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Spin-gap and magnetic excitations in the cuprate superconductors*

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We have analysed the spin-excitation spectrum as observed by neutron and NMR experiments in $YBa_2Cu_3O_{6+x}$ in the frame of a bidimensional t - t' - J model. Next-nearest neighbour hopping term t' is introduced in order to fit the shape of the Fermi surface revealed by photoemission. Within the slave-boson approach, we study as well the d-wave superconducting state, as the singlet-RVB state which is expected to describe the normal phase of heavily-doped systems. In the superconducting state, d-wave pairing leads to the prediction of a resonance and a gap-structure in the spin-excitation spectrum, in good agreement with neutron diffraction results for $x = 0.92$ and $x = 1.0$. Our calculations show a smooth evolution of the spectrum from one phase to the other: the value of the threshold of excitations E_G increases with doping, while the temperature T_m at which the spin-gap opens regularly decreases, reaching T_C only in the overdoped regime. This very atypical combined variation of E_G and T_m with doping results of strong-correlation effects in presence of the realistic band-structure considered here.

Experimentally, it is well admitted that while long range antiferromagnetic order is destroyed above $x = 0.4$ in $YBa_2Cu_3O_{6+x}$, the neutron scattering signal keeps its maximum of amplitude around the antiferromagnetic wavevector $\vec{Q} = (\pi, \pi)$. At low temperatures, the magnetic form factor $S(\vec{Q}, \omega)$ shows a depression of intensity when decreasing frequency, with a finite cut-off of order 50meV . A so-called pseudo-gap (or spin-gap) appears [1,2], the value of which continuously increases with doping ($E_G = 4, 16, 28$ and 26meV at $x = 0.51, 0.69, 0.92$ and 1.0). This pseudo-gap persists above T_C for heavily-doped systems ($x = 0.51, 0.69$ and 0.92), up to a temperature scale T_m which decreases with doping. For overdoped systems ($x = 1.0$) the gap disappears immediately above T_C , as in usual superconductors. In addition to the existence of a pseudo-gap, a resonance appears in the superconducting phase in $S(\vec{Q}, \omega)$ at $\omega = 41\text{meV}$ ($x = 0.92$ or 1.0) for $T = 5\text{K}$ [1,3]. This resonance is accompanied by an enhancement of the magnetic correlation length in its vicinity. NMR results are consistent with the opening of a pseudo-gap with the presence of a maximum of $(T_1T)^{-1}$ on ^{63}Cu at a temperature $T_m > T_C$ (with $T_m = T_C$ in overdoped

systems).

In the weak-coupling limit, we have studied in a previous paper [4] the superconducting state with a d-wave symmetry of the pairing parameter Δ_0 . The striking resemblance found between the spectrum of spin-excitations of the superconducting state in the weak-coupling limit, and the spectrum experimentally observed in the normal phase of heavily-doped systems, incited us to extend the d-wave pairing to the singlet-RVB state above T_C , in the strong coupling limit of the t - t' - J model.

In the slave-boson representation, we can write the t - t' - J hamiltonian as

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} c_{i\sigma} c_{j\sigma}^\dagger - t' \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} c_{i\sigma} c_{j\sigma}^\dagger + J \sum_{\langle i,j \rangle} \tilde{S}_i \tilde{S}_j$$

with $c_i^\dagger c_i + \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} = 1$. We have numerically solved the system of saddle-point equations [5], and studied the effect of d-wave pairing in both superconducting state, in which holons c_i are partially condensed ($T < T_{BE}$), and RVB state, in which the first excited levels are occupied ($T > T_{BE}$). We have computed the spin susceptibility $\chi''(\vec{q}, \omega)$ within this scheme includ-

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ing RPA renormalization. The strong-coupling effects make themselves felt through the renormalisation of the various parameters entering the expression of the susceptibility. We have plotted in Fig.1 the frequency-dependence of $\chi''(\vec{q}, \omega)$ at $T=0$ for two values of doping. Let us note the presence of a gap, the value of which increases with doping. In addition, the overdoped case shows a resonance at higher frequency in agreement with the neutron diffraction results: this resonance is analyzed as a Kohn anomaly of the second kind in the Cooper channel

Figure 1 Spectral weight $\chi''(\vec{Q}, \omega_0)$ versus frequency ω (a) overdoped system (b) heavily-doped system

We were able to establish the analytic expression of the spin-gap according to

$$E_G = 8\Delta_0 \sqrt{\frac{\mu}{4t'} - \left(\frac{\Delta_0}{2t'}\right)^2}$$

This result enables us to understand the characteristic increase of E_G with doping even though Δ_0 decreases in the meanwhile (see Fig 2). The calculations have been as well pursued at finite temperature. The spin-gap is gradually filled up and the resonance disappears when the temperature increases. Fig 2 reports the evolution with doping of the temperature scale T_m at which the gap opens. This study shows the importance of

having included self-consistent effects contained in the strong-coupling limit in order to recover the decrease of T_m with doping, experimentally observed by neutron scattering experiments. We have also explored the $\vec{q}$ -dependence of the magnetic susceptibility $\chi''(\vec{q}, \omega_0)$ ($\omega_0 \ll E_G$). It is quite remarkable that the result predicts a peak in the signal around the antiferromagnetic wavevector $\vec{Q} = (\pi, \pi)$, accompanied by a characteristic enhancement of the magnetic correlation length around the resonance frequency

Figure 2 Combined variation of the spin-gap E_G and T_m , as a function of the chemical potential μ

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