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ELECTRONIC TOPOLOGICAL TRANSITION IN 2D ELECTRON SYSTEM ON A SQUARE LATTICE AS A MOTOR FOR THE 'STRANGE-METAL' BEHAVIOUR IN HIGH-T_c CUPRATES

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Abstract—We show that a 2D system of free electrons on a square lattice with hoping between more than nearest neighbours is characterised by two quantum critical points associated with a change in topology of Fermi surface as a function of electron concentration. This simple model (when taking into account a positive interaction in a triplet channel) allows us to consistently explain some crucial experiments in the underdoped regime of hole-doped high-T_c cuprates (ARPES, neutron scattering). © 1998 Elsevier Science Ltd. All rights reserved

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1. TWO QUANTUM CRITICAL POINTS IN A 2D FREE ELECTRON SYSTEM ON A SQUARE LATTICE

We study a 2D system of noninteracting electrons on a square lattice with hoping between nearest neighbours (t) and next nearest neighbours (t'). We show that it is characterised by two quantum critical points, QCP1 and QCP2, associated with a change in topology of Fermi surface (FS) as a function of electron concentration, $1-\delta$. Their criticality shows up in the electron polarisability, $\chi^0(\mathbf{k},\omega)$, at $T=0$. The calculated $\chi^0(\mathbf{Q}_{AF}=(\pi,\pi),0)$ is shown in Fig. 1 as a function of hole doping δ. It reveals two singularities: a logarithmic one at QCP1, $\delta=\delta_{c1}$ ($\mu=4t'$), and a square-root one at QCP2, $\delta=\delta_{c2}$ ($\mu=0$), for each negative value of t'/t ($|t'/t|<1/2$).

The character of these two quantum critical points appears when $\chi^0(\mathbf{k},\mathbf{0})$ is analysed as a function of $\mathbf{k}$ for different δ, see Fig. 2. Around QCP2: for both $\delta<\delta_{c2}$ and $\delta>\delta_{c2}$ there is a closed (in the extended BZ) line of static Kohn (square-root) singularities (KS's), $\mathbf{k}=\mathbf{Q}_{s2}$ which reduces into the point $\mathbf{k}=\mathbf{Q}_{AF}$ at $\delta=\delta_{c2}$. An absolute value of $\mathbf{Q}_{s2}$ along a fixed direction is given by $Q_{s2}\propto|\delta-\delta_{c2}|$. Around QCP1: at $\delta>\delta_{c1}$ and $\delta<\delta_{c1}$ the line of KS's $\mathbf{k}=\mathbf{Q}_{s2}$ related to QCP2 is preserved; in addition there is a new closed line $\mathbf{k}=\mathbf{Q}_{s1}$ at $\delta>\delta_{c1}$ which is ended at $\delta=\delta_{c1}$ being reduced into the point $\mathbf{k}=\mathbf{Q}_{AF}$. An absolute value of $\mathbf{Q}_{s1}$ along a fixed direction is given by $Q_{s1}\propto\sqrt{\delta-\delta_{c1}}$. Exactly at QCP2 and QCP1 one has respectively: $\chi^0(\mathbf{k},0)\approx A-B\sqrt{|\mathbf{k}-\mathbf{Q}_{AF}|}$ and $\chi^0(\mathbf{k},0)\propto\ln|\mathbf{k}-\mathbf{Q}_{AF}|$.

The criticality of QCP1 from another point of view is seen as a Lifshitz's electronic topological transition [1] in a 2D system with a saddle point (SP) in the electron spectrum resulting in singularities in thermodynamic properties, and an additional singularity in superconducting response function. The critical exponents associated with QCP1 and QCP2 are respectively: $\nu_1=1/2$, $z_1=2$, $s_1=\nu_1 z_1=1$, $\alpha_1=2-[(D=2)+z_1]\nu_1=0$ (logarithmic singularity in the density of states) and $\nu_2=1$, $z_2=1$, $s_2=\nu_2 z_2=1$, $\alpha_2=2-[(D=2)+z_2]\nu_2=-1$ (no singularity in the density of states).

The distance between QCP1 and QCP2 diminishes with decreasing $|t'/t|$ and the two points coincide when $t'/t=0$. In the latter case (nesting) we arrive at a quantum multicritical point with a $(\ln)^2$ singularity.

