New Scenario for High-T_c Cuprates: Electronic Topological Transition as a Motor for Anomalies in the Underdoped Regime

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We have discovered a new nontrivial aspect of electronic topological transition (ETT) in a 2D free fermion system on a square lattice. The corresponding exotic quantum critical point, $\delta = \delta_c$, $T = 0$ ($n = 1 - \delta$ is the electron concentration), is at the origin of anomalous behavior in the interacting system on one side of ETT, $\delta < \delta_c$. Most important is the appearance of the line of characteristic temperatures, $T^*(\delta) \propto \delta_c - \delta$. Application of the theory to high-T_c cuprates reveals a striking similarity to the behavior observed experimentally in the underdoped regime. [S0031-9007(99)08666-4]

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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) [1,2], angle-resolved photoemission spectroscopy (ARPES) [3], infrared conductivity [4], etc., provide 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 where a consistent theory is necessary to understand this exotic from theoretical point of view (but quite well defined from an experimental point) metallic behavior. The issue has a significance beyond the field of high-T_c superconductivity—the fundamental question arises: What kind of metallic behavior is there, in addition to the well-understood Fermi liquid?

In this paper we propose our variant of the answer. We reexamine a free electron 2D system on a square lattice with hopping beyond nearest neighbors. We show that, when varying the electron concentration defined as $1 - \delta$, the system undergoes an electronic topological transition (ETT) [5] at a critical value $\delta = \delta_c$. The corresponding $T = 0$ quantum critical point (QCP) combines two aspects of criticality. The first standard one is related to singularities in thermodynamic properties, in density of states at $\omega = 0$ (Van Hove singularity), to additional singularity in the superconducting (SC) response function (RF) [6]. The second nontrivial aspect is that the same QCP *is the end of the critical line* $T = 0$, $\delta > \delta_c$, each point δ of which is characterized by static Kohn singularity (KS) in polarizability of 2D free fermions. [What we mean as a static KS is a singularity at the wave vector connecting two points of Fermi surface (FS) with parallel tangents [7]]. The two aspects of criticality are not related. It is the latter aspect (never considered before) which, as we will show, is a motor for anomalous behavior in the regime $0 < \delta < \delta_c$ of the system of noninteracting and interacting electrons (or of any fermionlike quasiparticles, e.g., of those [8] appearing in the $t - t' - J$ model describing the strongly correlated CuO_2 plane responsible for the main physics in the cuprates). The found anomalies have a striking similarity to anomalies in the underdoped high-T_c cuprates. The effect exists in all cases $t' \neq 0$ or/and $t'' \neq 0, \ldots$, except for special sets of the parameters corresponding to the perfect nesting in FS (including $t' = t'' = \ldots \to 0$) studied in many papers (see, e.g., Ref. [9]). For such sets, the QCP loses the latter aspect of criticality and the anomalies disappear.

A starting point is a 2D electron system on a square lattice with hopping beyond nearest neighbors,

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \cdots . \tag{1}$$

For any set of the parameters t, t', t'', ..., the dispersion law is characterized by two different saddle points (SP's) located at $(\pm\pi, 0)$ and $(0, \pm\pi)$ with the energy ϵ_s. When we vary the chemical potential μ or the energy distance from the SP, $Z = \mu - \epsilon_s$, the topology of the FS changes when Z goes from $Z > 0$ to $Z < 0$ through the critical value $Z = 0$. In vicinity of SP's the dispersion law is

$$\tilde{\epsilon}(\mathbf{k}) = \epsilon_{\mathbf{k}} - \mu = -Z + ak_\alpha^2 - bk_\beta^2 , \tag{2}$$

where $\mathbf{k}$ is measured from $(0, \pi)$ ($\alpha = x, \beta = y$) or from $(\pi, 0)$ ($\alpha = y, \beta = x$). Explicit expressions for a and b depend on t, t', ... We consider the following general case: $a \neq 0$, $b \neq 0$, $a \neq b$. We choose $a > b$ corresponding to $t'/t < 0$.

The $T = 0$ ETT has two characteristic aspects. The first (trivial) one is related to the *local change of FS topology* in the vicinity of SP. This leads to divergences in thermodynamic properties, in density of states at $\omega = 0$, etc. From this point of view the corresponding QCP is of a Gaussian-type with the dynamic exponent $z = 2$.

