NEW SCENARIO FOR HIGH-T_C CUPRATES : ELECTRONIC TOPOLOGICAL TRANSITION AS A MOTOR FOR ANOMALIES IN THE UNDERDOPED REGIME

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This is a particularly exciting time for high-T_c. The experimental knowledge converges. Almost all experiments, nuclear magnetic resonance (NMR), angle resolved photoemission spectroscopy (ARPES), tunneling spectroscopy etc., provide an evidence for the existence of a characteristic energy scale $T^*(\delta)$ in the underdoped regime (δ is hole doping). Below and around the line $T^*(\delta)$ the "normal" state (i.e. above T_c) has properties fundamentally incompatible with the present understanding of metal physics. The field has reached the point when a consistent theory is needed to understand this experimentally well defined but theoretically exotic metallic behaviour and its relevance to high T_c superconductivity.

We show that these phenomena can be naturally understood within the concept of a proximity of the underdoped regime to an electronic topological transition (ETT). The concept of electronic topological transition due to the variation of the topology of the Fermi surface was introduced in the early 60's by I. Lifshitz and applied to 3D systems [1]. It was shown that an ETT implies singularities in thermodynamic and transport properties at T=0 which are smoothed at finite temperature (this left Lifshitz in a difficult position concerning the classification of this transition as a phase transition). Due to (i) the weakness of the singularities in 3D case (the only dimension considered at Lifshitz's time) and (ii) the difficulty of classification, this phenomenon (which is as general as for example the phenomenon of phase transition) has been quite forgotten.

We analyse a 2D electron system on a square lattice (in direct application to the high-T_c cuprates) and show that it obligatory undergoes an ETT (the Fermi surface changes from open to closed) under change of electronic concentration n (or of hole doping $\delta=1-n$) and that the ETT occurs in the doping range where all anomalies in the high-T_c cuprates are observed. We show that the ETT point, $\delta = \delta_c$, $T = 0$, is a quantum critical point (QCP) (at Lifshitz's time the concept of QCP had not yet been introduced), which is very rich in the 2D case, and that its existence results in global anomalies of the system[2-6]. Firstly, in the presence of interaction of necessary sign (such interaction does exist in the strongly correlated CuO_2 plane being of magnetic origin, see [7]), a d-wave superconducting state with high T_c develops around the ETT QCP with maximum T_c at $\delta = \delta_c$; its symmetry and properties studied in [7] are in a good agreement with experiments. Secondly, the underdoped regime, $\delta < \delta_c$ above $T_{sc}(\delta)$ is a new type of metallic state: quantum spin-density wave (SDW) liquid re-entrant in temperature and frozen in doping [4,2]. The re-entrance means that the characteristics of the short range order behave in a re-entrant way: the system becomes more ordered with increasing T and it reaches a minimum disorder at some pseudocritical temperature $T^*(\delta)$ which increases with decreasing doping. Freezing means that the system keeps strong short range order (or strong quantum critical fluctuations) quite far in doping from the ETT QCP.

A detailed study of these phenomena allows to understand many effects observed in high-T_c cuprates by different experiments and unexplained until now. Below we present several examples of theoretical predictions of our theory. Notice that the different anomalies are explained within the same theory and that neither adjustable parameters nor phenomenological *anzatz* are used.

Nuclear magnetic resonance (NMR)

There are two glaring anomalies observed systematically in the underdoped high-T_c cuprates; (i) the nonmonotonical behaviour of the nuclear spin lattice relaxation rate $1/T_1T$ on copper with maximum at some T* (see Fig.1b) instead of the Korringa law $1/T_1T$=const for ordinary metals, (ii) qualitatively different behaviour of $1/T_1T$ measured on copper and oxygen (or for the wavevectors $\mathbf{q} \approx \mathbf{Q}_{AF}$ and $\mathbf{q} \approx 0$ from theoretical point of view), see Fig 1d. (The relaxation rate $1/T_1T$ is roughly proportional to the slope in the imaginary part of the spin dynamic susceptibility, $\lim_{\omega\to 0} \mathrm{Im}\chi^0(\mathbf{q},\omega)/\omega$). The results of our theory are in a very good agreement with experiment, compare Fig.1a and 1b (there are no adjustable parameters). The shown dependences are a manifestation of the quantum SDW liquid : the nonmonotonic behaviour reflects the re-entrance in T. The difference in behaviour for $\mathbf{q} \approx \mathbf{Q}_{AF}$ and $\mathbf{q} \approx 0$ is related to the different aspects of criticality of the ETT QCP. The detailed analysis is done in [4].

