Evidence for composite nature of quasiparticles in the 2D t–J model

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I. INTRODUCTION

The discovery of high-temperature superconductivity has motivated a considerable effort in the study of strongly correlated fermion systems. The question of spin-charge separation is an important issue in these systems. In the case of the 1D t-J model, it is known that a hole injected into the undoped system decays into two elementary excitations, a charge-1 spinless excitation (holon) and a neutral spin-1/2 excitation (spinon). Holons and spinons are independent excitations whose dispersion relations respectively scale with the hopping integral $t$ and with the spin-spin coupling constant $J$, so that the decay products of an injected hole get quickly separated. The question of spin-charge separation is more controversial in the case of the 2D t-J model, which is the simplest model used to describe the CuO planes of doped HTc materials. Anderson suggested that, in analogy with the 1-D case, a single hole in the 2D t-J model decays into elementary excitations of spinon- and holon-type. Other approaches describe the single hole as surrounded by a region with reduced antiferromagnetic order, leading to a charge-1 spin-1/2 quasiparticle.

Based on exact calculations for small systems, we present here evidences that the hole in the 2D t-J model decays into elementary excitations of spinon and holon type. Following Ref. ³ we make the case that the Drude conductivity and the total width of the spectral density of the hole, which are observed to depend mainly on parameter $t$, are inconsistent with the interpretation of the low energy behavior of the spectral density as a simple quasiparticle whose dispersion scales with $J$. All these properties of the hole can however be simply understood in terms of spinons and holons, provided that, in 2D, there exists a long ranged attraction between spinons and holons which scales with $J$. In the presence of such an attraction, the quasiparticle-like pole seen in the spectral density of the single hole can be regarded as a bound state of two constituents, a light one (holon) and a heavy one (spinon).

The long ranged attraction between the heavy constituent and the light constituent of the hole in 2D can be visualized using a string picture. In this picture, a hole is initially created in an antiferromagnet by removing an electron. The hole then hops away, leaving a wake of flipped spins behind. In absence of spin-flip terms in the Hamiltonian, the hole is bound to its initial position by the energy cost of the wake of flipped spins. A more formal description of this attraction can be obtained using the gauge theory of quantum antiferromagnets in which the fields of matter describing spinons and holons are coupled to a confining gauge field. This leads to the confinement of the constituents of the hole (spinon and holon), similar to the confinement of quarks which are the constituents of hadrons and mesons. The observation of spin-charge separation in the 2D t-J model at small time and length scales is therefore important, because it strongly suggests that elementary excitations with quantum numbers and interaction similar to those of quarks can be found in quantum antiferromagnets.

In this note, we consider the properties of holes in the t-J model which is defined by the Hamiltonian

$$H = T + \frac{J}{2} \sum_{< jl >} S_j \cdot S_l, \quad (1)$$

where the kinetic term $T$ is given by

$$T = P_G \left[ -t \sum_{< jl >\sigma} c_{jl\sigma}^\dagger c_{jl\sigma} \right] P_G \quad (2)$$

and where $P_G$ is the Gutzwiller projector which filters out states containing doubly occupied sites. The sum $< jl >$ is performed over near-neighbor pairs sites, with each pair counted twice to maintain hermiticity.
II. SINGLE HOLE PROPERTIES

Let us first consider the propagator of the hole, which is defined by

$$G_{k\sigma}(\omega) = \frac{1}{\omega + E^{(N)}_0 - \mathcal{H} + i\eta} \langle \Psi_{0}^{(N)} | c_{k\sigma}^\dagger c_{k\sigma} | \Psi_{0}^{(N)} \rangle,$$

(3)

where $| \Psi_{0}^{(N)} \rangle$ denotes the undoped (Néel) groundstate of the system with energy $E^{(N)}_0$, $c_{k\sigma} = N^{-1/2} \sum_{j} e^{i k \cdot r_j} c_{j\sigma}$, and $N$ is the number of sites. In Eq. (3) and in the following, we set $\hbar = 1$. In Fig. 3, we show the spectral density

$$A_k(\omega) = -\frac{1}{\pi} \text{Im} G_{k\sigma}(\omega)$$

(4)

obtained by exact diagonalization of 26-site and 32-site clusters for $J = 0$ and at different momenta. At $\Sigma (\pi/2, \pi/2)$, an 8t-wide continuum consisting of two lobes with a hole in the middle is clearly visible. When one goes along the $\Gamma$–M direction (from $(0,0)$ to $(\pi, \pi)$) weight is re-distributed from negative to positive frequencies. This is consistent with the calculation of Ref. 17 based on chiral spin liquid, in which these structures remain visible in the vicinity of $(\pi, \pi)$ as we shall discuss later on.

