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Spin Dynamics in high- T_c copper oxides

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We analyze the spectrum of magnetic excitations as observed by neutron diffraction and NMR experiments in $YBa_2Cu_3O_{6+x}$, in the frame of the single-band $t-t'$ - J model in which the next-nearest-neighbour hopping term has been introduced in order to fit the shape of the Fermi surface revealed in photoemission. Within the slave-boson approach, we have as well examined the d -wave superconducting state, and the singlet-RVB phase appropriate to describe the normal state of heavily-doped systems. Our calculations show a smooth evolution of the spectrum from one phase to the other, with the existence of a spin-gap in the frequency-dependence of $\chi''(\vec{Q}, \omega)$. The value of the threshold of excitations E_G is found to increase with doping, while the characteristic temperature-scale T_m at which the spin-gap opens, exhibits a regular decrease, reaching T_c only in overdoped regime. This very atypical combined variation of E_G and T_m with doping results of strong-correlation effects in presence of realistic band structure. We point out the presence of a resonance in the ω -dependence of $\chi''(\vec{Q}, \omega)$ in good agreement with the neutron diffraction results obtained at $x = 0.92$ and $x = 1.0$. This resonance is analyzed as a dynamical Kohn anomaly of the second kind in the Cooper channel. Finally, we examine the $\vec{q}$ -dependence of the dynamical susceptibility allowing to study the magnetic correlation length ξ as a function of doping, frequency and temperature.

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In this paper, we would like to address the problem of the theoretical understanding of the spin-excitations in high- T_c superconductors. The Inelastic Neutron Scattering and Nuclear Magnetic Resonance experiments performed in various cuprates both in the normal and in the superconductor states raise a number of fundamental questions that are very important to answer. Let us summarize here the essential features revealed in INS and NMR:

1. In the metallic phase above a critical value of doping, long-range antiferromagnetic order disappears but the dynamical spin structure factor $S(\vec{q}, \omega)$ keeps large amplitudes centered around the antiferromagnetic vector ($\vec{Q} = (\pi, \pi)$) in $YBa_2Cu_3O_{6+x}$ compounds^{1,2} or $\vec{q} = (\pi \pm \delta q, \pi)$ and $\vec{q} = (\pi, \pi \pm \delta q)$ in $La_{2-x}Sr_xCuO_4$ compounds³ signaling respectively commensurate or incommen-

surate spin-fluctuations.

2. The magnetic correlation length ξ deduced from the width of the $\vec{q}$ -dependence of $S(\vec{q}, \omega)$ regularly decreases with doping. The fact that ξ does not exhibit any significant dependence on temperature and frequency (except in the vicinity of the resonance outlined further) is undoubtedly an important point that has been thoroughly examined in the course of our work.

3. The study of the frequency dependence of $S(\vec{Q}, \omega)$ in $YBa_2Cu_3O_{6+x}$ shows a depression of intensity at low frequencies with a finite cut-off of order 50meV . Due to the difficulty of the measurements, specially at high doping for which the signal is largely broadened, there still exists a large controversy on the existence of a spin-gap. Some studies¹ indicate the formation of a pseudo-gap in the ω -dependence of $S(\vec{Q}, \omega)$ which persists well above T_c in the so-called "heavily doped" systems. Oppositely, on the other side of the optimally-doped regime associated to the maximum of T_c , the existence of the gap is restricted to the superconducting phase. The corresponding situation is schematized on the phase diagram reported in Fig.1(a). An interesting feature that has to be kept in mind is the difference in the doping-dependence of the threshold E_G of antiferromagnetic fluctuations, and the temperature-scale T_m signaling the opening of the gap. In the mentioned study, E_G increases with doping (reaching $3.5T_c$ only in the overdoped regime) while T_m simultaneously decreases until reaching T_c at high doping. Whatever will be the final issue concerning the experimental controversy about the existence of the spin-gap, it appeared crucial on the theoretical side to examine the question without any a priori assumptions on the existence of the spin-gap but by taking into account all the indications coming from the experiments, as for instance the shape of the Fermi surface determined by angle-resolved photoemission experiments.

4. Finally, and definitely established now is the existence of a resonance^{1,4} in the ω -dependence of $S(\vec{Q}, \omega)$ in $YBa_2Cu_3O_{6+x}$ ($x=0.92$ or 1.0) at a frequency of the order of 41meV . We propose an interpretation of this resonance in terms of dynamical Kohn anomaly in the Cooper channel (instead of the usual electron-hole channel). A remarkable point that we will also discuss concerns the observed enhancement of the magnetic correlation length ξ in the vicinity of the resonance.