The nontrivial aspect is related to *mutual change* in the topology of FS in vicinities of two different SP's and reveals itself when considering the electron polarizability,

$$\chi^0(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{n^F(\tilde{\epsilon}_{\mathbf{k}}) - n^F(\tilde{\epsilon}_{\mathbf{q+k}})}{\tilde{\epsilon}_{\mathbf{q+k}} - \tilde{\epsilon}_{\mathbf{k}} - \omega - i0^+} . \tag{3}$$

We show that the latter has a square-root singularity at

$\omega = 0$ and wave vector $\mathbf{q} = \mathbf{q}_m$ in a vicinity of $\mathbf{Q} = (\pi, \pi)$ *for any Z on the semiaxis* $Z < 0$: $\chi^0(\mathbf{q}, 0) - \chi^0(\mathbf{q}_m, 0) \propto \sqrt{|\mathbf{q}_m - \mathbf{q}|}$ for $|\mathbf{q}| > |\mathbf{q}_m|$. It is a static KS in the 2D electron system. The locus of the wave vectors $\mathbf{q}_m$ in the Brillouin zone (BZ) is a closed curve around $\mathbf{Q}$ with $|\mathbf{Q} - \mathbf{q}_m| \propto \sqrt{|Z|}$. With decreasing $|Z|$ the closed curve shrinks and is reduced to the point $\mathbf{q} = \mathbf{Q}$ at $Z = 0$, where $\chi^0(\mathbf{q}, 0)$ diverges logarithmically. The curve of the static KS's with $\mathbf{q}$ close to $\mathbf{Q}$ does not reappear for $Z > 0$: $\chi^0(\mathbf{q}, 0)$ is peaked at $\mathbf{q} = \mathbf{Q}$ in an intimate vicinity of ETT and it exhibits a wide plateau around $\mathbf{q} = \mathbf{Q}$ for larger Z. To illustrate this we show in Fig. 1 the $\mathbf{q}$ dependence of $\chi^0(\mathbf{q}, 0)$ calculated based on (3) and (1). [We use the model with only $t' \neq 0$ being a generic model for the family: $a \neq 0$, $b \neq 0$, $a \neq b$.] The curve discussed above is the curve of singularities in Fig. 1a closest to $\mathbf{q} = \mathbf{Q}$. In the plot, one sees only a quarter of the picture around $\mathbf{q} = \mathbf{Q}$; to see the *closed* curve around (π, π), one has to consider the extended BZ. (Few other curves of KS's seen in Fig. 1 are not sensitive to ETT; we discuss them elsewhere.)

As a result, the point $Z = 0$, $T = 0$ turns out to be the end point of the critical line $Z < 0$, $T = 0$.

Paradoxically, the *absence* of the discussed curve of static KS's for $Z > 0$ leads to an anomalous behavior of the system on this side of QCP. To see this, let us calculate ω dependencies of $\mathrm{Re}\,\chi^0(\mathbf{q}, \omega)$, $\mathrm{Im}\,\chi^0(\mathbf{q}, \omega)$ and $C(\omega) = \mathrm{Im}\,\chi^0(\mathbf{q}, \omega)/\omega$ for the characteristic for this regime wavevector $\mathbf{q} = \mathbf{Q}$. The results are shown in Fig. 2a. One can see that all functions are singular at some energy ω_c. Analytical calculations with the hyperbolic spectrum (2) give the following expression: $\mathrm{Im}\,\chi^0(\mathbf{Q}, \omega) = F(\omega/\omega_c, b/a)/2\pi t$, $\mathrm{Re}\,\chi^0(\mathbf{Q}, \omega) = \mathrm{Re}\,\chi^0(\mathbf{Q}, \omega_c) - \Phi(\omega/\omega_c, b/a)/t$ with

$$F(x,y) = \begin{cases} \ln \frac{\sqrt{1+xy}+\sqrt{1+x}}{\sqrt{1-xy}+\sqrt{1-x}}, & 0 \le x \le 1 \\ \ln \frac{\sqrt{1+xy}+\sqrt{1+x}}{\sqrt{x(1-y)}}, & x \ge 1 \end{cases},$$

$$\Phi(x,y) = \begin{cases} \gamma_1(y)(1 - x^2), & x - 1 < 0 \\ \gamma_2(y)\sqrt{x - 1}, & 0 \le x - 1 \ll 1 \end{cases} \quad (4)$$

$[\gamma_1(y) \ll 1]$. The *new energy scale* which appears and corresponds to the singularities in Fig. 2a is given by

$$\omega_c = Z(1 + b/a).$$

The singularities at $\omega = \omega_c$ are dynamic 2D KS's.