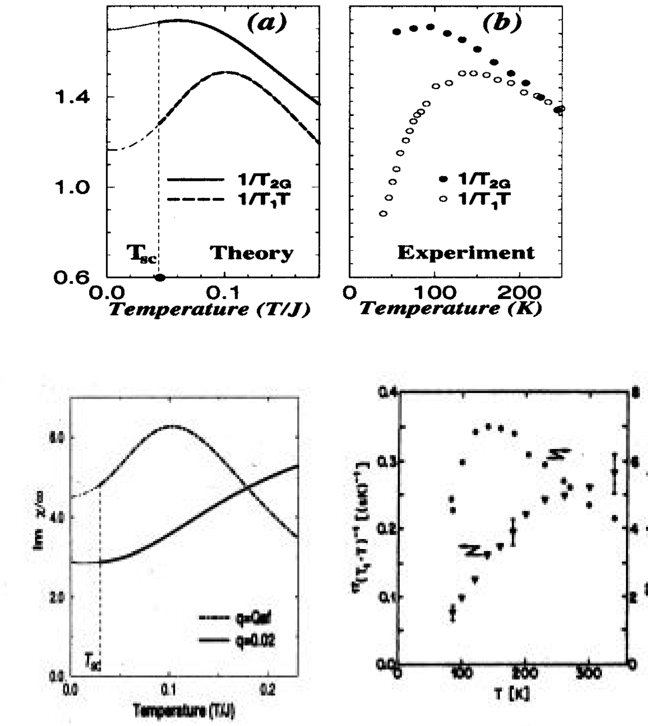

*Figure 1. Comparison between theory and experiment for $1/T_1T$ on copper and oxygen. (a) and (b) show the $1/T_1T$ and $1/T_{2G}$ (nuclear transverse relaxation rate) on copper, (a) calculated [2,4] (should be considered only above T_{sc}) and (b) measured by NMR for $YBCO_{6.6}$ [8]; (c) and (d) demonstrate the qualitatively different temperature dependences for copper (**q** » Q_{AF}) and oxygen (**q** » 0): (c) shows the theoretical results nonintegrated in **q** (the function for **q** » 0 is multiplied by factor 20), (d) shows experimental data for $1/T_1T$ on copper (Cu^{63}) and on oxygen (O^{17}) in $YBa_2Cu_4O_8$ [9].*

Angle resolved photoemission spectroscopy (ARPES)

There are numerous anomalies observed by photoemission in the underdoped regime (ARPES directly measures the electron spectral function as a function of energy and wavevector) which can be summarized as the so-called $(\pi,0)$ feature : the Fermi surface disappears in the normal state in the vicinity of $(\pi, 0)$ wavevector while in all ordinary metals it is well defined; the spectrum has a very unusual flat form as a function of wavevector; the electron spectral function $A(\mathbf{k}, \omega)$ is almost non-structured as a function of energy with a hump in the normal state and with the peak-dip-hump in the superconducting state instead of the usual almost δ-function form, etc. Within our theory all anomalies find a natural explanation. They are signatures of the quantum spin density wave (SDW) short range ordered liquid state, being a precursor of the ordered SDW phase. For example, the spectrum shown in Fig.2a, 2b is a result of a hybridization of the two parts of the bare spectrum in the vicinity of two different saddle points $(0,\pi)$ and $(\pi,0)$. The bare spectrum (dashed line) splits into two branches, $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$. The hybridization is static for the ordered SDW phase and is dynamic for the disordered (quantum SDW liquid) state. In the latter case the mode $\varepsilon_2(\mathbf{k})$ is strongly damped and appears above an incoherent background. The spectrum is in excellent agreement with ARPES data, see Fig.2c (ARPES measures only the part corresponding to negative energies ω). The existence below Fermi level of the incoherent background and of the damped mode $\varepsilon_2(\mathbf{k})$ explains the anomalous almost nonstructured ω dependence of the electron spectral function with the hump at energy $\approx \varepsilon_2(\pi,0)$ observed experimentally above T_{sc}. The effect of splitting into two branches leads to the pseudogap opening. The behaviour as a whole is strikingly similar to that observed experimentally. It concerns the very existence of pseudogap below T^*_{gap} which grows with decreasing δ, its doping and temperature dependences, the gradual disappea-rence of the Fermi surface with T, the shape of the spectrum around $(0,\pi)$, etc. Details are given in [3].

These were the features existing at intermediate temperature (above T_{sc}). At low temperature, the general picture of the spectrum is the same except that the upper branch $\varepsilon_1(\mathbf{k})$ (i) moves to lower energies and intersects the Fermi level [3], (ii) gets a gap, $E_1^{\pm}(\mathbf{k}) = \pm\sqrt{\varepsilon_1^2(\mathbf{k}) + \Delta^2(\mathbf{k})}$ in the presence of superconductivity with $\Delta(\mathbf{k}) = \Delta(\cos(k_x) - \cos(k_y))$ for the d-wave symmetry. Therefore two modes exist below Fermi level: the well- defined $E_1^-(\mathbf{k})$ and