5. The measurements of the nuclear relaxation rate on ^{63}Cu are consistent with the opening of a spin-gap in the spectrum of antiferromagnetic fluctuations. $^{63}(T_1T)^{-1}$ is large and does not exhibit a Korringa law but instead has a maximum as a function of temperature at the same temperature T_m as seen in INS, as expected if one realizes that the hyperfine constant of ^{63}Cu mostly filters the $\vec{Q} = (\pi, \pi)$ component. On the other hand, the nuclear relaxation rates on ^{89}Y and ^{17}O involving different $\vec{q}$ filtering, have different temperature behaviour. Both of these quantities show a decrease when lowering the temperature, starting from well above T_c in heavily-doped systems. Again the overdoped case is special since the decrease starts directly at T_c . In a non-conventional way, $(T_1T)^{-1}$ on ^{89}Y and ^{17}O vary linearly with the Knight shift.

The whole set of the INS and NMR data constitutes a puzzling problem in that the spin-excitation spectrum drastically differs from a traditional Fermi liquid. We will just mention that a number of theories have been developed these last years to understand this class of behavior starting from rather different points of view : quantum disordered description of the normal phase,⁵ Marginal Fermi liquid,⁶ or

more microscopic approaches starting from an electronic description of the CuO_2 layers. It is widely accepted now that the high- T_c cuprates come under the strong coupling regime reached either in multi-band⁷ or single-band descriptions⁸ formed from the Zhang and Rice singlets Cu-O in the layers. The role of the next-nearest hopping term t' is then crucial in order to reproduce a fermiology in agreement with the angle-resolved photoemission results⁹ on the shape of the Fermi surface. As has been pointed out in previous works for the weak coupling limit^{10,11} (t - t' -U Hubbard model), the effect of t' ($t' < 0$) makes the model a better starting point from a perturbative point of view :

- the Fermi surface is found to be rotated of 45° compared to the diamond shape and centered around the point $S(\pi, \pi)$ instead of $\Gamma(0, 0)$.

- it leads to the right sign of the Hall effect (cf. curvature of the Fermi surface) and the correct doping dependence of the Knight shift. As concerns the spin-excitations, the prediction for the weak-coupling regime gives no gap in the frequency dependence of $\chi''(\vec{Q}, \omega)$ for the current regime of interest ($4t' < \mu < t'$) as long as pairing effects are not considered ($4t'$ locates the position of the Van Hove singularity in the density of states). On the other hand, when pairing effects are introduced, with for instance a d-wave symmetry of the order parameter, we have shown¹¹ that the frequency-dependence of $\chi''(\vec{Q}, \omega)$ gains a gap with a very characteristic evolution of the threshold of excitations E_G with doping. In addition to the gap, the model leads to the prediction of a resonance in clear analogy with the experimental results obtained in $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ at $T_r < T_c$. The resonance has been analyzed as a dynamical Kohn anomaly of the second kind in the Cooper channel and is typical of axial superconductivity.

Motivated by the striking resemblance existing between the spectrum of magnetic excitations in the superconducting state of the weak-coupling regime, and the spectrum effectively observed in the normal phase of heavily doped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, we propose to examine in this paper the strong-coupling limit expressed in the t - t' -J model with the idea of extending the pairing effects to the singlet Resonant-Valence-Bond (RVB) phase above T_c . This problem, already addressed in some recent works¹² will be considered here¹³ closer to the systematics that we developed earlier in the weak-coupling limit.

In the slave-boson representation, the t - t' -J hamiltonian is written as:

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} c_{ie}^\dagger e_j^\dagger - t' \sum_{\langle i,j \rangle'} c_{i\sigma}^\dagger c_{j\sigma} c_{ie}^\dagger e_j^\dagger + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad (1)$$

in which the spin $\vec{S}_i$ is noted $S_i^\alpha = \sum_{\sigma\sigma'} c_{i\sigma}^\dagger \tau^\alpha c_{i\sigma'}$. It exists a local constraint:

$$e_i^\dagger e_i + \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} = 1$$