The dynamic KS's at $T = 0$ transform into static Kohn anomalies at finite temperatures (see Fig. 2b). When comparing with Fig. 2a, one can see that the behavior is similar to being smoothed by the effect of finite T. The important difference is that the characteristic temperatures of the Kohn anomalies for $\mathrm{Re}\,\chi^0(\mathbf{Q}, 0)$ and for $\lim_{\omega\to 0} \mathrm{Im}\,\chi^0(\mathbf{Q}, \omega)/\omega$ being both scaled with Z,

$$T^*_{\mathrm{Re}} = AZ, \qquad T^*_{\mathrm{Im}} = BZ, \qquad A < B,$$

are different; that is a usual effect of finite T.

Another remarkable signature of *asymmetry in Z* is the following. Taken for the characteristic for each regime

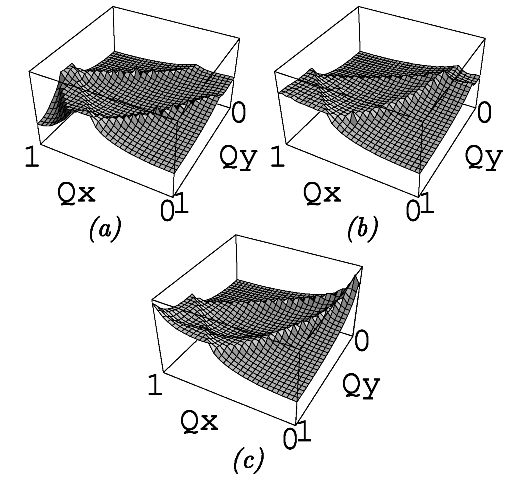

FIG. 1. $\mathbf{q}$ dependence of $\chi^0(\mathbf{q}, 0)$ through the BZ for (a) $Z < 0$, (b) $Z > 0$, (c) $Z = 0$. $Q_x = q_x/\pi$, $Q_y = q_y/\pi$. The point $\mathbf{q} = \mathbf{Q}$ corresponds to the left corner. ($t'/t = -0.3$.)

wave vector, $\mathbf{q} = \mathbf{q}_m$ for $Z < 0$ and $\mathbf{q} = \mathbf{Q}$ for $Z > 0$, $\chi^0(\mathbf{q}, 0)$ decreases rapidly with $|Z|$ for $Z < 0$ while for $Z > 0$ it remains *practically constant* (and quite high) for not too small Z. Moreover, for finite T, $\chi^0(\mathbf{Q}, 0)$ has a maximum at $Z = Z^*(T) > 0$. As a result of the described T and Z dependencies of $\chi^0(\mathbf{Q}, 0)$ in the regime $Z > 0$, the lines $\chi^0(\mathbf{Q}, 0) = \mathrm{const}$ have an unusual form in the $T - Z$ plane: They develop rather around the "critical" lines $T^*_{\mathrm{Re}}(Z)$ and $T^*_{\mathrm{Im}}(Z)$ than around the QCP, $T = 0, Z = 0$.

On the contrary, the behavior of SC RF (in both cases isotropic s-wave or d-wave symmetry) is symmetrical in Z being related to the first aspect of ETT. For the same reason, the SC RF decreases quite rapidly with increasing a distance from QCP, i.e., with increasing T and $|Z|$.

Above we considered a system of noninteracting electrons. In fact, the same picture takes place for any system of fermion or fermionlike quasiparticles when the dispersion law is determined by the topology of 2D square

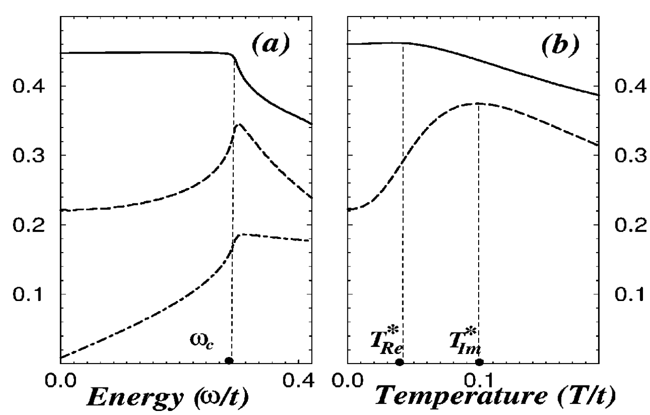

FIG. 2. $\mathrm{Re}\chi^0(\mathbf{Q}, \omega)$ (solid line), $\mathrm{Im}\,\chi^0(\mathbf{Q}, \omega)$ (dot-dashed line), and $C(\omega) = \mathrm{Im}\,\chi^0(\mathbf{Q}, \omega)/\omega$ (dashed line) in the regime $Z > 0$ (a) as a function of ω for $T = 0$ and (b) as a function of T for $\omega \to 0$. Here $t'/t = -0.3$ and $Z/t = 0.21$.