As $\delta_{c1}>0$ and $\delta_{c2}<0$ (for any t'/t), it is a doping range around QCP1 which is actual for the hole doped cuprates and around QCP2 for the electron doped. As we are interested here in the former we consider below only properties around QCP1 which are also influenced by QCP2. We assume $|t'/t|$ to be not small in order to correspond to the experimental FS observed by ARPES.

One can check that $Re\chi^0$ and $Im\chi^0$ behave in a strongly anomalous way in the regime $\delta_{c2}<\delta<\delta_{c1}$. First of all taken at the characteristic for this regime wavevector $\mathbf{q}=\mathbf{Q}_{AF}$, $Re\chi^0(\mathbf{q},0)$ changes very weakly with doping starting from some threshold value of δ (see Fig. 1) as a consequence of the interplay between QCP1 and QCP2. Secondly, energy dependences of $Re\chi^0$ and $Im\chi^0/\omega$ for $T=0$ and their temperature dependences for $\omega\to 0$ are characterised by a characteristic energy $\omega=\omega_c\propto\delta_{c1}-\delta$ and a characteristic temperature $T=T^*\propto\delta_{c1}-\delta$ both being scaled with the doping distance from QCP1. The behaviour is anomalous in the regimes $\omega<\omega_c$, $T<T^*$. For example, $Re\chi^0(\mathbf{Q}_{AF},0)$ taken at fixed δ increases with increasing T for $T<T^*$. Thirdly, $Re\chi^0(\mathbf{q},0)$ exhibits a plateau as a function of $|\mathbf{q}|$ (see Fig. 1c) until very high temperature, $T<T^*_{\mathbf{q}}\propto\delta-\delta_{c2}$, which scales with the distance from QCP2. These and other anomalies are discussed in more detail in [2].

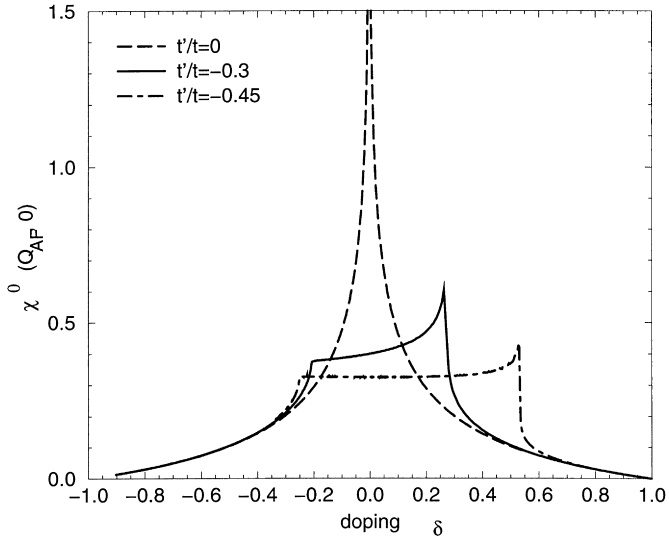

Fig. 1. Electron-hole susceptibility $\chi^0(\mathbf{Q}_{AF},0)$ around two quantum critical points, QCP1 and QCP2.

2. 2D INTERACTING SYSTEM: PROPERTIES OF CUO_2 PLANE

The anomalous behaviour of the free electron system in the presence of the two QCP is at the origin of an anomalous behaviour of interacting system. We concentrate below on properties related to long-range and short-range density wave (DW) order. (Obviously, in the presence of interactions of a certain sign, QCP1 gives rise to DW and superconducting (SC) instabilities around it due to logarithmic divergences of the corresponding response functions. What is important is that a positive interaction in a triplet channel (exchange interaction) is enough to create *both* instabilities. Such an interaction exists in the t–J model.)

A phase diagram is shown in Fig. 3. As T_{sc} is maximum at $\delta = \delta_{c1}$ (see [3]), the regime $\delta < \delta_{c1}$ is underdoped and $\delta > \delta_{c1}$ is overdoped. Although the DW phase for realistic values of t/J is hidden under the SC phase, it is DW critical fluctuations which determine a fundamentally anomalous metal behaviour below T^* and above T_{sc} (regime I) (the temperature $T = T^*(\delta)$ discussed above for the non-interacting system appears as a characteristic

