band of width $\sim 4J$. With the additional assumption that the density operator acts only on the bosons, the spin operator only on the Fermions, this ground state clearly would have an excitation spectrum which is consistent with the numerical results; the justification of this assumption as well as the possible agreement with details of the cluster results remains to be clarified.

In summary, we have studied the dynamical spin and density correlation function for the 2D $t-J$ model near half-filing. Whereas these correlation functions should be closely related in a Fermi liquid, we found them to differ substantially for this strong correlation model: the density correlation function has a Boson-like dependence on the hole density and the hopping integral $t$ as its characteristic energy scale, the doping dependence of the spin correlation function is consistent with Fermions and it has the exchange constant $J$ as energy scale. While the remarkably systematic scaling of the correlation functions suggests the existence of a simple ‘effective theory’ for the excitation spectrum, the familiar particle-hole picture thus is clearly insufficient. The familiar spin bag picture then provides a promising framework for such an effective theory: the strong dressing of the hole with spin fluctuations and the resulting complex internal structure of the spin bag-type quasiparticles lead to a qualitatively new type of excitations, namely the excitation of internal degrees of freedom of the quasiparticles. Spin and density operator differ markedly in their ability to excite the various degrees of freedom of the spin bag liquid, hence their very different spectra. While details need to be worked out, it seems obvious that the existence of such new types of excitations, as well as the apparently very different response of the spin bag liquid to ‘spin-like’ and ‘charge-like’ perturbations may lead to experimentally observable anomalies e.g. in high-temperature superconductors.

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DCF divided by $n_h$ for various $n_h$ $(t/J = 2.5$, Lorentzian broadening $\epsilon=0.2t$).

DCF for 2 holes in 16-sites for different $t/J$ ($\epsilon=0.2t$).

SCF for different $n_h$; the $(\pi, \pi)$ spectra are multiplied by 0.2 $(t/J = 2.5, \epsilon=0.5J)$.

SCF for 2 holes in 16 sites for different $t/J$; the $(\pi, \pi)$ spectra are multiplied by 0.2, $\epsilon=0.2J$.

SCF for 2 mobile and static holes. The $(\pi, \pi)$ spectra are multiplied by 0.2, $\epsilon=0.5J$. 

TABLE I. (a) $\Delta_{q} (k)$ for spin and charge operator with $q = (\pi, \pi)$ (16 sites, 2 holes, $t/J = 2.5$). (b) $n_{shf}(q)$ for the same system.

| $k, q$ | $(0, 0)$ | $(\pi/2, 0)$ | $(0, \pi)$ | $(\pi/2, \pi/2)$ | $(\pi, \pi/2)$ | $(\pi, \pi)$ |
|--------|----------|--------------|-----------|----------------|--------------|------------|
| (a), $O_s$ | -0.001 | -0.004 | -0.037 | +0.001 | +0.017 | +0.016 |
| (a), $O_d$ | -0.130 | -0.114 | +0.014 | 0.000 | +0.111 | +0.114 |
| (b), $O_s$ | 0.000 | 0.3174 | 0.2826 | 0.2863 | 0.1930 | 0.1778 |
| (b), $O_d$ | 0.000 | 0.7437 | 0.7911 | 1.0568 | 1.1673 | 1.1714 |

TABLE II. Hole occupation numbers $\bar{n}(k)$ divided by $n_h$ for different $k$ and $n_h$ (16 sites, $t/J = 2.5$).

| $n_h$ | 1 | 2 | 3 | 4 |
|-------|---|---|---|---|
| $\bar{n}(\pi, \pi)/n_h$ | 0.1679 | 0.1567 | 0.1549 | 0.1460 |
| $\bar{n}(\pi, \pi/2)/n_h$ | 0.1406 | 0.1537 | 0.1427 | 0.1373 |

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Figure 1

C_d(q,w) / n_h

1 hole
2 holes
3 holes
4 holes

(1/3,1/3) (0,2/3)
(1/2,1/2) (0,1)
(2/3,2/3) (1/3,1)
(1,1) (1/2,1)
Figure 2

\[ C_d(q,w) \]

- \( t/J = 1 \)
- \( t/J = 2 \)
- \( t/J = 4 \)
- \( t/J = 8 \)

\( w/t \)

- \((0, 1/2)\)
- \((1/2, 1/2)\)
- \((0, 1)\)
- \((1, 1)\)
- \((1/2, 1)\)
Figure 3

\[ C_s(q,w) \]

- 2 holes
- 3 holes
- 4 holes

- (0, 1/2)
- (1/3, 1/3)
- (0, 2/3)
- (1/2, 1/2)
- (0, 1)
- (2/3, 2/3)
- (1/3, 1)
- (1, 1)
- (1/2, 1)

\( w/J \)

\( x 0.2 \)

- 2 holes
- 3 holes
- 4 holes
Figure 4

\[ C_s(q, w) \]

- \( t/J = 1 \)
- \( t/J = 2 \)
- \( t/J = 4 \)
- \( t/J = 8 \)

- (0, 1/2)
- (1/2, 1/2)
- (0, 1)

- (1, 1)
- (1/2, 1)

\[ x 0.2 \]

\[ w/J \]

\[ C_s(q, w) \]
Figure 5

\[ C_s(q,w) \]

- \( t/J=0 \)
- \( t/J=2.5 \)

Different points and lines for various values of \( (q,w) \):
- \((1/3,1/3)\)
- \((1/2,1/2)\)
- \((1/3,1/2)\)
- \((1/2,1)\)
- \((1,1)\)
- \((1/2,1)\)

Axes:
- \( w/J \) on x-axis
- \( C_s(q,w) \) on y-axis

Legend:
- \( x \times 0.2 \)