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Spin excitations in high- T_c superconductors : discussion of neutron and NMR experiments

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The spin excitation spectrum as observed in neutron diffraction and NMR experiments in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ is theoretically examined on the basis of a bidimensionnal extended t - t' - J model in which next-nearest neighbour hopping term t' is considered in order to fit the shape of the Fermi surface observed in angle-resolved photoemission experiments. We study more specifically the superconducting phase in which d -wave pairing leads to the prediction of a resonance in $S(Q_0, \omega)$ surimposed to a gap-structure in agreement with the neutron results. We also extend our calculations to the study of the RVB (resonant-valence-bond) singlet state and show that the latter is a good candidate to describe the normal phase above T_c of heavily-doped systems.

In addition to their high superconducting temperature, the new superconducting oxides are noticeable by the aspect of the spin-excitation spectrum that they exhibit both above and below T_c . Long-range antiferromagnetic order exists at low doping. Antiferromagnetism disappears above a critical concentration of Oxygen for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. However, the neutron scattering signal keeps its maximum of amplitude around the AF vector $Q_0 = (\pi, \pi)$, showing a depression of intensity at low-frequencies with the existence of a so-called pseudo-gap (or spin-gap) which persists above T_c for heavily-doped systems. For surdoped systems ($x=1.0$), the gap disappears immediately above T_c as usual in superconductivity theory. In addition, the superconducting state is marked by the presence of a resonance at a characteristic frequency ω_0 situated above the gap value E_G . NMR results are consistent with the opening of a pseudo-gap with the presence of a maximum of $(T_1 T)^{-1}$ on ^{63}Cu at a temperature $T_m > T_c$ (with $T_m = T_c$ in surdoped systems).

We propose to understand the whole set of these experimental observations in the frame of a t - t' - J model on a square lattice appropriate to describe the electronic structure of the CuO_2 layers. The hamiltonian is :

$$H = \sum_{\langle i,j \rangle, \sigma} (-t f_{i\sigma}^\dagger f_{j\sigma} + J \vec{S}_i \cdot \vec{S}_j) - \sum_{\langle i,j \rangle', \sigma} t' f_{i\sigma}^\dagger f_{j\sigma}$$

where $f_{i\sigma}^\dagger$ is the creation operator of the Zhang-Rice singlet constituted by Copper spin and Oxygen spin

formed after doping; $\vec{S}_i$ represents the spin of Copper interacting via the superexchange coupling J ; t and t' are the hopping integral between nearest-neighbours $\langle i,j \rangle$ and next-nearest-neighbours $\langle i,j \rangle'$. The latter one is introduced to fit the shape of the Fermi surface observed in angle-resolved photoemission experiments which is found to be rotated of an angle 45° compared to the case $t'=0$, and is centered around the point (π, π) of the Brillouin zone (cf.figure1).

The severe constraint ($n_{fi} \leq 1$) which governs the $f_{i\sigma}^\dagger$ operator is treated within the standard slave-boson technique in which $f_{i\sigma}^\dagger \rightarrow c_{i\sigma}^\dagger e_i$ and the equality constraint: $e_i^\dagger e_i + \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} = 1$ is treated with the aid of Lagrange multipliers. In the saddle-point approximation, the mean-field parameters are : $\langle e_i^\dagger e_j \rangle = \delta$ at low temperatures (let the slave-bosons be either in the condensate or in the first excited states); $\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle = F$ independent of the bond in the fluxless state; $\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle = \Delta_0 (-1)^n$ where, for d -wave pairing, $n=1$ (or 2) depending whether vertical (or horizontal) bond is considered. The saddle-point equations (one of which being equivalent to the gap equation in BCS theory), determine the temperature and doping dependence of F , Δ_0 and chemical potential μ for given parameters t , t' and J . The spectrum of excitations is given by:

$$\varepsilon_k = \sqrt{(\xi_k - \mu)^2 + \Delta_k^2} \quad (1)$$

where $\xi_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$

and $\Delta_k = 2\Delta_0(\cos k_x - \cos k_y)$

($\tilde{t}$ and $\tilde{t}'$ are effective hopping integrals renormalised by mean-field parameters). The corresponding equienergetics are represented in figure 1. Close to the original Fermi surface, it develops four "superconducting bags" (ellipses) centered around the points A,B,C,D for which $\varepsilon_k = 0$ (intersection of the Fermi surface with the first bissectors).

Figure 1: Equienergetics $\varepsilon_k = \text{cste}$ derived from equation(1) for $\tilde{t}' / \tilde{t} = -0.45$, $\Delta / \tilde{t} = 0.05$ and $\mu / \tilde{t} = -0.6$. Note the presence of a Van Hove singularity at $\varepsilon_k = 4\tilde{t}'$ and the formation of 4 superconducting bags.

The unrenormalized dynamic susceptibility is given by:

$$\chi_o(\vec{q}, \omega) = \sum_k \frac{1}{4} \left(1 - \frac{\xi_k \xi_{k+q} + \Delta_k \Delta_{k+q}}{\varepsilon_k \varepsilon_{k+q}} \right) \frac{1 - n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})}{\omega - \varepsilon_k - \varepsilon_{k+q}} + \frac{1}{2} \left(1 + \frac{\xi_k \xi_{k+q} + \Delta_k \Delta_{k+q}}{\varepsilon_k \varepsilon_{k+q}} \right) \frac{n_F(\varepsilon_{k+q}) - n_F(\varepsilon_k)}{\omega - \varepsilon_{k+q} + \varepsilon_k}$$

and the renormalized susceptibility is obtained in the RPA scheme by :

$$\chi(\vec{q}, \omega) = \frac{\chi_o(\vec{q}, \omega)}{1 + J(\cos q_x + \cos q_y) \chi_o(\vec{q}, \omega)}$$

The result for the frequency-dependence of $\chi''(Q_0, \omega)$ at zero temperature is reported in figure 2 for $\delta = 0.16$. One notices the presence of a gap followed by a resonance which may account for the neutron results obtained in $\text{YBa}_2\text{Cu}_3\text{O}_{6.92}$ at $T = 5\text{K}$. To our point of view, this behaviour can be viewed as a signature of a d-wave superconductivity in the realistic structure considered here.

We have been able to establish the analytic expression of the gap E_G in $\chi''(Q_0, \omega)$ and its dependence as a function of the chemical potential μ has been analyzed. There are clearly two regimes: at

high doping when μ is of order $4\tilde{t}'$, E_G is of order $2(4\Delta_0)$ i.e. $3.5 T_c$ as in the standard BCS theory while at low doping, the value of the gap is radically different reaching the value $2|\mu|$ in the limit of low μ . In the latter case, the resonance is found to occur at much upper values of the frequency and then is expected to be suppressed as soon as the self-energy-corrections are included.

Figure 2 : Frequency-dependence of the RPA-renormalized $\chi''(Q_0, \omega)$ at $\delta = 0.16$ in the t - t' - J model in the $T = 0$ superconducting phase.

We have extended our calculations to the study of the RVB phase in which the pairing-temperature T_{RVB} of spinons $c_{i\sigma}$ does not coincide with the superconducting temperature which, in this scheme, requires the additional Bose-Einstein condensation of slave-bosons. The prediction of a gap of order $2|\mu|$ in the intermediate-doping regime of interest, persisting well above T_c provides strong arguments, when put together with the experimental data, in favour of a RVB description of the normal phase of heavily-doped systems.

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