Spin susceptibility and the $\pi$-excitation in underdoped cuprates.

Jan Brinckmann and Patrick A. Lee
Massachusetts Institute of Technology, Cambridge MA 02139
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The dynamical spin susceptibility $\chi''_\pi$ at wave vector $(\pi, \pi)$ and the spectrum $\pi''$ of the spin-triplet particle–particle excitation with center of mass momentum $(\pi, \pi)$ ($\pi$-excitation) are considered in the slave-boson formulation of the t–J-model. Propagators are calculated in a diagrammatic t-matrix approximation in the d-wave superconducting state for a wide doping range. The resulting spectra $\chi''_\pi$ and $\pi''$ both show a resonance at a doping dependent energy, in qualitative agreement with recent numerical cluster calculations. In underdoped systems, the peak position is comparable to that found in neutron scattering experiments. The peak in $\chi''_\pi$ as well as $\pi''$ is at low doping entirely caused by spin fluctuations, whereas the triplet particle–particle channel does not contribute as a collective mode.

The spin-triplet particle–particle excitation (‘$\pi$-excitation’)

$$\hat{\pi} = \sum_k (\cos(k_x) - \cos(k_y)) c_{k+q}^\dagger c_{k+q+\uparrow}$$

at wave vector $q = (\pi, \pi)$ has been introduced in [1] as a possible explanation for the ‘41 meV resonance’ observed in neutron scattering on cuprates in the superconducting state (see e.g. [2,3]). It has been argued that $\hat{\pi}^\dagger$ is an approximate collective eigenmode of the t–J or Hubbard model. The coupling of spin-triplet particle–particle excited states and spin-singlet particle–hole states in the superconducting phase then should lead to a resonance in the susceptibility $\chi''_\pi(\omega)$ at $q = (\pi, \pi)$ at the energy $\omega_0$ of this mode.

We compare the susceptibility and the propagator of the $\pi$-excitation in a slave-boson theory for a wide range of hole concentrations (doping). Both calculated spectra $\chi''_\pi$ and $\pi''$ show a pronounced resonance at the same energy $\omega_0$, which is roughly given by the chemical potential $\mu$ as $\omega_0 \approx 2|\mu|$. The outcome is in qualitative agreement with the aforementioned prediction and with recent numerical [4,5] and diagrammatic calculations [6]. However, our interpretation differs from that originally envisioned in [1]: The diagrammatic spin-triplet particle–particle channel does not contribute as a collective mode to $\chi''_\pi$ or $\pi''$. In underdoped systems not far from the Néel state, the resonance is solely caused by the ‘RPA channel’, which describes spin fluctuations mediated through spin-singlet particle–hole excitations of fermions. The ‘$\pi$-propagator’ is given as

$$\pi(\omega) = \langle T_\tau \hat{\pi}(\tau)\hat{\pi}^\dagger(\tau') \rangle^{\omega} .$$

We start from the t–J-model and consider a Gutzwiller-projected $\pi$-propagator, Eq. [1] with $\hat{\pi} \rightarrow P_G \hat{\pi} P_G$. The calculations for $\pi(\omega)$ as well as the susceptibility $\chi_\pi(\omega)$ are performed within the standard slave-boson scheme. Diagrammatic expressions are based on a self-consistent perturbation theory with self energies taken at Hartree-Fock (mean-field) level. We consider the superconducting state at very low temperature, i.e., the d-wave pairing phase of fermions and fully condensed bosons. The t-matrix approximation for $\chi_\pi(\omega)$ and $\pi(\omega)$ are indicated in Figs. [1.a] and [1.b] respectively. The susceptibility is given by the vertex-renormalized mean-field bubbles displayed in Fig. [1.a], which are to be inserted into

$$\chi_\pi(\omega) = \chi_\pi(\omega)/(1 - 2J\chi_\pi(\omega)) .$$

Eq. [2] represents the particle–hole RPA channel (random phase approximation).

The single and double arrowed lines in Fig. [1] stand for the normal and pairing Green’s functions of auxiliary fermions. The dashed line in Fig. [1.a] is the t–J-model’s spin and density interaction for fermions on two nearest neighbor lattice sites i, j,

$$J \sum_{<i,j>} [S_i S_j - \frac{1}{4} n_i n_j]$$

with $n_i = \sum_\sigma f_\sigma^\dagger f_\sigma$.
\[ \pi_f = 2 + 2 + 4 \]

FIG. 2. t-matrix approximation for the \( \pi_f \)-propagator. The box indicates the phase factor \( \cos(k_x) - \cos(k_y) \), \( k \) is the summed (loop) wave vector. The double dashed line stands for the effective interaction \( J(q, \omega) \) (see text). Prefactors count degenerate exchange parts.

The vertex corrections entering \( \chi' \) consist of the spin-singlet particle-hole (ph) ladder diagrams shown in Fig. 1b. The double arrowed (anomalous) Green’s function introduces the ph channel in both time directions. In general it also allows for a coupling of the spin-triplet particle-particle (pp) channel into the singlet ph correlation function \( \chi'' \) by transforming e.g. a spin-up fermion into a spin-down hole and vice versa. However, the pp channel would appear in \( \chi'' \) as a vertex-function, involving at least one interaction vertex Eq. (3) with equal spin on both sites, which is zero [7]. This reflects the fact that Pauli’s principle blocks any exchange process involving at least one interaction vertex Eq. (3) with equal spin on both sites, which is zero [7]. This reflects the fact that Pauli’s principle blocks any exchange process. Thus the pp channel contributes no spectral weight to \( \chi'' \). This also holds if the pp channel is ‘artificially’ switched on by replacing \( n_i n_j \) in Eq. (3) with \( g n_i n_j \) and turning \( g = 1 \rightarrow g = 0 \): Recent numerical cluster calculations for the t–J-model [5] show that \( \chi'' \) is not affected by varying the coefficient of the density–density interaction. In the following we stick to the case \( g = 1 \).