In Fig. 2(b,c), low energy poles located at the bottom of the spectrum become visible when the antiferromagnetic coupling $J/t$ is turned on. They can be interpreted as signatures of quasiparticles with a definite dispersion relation. Note that, although the quasiparticle-like pole is present for all momenta (only $\Sigma$ is shown on Fig. 2), it has a much smaller weight at momentum $k = (\pi, \pi) (M)$ as we shall discuss later on.

Fig. 2(d-f) shows the same quantities evaluated using a perturbative approach based on linear spin-wave theory. In this approach, the fermionic operator $c_{k\sigma}$ is expressed in terms of the spin-wave bosonic operator and a fermionic spinless hole operator. The hole propagator is then approximated by the propagator of the spinless hole, which is numerically evaluated within the self-consistent Born approximation. In this approximation, the line of the spinless hole propagator is dressed by non-crossing spin-wave lines. The perturbative results of Fig. 2(d-f) agree well enough with the exact results of Fig. 2(a-c) to help to understand the structure seen in Fig. 2(b-c), as we shall discuss later on.

The quasiparticle dispersion relation vs momentum is shown in Fig. 3(a) from an interpolation between the data obtained at the allowed $K$-values of the 26-cluster. It agrees remarkably well with the Green Function Monte Carlo data showing in particular a pronounced minimum at momentum $(\pi/2, \pi/2)$ and a flat band in the vicinity of $(\pi, 0)$. Fig. 3(b) shows the linear behavior of the total bandwidth defined as the difference in quasiparticle energy between the top of the band at $\Gamma$ (expected to become exactly degenerate with M in the thermodynamic limit) and the bottom of the band at $\Sigma$.

In Figs. 3(a-c), we show the weights

$$Z_k = \left| \frac{\langle \Psi_{k}^{(N-1)} | \cdots c_{k\sigma} | \Psi_{0}^{(N)} \rangle}{\langle \Psi_{0}^{(N)} | \cdots c_{k\sigma}^\dagger c_{k\sigma} | \Psi_{0}^{(N)} \rangle} \right|^2,$$

(5)

of the quasiparticle poles as a function of $J/t$ for the bottom (Fig. 3(a)) and the top of the band (Fig. 3(b,c)), where $| \Psi_{k}^{(N-1)} \rangle$ denotes the groundstate of the system with one hole and momentum $k$. The vanishing of $Z_k$ in the limit $J/t \to 0$ reflects the divergence of the "quasiparticle" size, i.e. the region of reduced antiferromagnetic order.

At this point, it is important to notice that the spectral density extends on an energy interval of order $8t$ as seen in Fig. 3. It is remarkable that this energy width is basically almost independent of $J$ while, on the other hand, the quasiparticle bandwidth varies linearly with $J$. As mentioned previously, the spectral function at higher energy also shows a strong $k$-dependence. These facts are clearly difficult to explain without taking into account the complex nature of the quasiparticle.

The description of the hole propagator in terms of a simple quasiparticle dispersing like $J$ is also a priori difficult to reconcile with the observation that the optical conductivity of the hole depends mainly on $t$ as first noticed by one of us. The optical conductivity is defined by

$$\sigma_{xx}(\omega) = 2\pi D\delta(\omega) + \frac{\pi e^2}{N} \sum_{n \neq 0} \frac{|\langle n | j_x | 0 \rangle|^2}{E_n - E_0} \delta(\omega - E_n + E_0),$$

(6)

where the weight $\pi D$ of the Drude peak is simply proportional to the charge stiffness $D$ given by

$$D = -\frac{e^2}{4N} \langle \langle 0 | T | 0 \rangle \rangle - \frac{e^2}{N} \sum_{n \neq 0} \frac{|\langle n | j_x | 0 \rangle|^2}{E_n - E_0},$$

(7)

where $\langle 0 \rangle$ and $| n \rangle$ respectively denote the groundstate and excited states with energies $E_0$ and $E_n$ of the system with a given number of electrons and where

$$j_x = it \sum_{l} \left[ c_{l\sigma}^\dagger c_{l+\hat{x} \sigma} - c_{l+\hat{x} \sigma}^\dagger c_{l\sigma} \right]$$

(8)

with $\hat{x}$ denoting the vector connecting two neighboring sites along the $x$ direction.