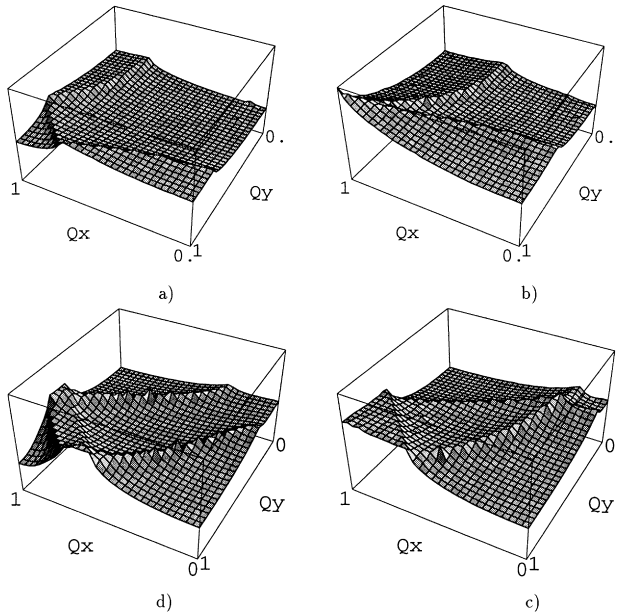

Fig. 2. Wavevector dependences of $\chi^0(\mathbf{q},0)$ for increasing doping (a) $\delta < \delta_{c2}$, (b) $\delta = \delta_{c2}$, (c) $\delta_{c2} < \delta < \delta_{c1}$ and (d) $\delta > \delta_{c1}$ ($Q_x = q_x/\pi$, $Q_y = q_y/\pi$, $t'/t = -0.3$).

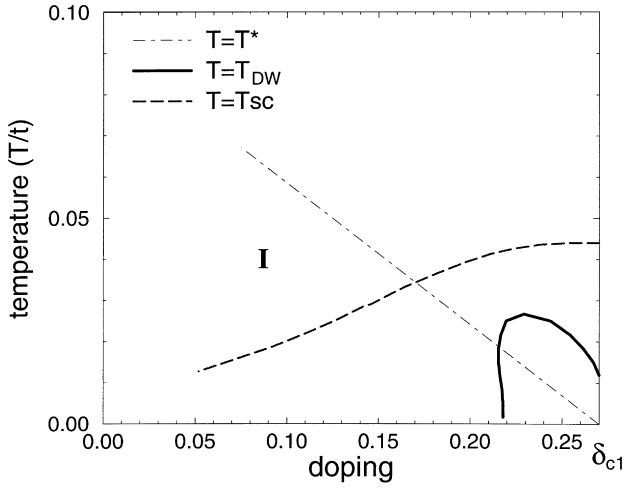

Fig. 3. Phase diagram with the lines of DW and SC instabilities and the line $T^*(\delta)$ ($t'/t = -0.3$, $t/J = 1.9$).

temperature for the interacting system). The state in regime I is reentrant in temperature and frozen in doping rigid DW liquid [2]: the correlation length slightly *increases* with T (being maximal at $T = T^*(\delta)$) and *almost does not change with doping*. Moreover, the parameter determining a proximity to the ordered DW phase does not practically change along the line $T = T^*(\delta)$, therefore remaining quite low in regime I. (All this stems from the properties of χ^0 discussed at the end of the previous section and is valid when the interaction J/t is not too small.) The ordered DW phase is also 'reentrant': T_{DW} increases with increasing $\delta_{c1} - \delta$.

All properties in the metal DW phase and in the metal regime I are anomalous. Below we show several examples.

First in Fig. 4 we show the electron spectrum in the long-range ordered DW phase. Prominent features of the spectrum are:

1. *flat shape around SP;*
2. *'disappearance' of the spectrum* in the direction $(k,\pi) - (\pi,\pi)$ above some threshold value of wavevector k (the residue tends to zero), both features being consequences of the hybridisation of the two parts of the bare spectrum around two SP's with a different curvature;
3. existence of the gap in a vicinity of SP $\Delta \propto \delta_{c1} - \delta$ *(the increase of the gap with decreasing doping* is the other side of the reentrant behaviour of DW phase). Details are given in [4].