Numerical calculations in the t-matrix approximation are performed with mean-field parameters set to reflect a fermion bandwidth of 4\( J \) and a superconducting gap \( \Delta_0 = 40 \text{ meV} \approx 0.3 J \). As has already been observed in earlier RPA calculations [5], an instability to the Néel state occurs at an unphysically high hole concentration \( x > x_c \). Since the vertex corrections of the t-matrix approximation turn out to have no significant effect, we assume a further renormalization of \( J \rightarrow \alpha J \) in Eq. (2). We have chosen \( \alpha = 0.5 \) such that \( x_c \) is reduced to \( \approx 0.02 \).

Results for \( \chi''(\omega) \) are shown in Fig. 3 (top) as continuous curves for several hole densities in the underdoped regime. The dominant feature is apparently a sharp and strongly doping dependent resonance. Its position \( \omega_0 \) shifts from \( \approx 0 \) at the magnetic instability \( (x = x_c = 0.02) \) to higher energies with increased doping, crossing the anticipated value \( 40 \text{ meV} \approx 0.3 J \) around \( x = x_m = 0.12 \). \( \omega_0 \) is for \( x > x_c \) roughly given by the chemical potential \( \mu \approx 2|\mu| \). This shift of the resonance with hole concentration is found in neutron scattering experiments on optimal [8] and underdoped YBCO-compounds [9,10]. The ‘optimal’ doping \( x_m \approx 0.12 \) found here also compares to experimental values. However, the spectral weight \( \int d^2 q \chi''(q, \omega) / \int d^2 q \) comes out too small with respect to the experiment [11].

The resonance is caused by the spin-fluctuation RPA channel Eq. (3): For comparison, dashed curves in Fig. 3 (top) show the results for \( \tilde{\chi}''_\pi(\omega) \), i.e., the renormalized bubble diagrams in Fig. 1b. The position of the doping dependent peak here is bound from below by \( \approx 2\Delta_0 = 0.6 J \), even for lowest doping. The contribution from the \( ph \) vertex corrections is quite small, \( \tilde{\chi}''_\pi \) differs only slightly from the well known mean-field susceptibility.

The results for the susceptibility may be compared to the \( \pi \)-propagator Eq. (4). In slave-particle formulation, with bosons completely condensed at very low temperature, it reads \( \pi(\omega) = x^2 \pi_f(\omega) \). The prefactor \( x^2 \) is the (mean-field) probability of finding two empty lat-
tice sites when adding a spin-triplet pair of particles. The \( \pi \)-propagator for fermions \( \pi_f(\omega) \) appearing here is formally identical to Eq. (1), its t-matrix approximation is displayed in Fig. 2. According to the discussion given above, the triplet \( pp \) channel may contribute only as the mean-field bubble (1st diagram). The singlet \( ph \) channel appears in vertex renormalizations in the 2nd and 3rd diagram. The 3rd diagram contains the contribution from the RPA channel via \( J(q, \omega)/2 = \frac{1}{2} J(q) + \frac{1}{2} J(q) \chi(q, \omega) J(q) \), indicated as a double dashed line in Fig. 2.

The resulting spectrum \( \pi''(\omega) \) in the underdoped regime is shown in Fig. 3 (bottom) for the same set of parameters and hole densities \( x \) as the susceptibility. Continuous lines correspond to the t-matrix approximation, dashed lines are calculated with the 3rd diagram in Fig. 2 (the coupling to the RPA channel) ignored. Again, the effect of the vertex corrections is negligible, the dashed curves differ only slightly from the mean-field theory (given by the 1st diagram in Fig. 2). Apparently \( \pi'' \) shows a pronounced peak which occurs at exactly the same position as the resonance in \( \chi'' \), if the same approximation is used for both quantities. As has been pointed out, the spin-fluctuation (RPA) channel has to be taken into account in the underdoped regime \( |\mu| < \Delta_0 \), where the system is not far from the instability to the Néel state, and the RPA dominates \( \chi'' \). In this case the peak in \( \pi'' \) is entirely caused by the coupling to spin fluctuations through \( J \). Note that its spectral weight decreases with reduced \( x \), and vanishes at the transition to the Néel state (\( x = x_c \approx 0.02 \)).

The picture changes in a highly overdoped situation \( |\mu| \gg \Delta_0 \): Fig. 4 shows curves for a large chemical potential \( \mu = -J \) (the breakdown of superconductivity in favor of the fermi-liquid state \( \Delta_0 = 0 \) is ignored for the moment). The peaks in \( \chi'' \) and \( \pi'' \) still occur at the same position \( \approx 2|\mu| \), but the RPA induces only a slight shift, besides an enhancement of \( \chi'' \). In the normal state \( \Delta_0 = 0 \) the resonance in \( \chi'' \) vanishes, whereas the peak in \( \pi'' \) remains as a delta function, \( \pi''(\omega) \sim x^2 \delta(\omega + 2\mu) \), as has also been observed in numerical calculations on highly doped clusters (referenced in (12)). In contrary to the low doping region, the highly overdoped regime \( |\mu| \gg \Delta_0 \) is well described by mean-field theory.

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FIG. 4. Set of curves for a large chemical potential \( \mu = -J \) in the superconducting state (see text). \( \chi'' \) and \( \pi'' \) (scaled \( \times 1/4 \)) are shown with the RPA-channel taken into account (continuous and dashed line respectively) and with the RPA channel omitted (dotted and dashed-dotted line resp.).

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