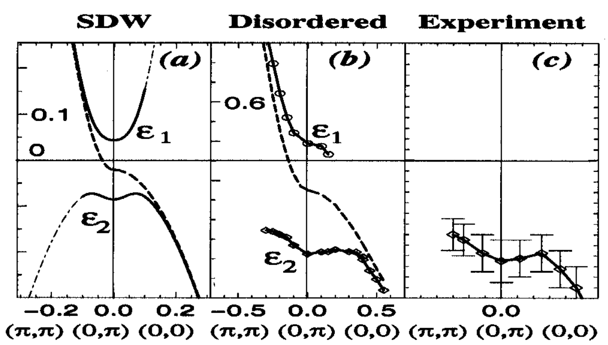

*Figure 2. Electron spectrum e(**k**)/t as a function of wavevector along G - X symmetry lines in the Brillouin Zone, (a) in the ordered SDW phase, (b) in the quantum SDW liquid state above T_{sc}. (c) ARPES data[10] for underdoped BSCO above T_{sc}. The dashed lines correspond to the bare spectrum, the thick lines to the two branches of the splitted spectrum, the dot-dashed line in (a) to the spectrum with the spectral weight less than 0.1.*

the strongly damped $\varepsilon_2(\mathbf{k})$ which leads to the peak-dip-hump form of $A(\mathbf{k},\omega)$ as a function of ω observed experimentally in the superconducting (SC) state (E_1 corresponds to the peak and ε_2 to the hump).

Tunneling spectroscopy

The typical form of the tunneling function with peak-dip-hump features at negative energies, $\omega<0$ as well as the asymmetry between $\omega<0$ and $\omega>0$ observed experimentally (see Fig.3b) and not understood until now are also explained well by our theory, compare Fig.3a and 3b. The effects are direct consequences of the discussed above form of the electron spectrum in the quantum SDW liquid state (tunneling spectroscopy measures the density of states, i.e. the electron spectral function integrated in $\mathbf{k}$). The peak-dip-hump structure seen in Fig.3 at negative ω results from the existence of two modes below the Fermi level (FL). So far, as it is not the case above FL, the picture in ω is quite asymmetrical.

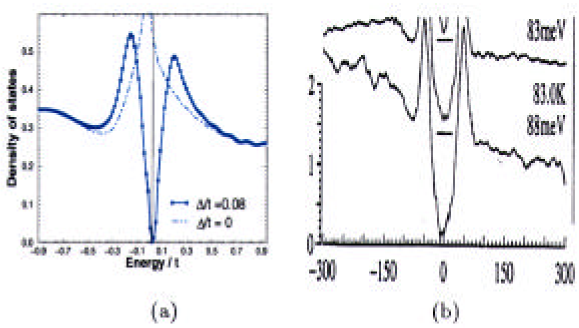

Figure 3. The density of states (a) calculated in the normal state (dotted line) and in the superconducting state (full line), (b) measured by tunneling [11] at T=4.2K: the lowest curve corresponds to the underdoped Bi2212 (T_c=83K); the energy scale is given in meV.

Inelastic neutron scattering (INS)

The existence of the quantum SDW liquid state and of the corresponding quantum spin fluctuations have a direct consequence for the spin dynamics measured by INS. Firstly, it explains the very fact of magnetic response so strong that it can be measured by INS (in ordinary metals it is impossible). Secondly, it explains practically all details observed by INS. Most interesting among the theoretical predictions are maybe the existence in the SC state (i) of the resonance spin mode (with almost horizontal dispersion in the vicinity of $\mathbf{Q}_{AF}$) developing out of two particle electron-hole continuum and (ii) of the incommensurability at low energies[5]. The former explains well the resonance peak at $\mathbf{q}=\mathbf{Q}_{AF}$ and $\omega \approx$ 40 meV with resolution-limited energy width and a finite q width observed systematically in the SC state from the beginning of high-T_c era[12]. The latter explains recent results obtained with a high resolution spectrometer, see Fig.4b[13]. The agreement with experiment is remarkable, compare Fig.4a and 4b.

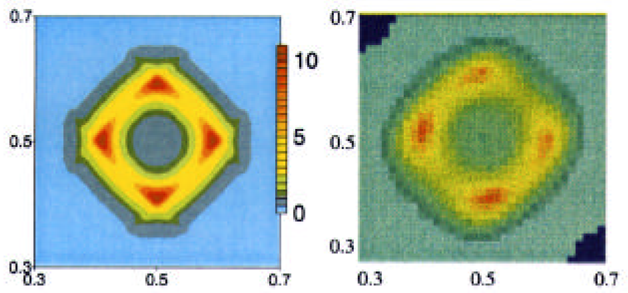

*Figure 4. **q** dependence of Imc(**q**,w) (a) theoretical for w/J = 0.25, (b) experimental [13] ($YBCO_{6.6}$ for w = 25 meV). The point (0.5,0.5) corresponds to (π/a,π/a). Note that J »120 meV for the cuprates.*

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