enforced at each site by time-independent Lagrange multipliers λ_i . Two characteristic temperatures arise from the mean-field approximation : the Bose condensation temperature of holons T_{BE} (defined by $\mu_B(T_{BE}) = 0$), and the pairing temperature of spinons T_{RVB} (defined by $\langle c_{i\uparrow}^\dagger c_{j\uparrow}^\dagger - c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger \rangle \neq 0$). Note that strictly speaking, T_{BE} should be zero whatever the doping is, resulting from general arguments on Bose condensation in two dimensions. This is no longer true if one allows for additional coupling between layers with a variation of T_{BE} with doping as represented

in Fig.1(b). The superconducting state is obtained when simultaneously spinons are paired and holons condensed, such that T_c is given by T_{BE} below δ_c , T_{RVB} above δ_c and then exhibits the nonmonotonic behavior quoted before. The RVB-state corresponds in the slave-boson representation to $T_{BE} < T < T_{RVB}$ for which pairing of spinons does not transpose into pairing of physical particles since the condensate of holons has lost its macroscopic occupation. In the case of the t - t' - J model within its slave-boson representation, we have numerically solved the saddle-point equations and found for instance a decrease of T_{RVB} with doping.

Fig.1 : Schematic phase diagram for $YBa_2Cu_3O_{6+x}$ (a) Sketch of experimental results (b) Sketch of theoretical results within the RVB hypothesis.

In the random-phase approximation, the dynamical susceptibility is calculated from :

$$\chi(\vec{q}, i\omega_n) = \frac{\chi_o(\vec{q}, i\omega_n)}{1 + J(\cos q_x + \cos q_y)\chi_o(\vec{q}, i\omega_n)} \quad (2)$$

in which $\chi_o(\vec{q}, i\omega_n)$ is the bare susceptibility involving both normal and anomalous contributions as usual in the BCS theory of superconductivity. At zero temperature, we have reported in Fig.2 the ω -dependence of $\chi(\vec{Q}, \omega)$ that we obtained for two different values of doping corresponding to under and overdoped cases. Note in the latter case the presence of a gap of value $E_G = 37\text{meV}$ followed by a resonance at $\omega_R = 47\text{meV}$ (T_{RVB} in this case is 120 K). The former case corresponds to a lower value of the gap $E_G = 14\text{meV}$ even though the characteristic temperature T_{RVB} is larger, of order 210K. Apart from the high-energy part of the spectrum which drags much too far compared to the experimental cut-off of order 50meV , our predictions concerning the value of the spin-gap and the position of the resonance are in good agreement with the measurements performed in $YBa_2Cu_3O_{6+x}$ by neutron diffraction. It is believed that self-energy corrections neglected in our mean-field approach would depress the energy tail and restore the correct order of magnitude for the cut-off. More work is required for a proper discussion of the high-energy contribution. Nevertheless, the results at low frequencies show very interesting features that we would like to comment :

1. The value of the spin-gap E_G is found to increase with doping. This result may surprise at the first sight, since conjointly, the characteristic pairing temperature T_{RVB} decreases. Actually, this very atypical behavior results in the interplay

of the anisotropy of the Fermi surface and of the anisotropy of the pairing parameter Δ_k . For instance, we have shown¹¹ that in the range of doping such as :

$$\{\mu_{c_1} = 4t' + \frac{2\Delta_0}{t'}\} < \mu < \{\mu_{c_2} = \frac{2\Delta_0}{t'}\} \quad (3)$$

the value of the threshold of antiferromagnetic excitations is :

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

The last equation settles the relation between E_G and the pairing parameter Δ_0 . Coming from the anisotropy of the gap parameter Δ_k , one can see that E_G scans a whole spectrum of values from 2μ (insensitive to the effect of Δ_0) to $2\sqrt{(4t' - \mu)^2 + (4\Delta_0)^2}$ (feeling the full effect of Δ_0) when μ goes from μ_{c_1} to μ_{c_2} . This effect is indeed at the origin of the opposite variation of E_G and T_{RVB} that we get as a function of doping.

2. The resonance that we obtain at $\omega_R = 47\text{meV}$ has to be brought closer to the surstructure observed by INS in $YBa_2Cu_3O_{6+x}$ ($x=0.92$ and 1.0). In our scheme, it arises as a Kohn anomaly of the second kind in the Cooper channel, i.e. the proximity of a Van Hove singularity in the density of double excitations ($\varepsilon_k + \varepsilon_{k+Q}$) obtained from pair breaking. The resonance appears as soon as $\mu \geq \mu_{c_1}$ and is progressively shaded off when μ becomes larger than μ_{c_2} .

Fig.2 : Dynamical susceptibility $\chi''(\vec{Q}, \omega)$ versus frequency ω (a) Overdoped (b) Heavily-doped systems.