Following Ref. 7 it is convenient to consider the ratio $D/e^2 n_h$ since we expect $D$ to scale with the hole doping $n_h$. This ratio has then the physical meaning of an inverse mass. Fig. 4 shows the dependence of the quantity $D/e^2 n_h$ given in units of $t$ as a function of $J/t$ for a system of 26 sites containing a single hole. Previous data
obtained by averaging over the boundary conditions (to reduce finite size effects) of a $4 \times 4$ cluster with one or two holes. Using Eq. (9), the quantity $1/2m$ can be expressed as a sum of two terms, (i) $D/e^2 n_h$ shown in Fig. 3 (called “inverse optical mass” in Ref. 3) and (ii) the finite frequency integrated weight $\int_0^\infty \sigma_{xx}(\omega) d\omega/(\pi e^2 n_h)$ also shown in Fig. 3. This leads to

$$m \approx 0.7 \frac{1}{t}$$

in units where the lattice bound length is set equal to one, i.e. the holon mass depends mainly on parameter $t$. Note that this estimate for the holon mass agrees well with that of chiral spin liquid theory. Both Eqs. (10) and (11) are consistent with exact results for systems with several holes, in which the total weight is found to be nearly independent of $J$ and proportional to doping.

The quasiparticle-like pole appearing in the spectral density of Fig. 3 for finite $J$ can be attributed to the spinon-holon bound state. The dispersion of the spinon-holon pair is characterized by the dispersion of the heaviest object, which is the spinon in the case of interest $J \approx 0.2t$. This is consistent with the finding that the quasiparticle bandwidth scales with $J$, shown in Fig. 3. Also, the vanishing of the quasiparticle weight $Z$ in the limit $J \rightarrow 0$ seen in Fig. 3 reflects the divergence of the size of the spinon-holon bound state, consistent with the vanishing of the confining potential $V(r) = \alpha J|\mathbf{r}|$ in this limit.

As can be seen in Fig. 3(c,f), the spectral density evaluated perturbatively for finite $J$ shows a series of resonances above the quasiparticle-like pole. These so-called string resonances can be interpreted as higher energy bound states of the spinon-holon pair. The energy dependence of both the quasiparticle-like pole and the first higher-energy resonance is displayed in Fig. 3. In this figure, the straight lines correspond to the fit

$$E_n = \beta t + \gamma_n (J/t)^{2/3} t,$$

where $\beta = -3.28$, $\gamma_0 = 2.16$ for the quasiparticle-like pole and $\gamma_1 = 5.46$ for the first higher-energy resonance. This is the behavior expected for the spectrum of a light particle in orbit around a heavy one, described by the Hamiltonian

$$H = -\frac{1}{2m} \nabla^2 + \alpha J|\mathbf{r}| + \beta t,$$

where $m$ is the mass of the light particle (holon) estimated using the f-sum rule. Using the energy dependence of either the quasiparticle-like pole or the first higher-energy resonance, one respectively finds $\beta = 1.64$ or $\alpha = 2.16$ for the string tension. Exact results for the quasiparticle-like pole are also well fitted using Eq. (11) with constants $\beta = -3.359$ and $\gamma_0 = 2.77$, leading to $\alpha = 2.39$. Nevertheless the observation of high-energy resonances in exact diagonalizations of small clusters has been more controversial. Although some authors have attributed some peaks in the spectral function of the $4 \times 4$ cluster to these resonances, similar studies carried out on larger clusters failed to detect any sharp structure. However, it is tempting to attribute the structure appearing at $\omega \approx -2.3t$ in Fig. 3(b) and at $\omega \approx -1.7t$ in Fig. 3(c) (indicated by arrows on the plot) to the first higher-energy string resonance. This structure can be fitted using Eq. (11) with constants $\beta = -3.359$ and $\gamma_1 = 4.95$, leading to $\alpha = 1.86$. Note that these data correspond to quite small $J/t$ ratios. For increasing $J/t$ (let’s say $J/t > 0.2$) the lifetimes of the string states becomes rapidly too small to be observable.

As seen in Figs. 3 and 3 significant spectral weight appears on a broad 8$t$-wide energy range. This continuum can be crudely viewed as the excitation spectrum of the light particle (holon) whose oscillator strength lies mainly at high frequencies.