The density of states (DOS) is shown in Fig. 5. It deviates from the bare DOS in two parts, A and B, related to QCP1 (A) and QCP2 (B). For the doping range around $\delta = \delta_{c1}$ it is the A-feature which determines properties of the system. It is characterised by a logarithmic singularity at ϵ^0 and by two jumps at ϵ^+ and ϵ^- instead of the

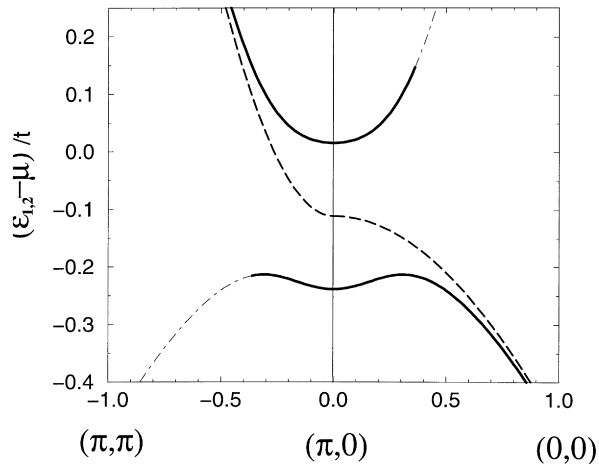

Fig. 4. Electron spectrum in DW phase around SP. The thin dot–dash line corresponds to the spectrum with residue < 0.1, and the dashed line to the bare spectrum ($t'/t = -0.3$, $t/J = 1.85$, $\delta = 0.19$).

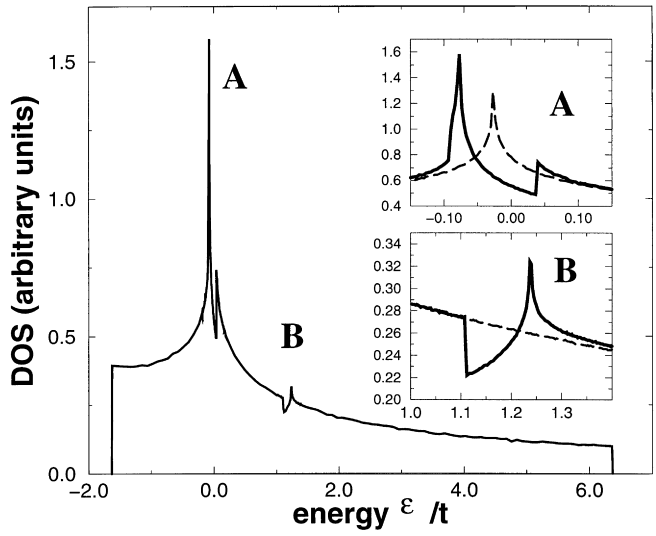

Fig. 5. Density of states with renormalised spectrum. The dashed line corresponds to the bare spectrum ($t'/t = -0.3$, $t/J = 1.8, \delta = 0.25$).

logarithmic singularity in the bare spectrum. There is a pseudogap on Fermi level.

The electron spectral function $A(\boldsymbol{k},\epsilon)$ in regime I calculated in a standard way based on the loop containing the electron Green function and the boson Green function corresponding to the susceptibility is shown in Fig. 6. The 'spectrum' deduced from it has the same shape as in Fig. 4 for $\omega < 0$. The pseudogap Δ is also proportional to $\delta_{c1} - \delta$. The difference is that for regime I the spectral function has a characteristic damped form for $\omega < 0$. The form of the 'spectrum', of the spectral function and the trend of increasing Δ with decreasing doping are in very good agreement with ARPES data above T_c [5].

The dynamic spin properties are also unusual. In Fig. 7a we show how $Im\chi(\mathbf{Q}_{AF},\omega)$ changes with decreasing T when one crosses the line $T = T^*$. One can clearly see the existence in the regime $T < T^*$ of the characteristic energy $\omega = \omega_0 \propto \delta_{DW}(0) - \delta$ (unchanging with T) at which $Im\chi$ is strongly peaked. For $T \gg T^*$ the curves lose a maximum and resemble $Im\chi^0$. In Fig. 7b we see that for low $\omega, \omega \ll \omega_c$, $Im\chi$ peaks at $\mathbf{k} = \mathbf{Q}_{AF}$. For larger ω, $Im\chi^0$ becomes flat and then even 'incommensurate' with a maximum determined by the wavevector $\mathbf{Q}_{s2}(\omega)$ related to QCP2 (a dispersion like effect). These results are in good agreement with recent INS data [6].