Fig.3 : Combined variation of the spin-gap E_G and T_m as a function of the chemical potential μ .

Our calculations have been as well pursued at finite temperatures. The effect of temperature is to fill up the spin-gap in the regime $4t' < \mu < 0$, and to shade off the resonance. The temperature scale T_m at which the spin-gap opens has been determined from the position of the maximum of $\chi''(\vec{Q}, \omega_0)$ ($\omega_0 \ll E_G$) with temperature. Let us gather the doping dependence that we get for both T_m and E_G in Fig.3. The apparently contradictory behavior of E_G and T_m observed in neutron-diffraction experiments receives a natural explanation in the strong-coupling limit. T_m decreases with doping as T_{RVB} does, until reaching $T_m = T_{RVB} = T_c$ at high doping. In the meanwhile, E_G increases coming from anisotropy effects mentioned above.

Extending the calculation of $\chi''(\vec{q}, \omega)$ to any value of the momentum $\vec{q}$, our conclusion is that, for the chosen value of t' , $\chi''(\vec{q}, \omega)$ is always peaked around the antiferromagnetic vector $\vec{Q} = (\pi, \pi)$ with a $\vec{q}$ -widening $\delta\vec{q}$ which evolves with doping, frequency and temperature, giving access to the magnetic correlation length ξ . We found a characteristic reduction of ξ with doping. It is remarkable that our approach predicts an enhancement of the magnetic correlation length ξ just at the resonance frequency. To our point of view, this gives strong support to our analysis of the resonance as a Kohn anomaly. In the same way, we found that ξ is almost independent on temperature.

To conclude, we have sketched in this paper the consequences on the spectrum of spin-excitations of a $d_{x^2-y^2}$ pairing in presence of realistic band-structures and strong-coupling effects as contained in the t-t'-J model. This pairing may as well appear in the superconducting phase, as in the singlet-RVB phase above T_c for the underdoped systems. Our calculations show a smooth evolution of the spectrum from one phase to the other, with the existence of a spin-gap in the frequency-dependence of $\chi''(\vec{Q}, \omega)$, and very typical doping-dependence of the threshold E_G as compared to the temperature-scale T_m associated to the opening of the gap. We were also able to understand the resonance observed for $x = 0.92$ or 1.0 as a manifestation of a Kohn anomaly in the Cooper channel. The approach also leads to interesting predictions on NMR quantities which are reported elsewhere¹³. The direction for future work would concern quasi 3-D effects with the consideration of interlayer coupling which seems to play an important role in underdoped regime. On the other hand, it would also remain to consider the effects of gauge field fluctuations in the lattice model considered here, which is likely to be a more delicate problem compared to the continuum limit considered so far¹⁴.

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REFERENCES

1. J.Rossat-Mignod et al *PhysicaB* **169**,58 (1991); *Selected Topics in Superconductivity*, ed. by L.C.Gupta and M.S.Multani **1**,295 (1993).
2. P.M.Gehring et al *Phys.Rev.B* **44**, 2811 (1991).
3. T.E.Mason et al *Phys. Rev. Lett* **68**,1414 (1992)
4. H.A.Mook et al *Phys.Rev.Lett.* **70**, 3490 (1993).
5. A.Sokol, D.Pines *Phys. Rev. Lett.* **71**, 2813 (1993).
6. C.M.Varma et al *Phys. Rev. Lett.* **63**, 1996 (1989).
7. Q.Si et al *Phys. Rev. B* **47**, 9055(1993).
8. T.Tanamoto et al *J.P.S.J.* **62**, 1455(1993); D.R.Grempel, M.Lavagna *Sol.St.Com.* **83**, 595 (1992); S.V.Maleyev *J.Phys.* **2**, 181 (1992); K.Maki, H.Won *Phys.Rev.Lett.* **72**,1758 (1994).
9. J.C. Campuzano et al *Phys.Rev.Lett.* **64**,2308 (1990).
10. P.Bénard et al *Phys.Rev.B* **47**, 15217 (1993).
11. M.Lavagna et al *Phys.Rev.B* **49**,4235 (1994).
12. T.Tanamoto et al *J.P.S.J.* **62**, 717 (1993); **63**, 2739 (1994).
13. G.Stemmam et al *Phys.Rev.B* **50**,4075 (1994).
14. P.A.Lee and N.Nagaosa *Phys.Rev.B* **46**, 5621 (1992).