We conclude by a comment on the rather weak dependence of the Drude weight on $J$ shown in Fig. 3 for one or several holes in small t-J clusters. This implies that a hole doped into the system has a dynamic mass which depends on $t$ only. This is in contradiction with the linear behavior of the quasiparticle bandwidth as a function of $J$ seen in Fig. 3(b), which implies that the mass of the hole depends on $J$ only. It is very likely that one of these results is contaminated by finite size effects but, so far, it is impossible to determine which one without computations on larger samples. It is however important to settle the question of which of these results holds in
the thermodynamic limit in order to determine wether or not holes decay into more elementary constituents at low doping: If our observation that the Drude weight is independent of J is not seen on larger systems, this would mean that this decay is indeed not possible. This would be the case if the Drude “pole” separates, in the thermodynamic limit, into a legitimate Drude pole containing a small fraction $\propto J$ and a very low frequency band containing the rest.

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FIG. 1. Single hole spectral functions for $J=0$ calculated on small 2D clusters with 32 and 26 lattice sites. The $\Gamma$, M and $\Sigma$ points in reciprocal space corresponds to momenta $(0,0)$, $(\pi, \pi)$ and $(\pi/2, \pi/2)$ respectively as shown in the insert. The spectral function at $(\pi/2, \pi/2)$ is in fact obtained by averaging the two spectral functions taken at the two nearest momenta.

FIG. 2. Spectral function at $\Sigma$ for various $J/t$ values calculated on the same 26-site cluster. (a-c) corresponds to the exact results and (d-f) to the spin-wave calculations. In (b,c) arrows indicate the location of the first string resonance. The dashed curves in panel (d-f) correspond to a 40×40-site cluster, for which finite size effects are negligible.

FIG. 3. (a) Quasiparticle dispersion along some symmetry directions of the Brillouin zone obtained by interpolating exact results for a 26-sites cluster ( full line ) and obtained from spin-wave calculation for a 40×40-sites cluster (dashed line). (b) Quasiparticle bandwidth vs J/t calculated on a 26-site cluster. Hexagons and triangles respectively denote exact and perturbative results. A linear behavior like 2.2 J/t is also shown for comparison.

FIG. 4. Quasiparticle weights vs J/t calculated on a 26-site cluster for various location in k-space. (a), (b) and (c) correspond to the $\Sigma$, $\Gamma$ and $M$ points as indicated on the figures. Filled and empty squares respectively correspond to exact and perturbative results.

FIG. 5. $D/c^2\rho_h$ for a single hole on a 26-site cluster (filled hexagons) in units of $t$. The finite frequency integrated weight $\int_0^\infty \sigma_{xx}(\omega) d\omega/\pi c^2\rho_h$ is also shown (empty hexagons). Similar results are given for one (triangles) or two (squares) holes on a 4×4 cluster. In that case an average over the boundary conditions was used, leading to values larger than those obtained in Ref. [4].
FIG. 6. Ground-state energy for a single hole as a function of $J$, obtained from exact calculations for a 26-site cluster (filled triangles) and from spin-wave calculations (empty triangles). Similar results are given for the energy of the first string resonance (squares) at momentum corresponding to the band bottom of the quasiparticle-like pole. In the case of exact results, the first string resonance is identified as the structure in the spectral density visible at $\omega = -2.3t$ in Fig. 2(b) and at $\omega = -1.7t$ in Fig. 2(c).
\[ t - J \]
\[ \sqrt{26} \times \sqrt{26} \]
\[ \sum \]
\[ J = 0 \]

\[ (a) \]

\[ J = 0.1 \]

\[ (b) \]

\[ J = 0.2 \]

\[ (c) \]

\[ A_k(\omega) \]

\[ \omega / t \]
\( t - J \)
\( \sqrt{26} \times \sqrt{26} \)
\[ \sum \]

(d) \( J = 0 \)

(e) \( J = 0.1 \)

(f) \( J = 0.2 \)
\( \sqrt{26} \times \sqrt{26} \)

\( J/t = 0.3 \)
(b) $t - J$

$\sqrt{26} \times \sqrt{26}$
\[ t - J \]
\[ \sqrt{26} \times \sqrt{26} \]

(a)
$t - J$

$\sqrt{26} \times \sqrt{26}$

(b)

$Z_k$

$0.5$

$0.25$

$0$

$0.5$

$1$

$J / t$

$\Gamma$