Summarising, a simple model taking into account the existence of two QCP's in a 2D electron system on a square lattice consistently explains certain experimental

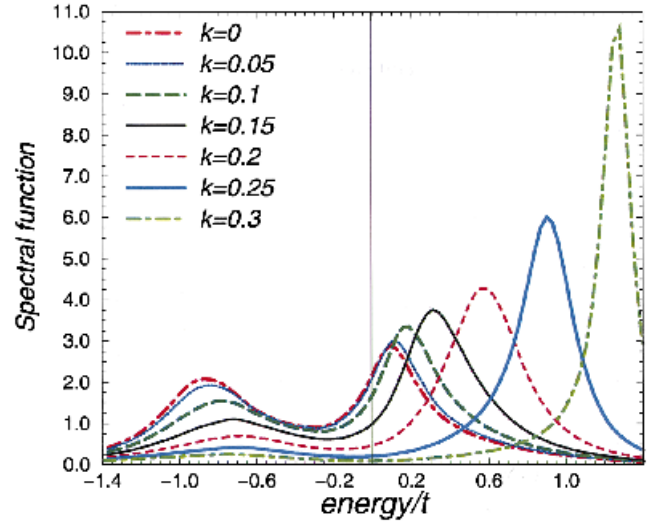

Fig. 6. Spectral function $A(\boldsymbol{k},\epsilon)$ in regime I calculated for the direction $(q,\pi) - (\pi,\pi)$. ($k = q/\pi, t'/t = -0.3$, $t/J = 1.8$, $T/t = 0.12$, $\delta = 0.1$).

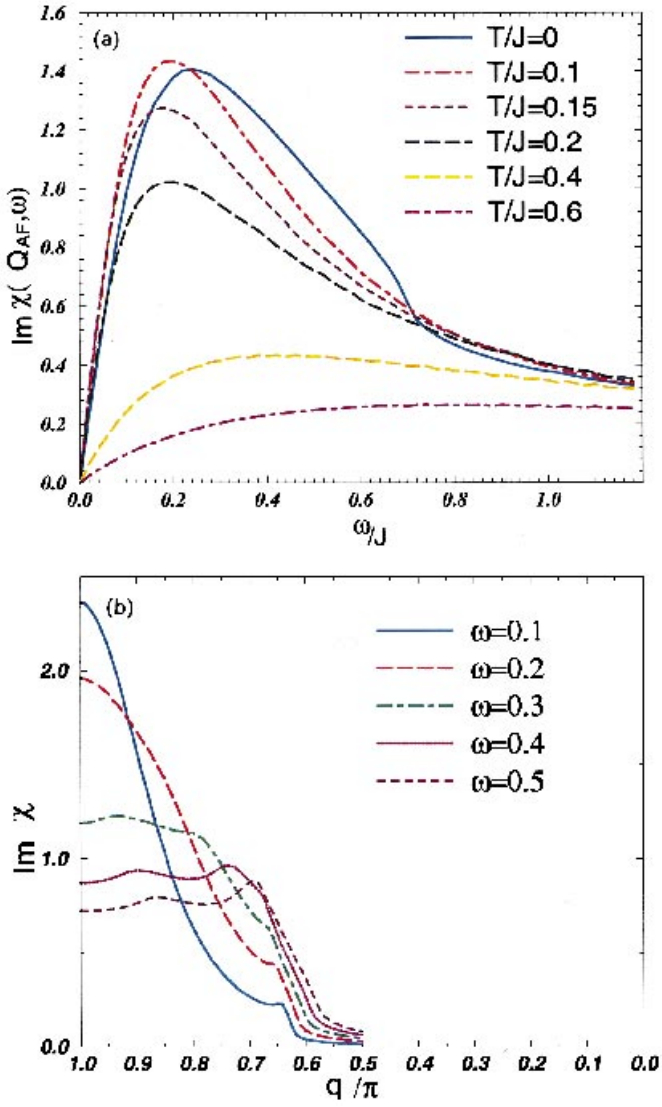

Fig. 7. *Im*χ for the underdoped regime at fixed doping $t/J = 1.83$, $t'/t = -0.3$, $\delta = 0.1$: (a) as a function of ω for different temperatures ($T^*/J = 0.2$); (b) as a function of q in the direction (q,π) for different values of ω/J (the existence of SC state is ignored).

facts considered today as crucial for understanding high-T_c cuprates.

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