lattice and has a form (1). In [8], where we discuss some problems of strongly correlated systems, we show that such quasiparticles (with spin and charge) do exist in the $t - t' - J$ model describing the strongly correlated CuO_2 plane. On the other hand, the shape of FS observed by ARPES does imply the existence of *nnn* hopping $t' \neq 0$, so that the condition of the asymmetry $a \neq b$ necessary for the existence of the discussed ETT is fulfilled. Moreover, this shape implies $t'/t < 0$, the case for which the critical doping δ_c is positive. Below we will pass from the energy distance from ETT Z to the doping distance $\delta_c - \delta$, using a large FS condition: $1 - \delta = 2\sum_{\mathbf{k}} n^F(\tilde{\epsilon}_{\mathbf{k}})$ [8].

Let us now consider the system in the presence of interaction. A quite trivial consequence of the ETT is a developing of density wave (DW) and SC instabilities around the point $\delta = \delta_c, T = 0$. [The effects are related to the logarithmic divergence of $\chi^0(\mathbf{Q}, 0)$ and $\ln Z \ln T$ divergence of the SC RF as $T \to 0$, $Z \to 0$.] Nontrivial consequences concerning the DW degrees of freedom and related to the Kohn singularity aspect of ETT are (*i*) strong asymmetry between regimes $\delta < \delta_c$ and $\delta > \delta_c$, and (ii) very long (in doping and temperature) memory about DW instability in the disordered state on one side of ETT, $\delta < \delta_c$. To see this, let us consider the electron-hole RF which in the random-phase approximation is given by $\chi(\mathbf{q}, \omega) = \chi^0(\mathbf{q}, \omega)/[1 + V_{\mathbf{q}}\chi^0(\mathbf{q}, \omega)]$. In the case of interaction $V_{\mathbf{q}}$ in a triplet (singlet) channel the instability and normal state fluctuations are of spin-density wave (SDW) [charge-density wave (CDW)] type. We will consider the former interaction: $V_{\mathbf{q}} = J_{\mathbf{q}} = 2J(\cos q_x + \cos q_y)$ $(J > 0)$ as strongly supported by neutron scattering and NMR experiments for the cuprates and on the other hand, as an interaction between the above discussed quasiparticles in the $t - t' - J$ model [8]. For such interaction both instabilities d-wave SC (see details in [8]) and SDW take place around QCP. Because of the symmetry of SC RF in Z, $T_{\mathrm{SC}}(\delta)$ is symmetrical on two sides of δ_c with a maximum at $\delta = \delta_c$ (see Fig. 3). Therefore the regimes $\delta < \delta_c$ and $\delta > \delta_c$ can be considered as underdoped and overdoped, respectively. On the contrary, the line of SDW instability, $T_{\mathrm{SDW}}(\delta)$, given by $\chi^0(\mathbf{q}, 0) = -1/J_{\mathbf{q}}$ ($\mathbf{q} = \mathbf{Q}$ for $\delta < \delta_c$ and $\mathbf{q} = \mathbf{q}_m$ for $\delta > \delta_c$) has an anomalous form in the regime $\delta < \delta_c$: It develops rather around the lines $T^*_{\mathrm{Re}}(\delta)$ and $T^*_{\mathrm{Im}}(\delta)$ than around QCP (see Fig. 3), reproducing the form of lines $\chi^0(\mathbf{Q}, 0) = \text{const}$ discussed above.

When, at certain doping, $\delta = \delta_{\mathrm{SDW}}$, the ordered SDW solution disappears, it is the disordered metallic state which retains this type of behavior: the regime $T^*_{\mathrm{Re}}(\delta) < T < T^*_{\mathrm{Im}}(\delta)$ (II) turns out to be a regime of a *minimum disorder* and the regime $T < T^*_{\mathrm{Re}}(\delta)$ (I) is a regime of *a reentrant in temperature quantum SDW liquid.* Indeed, the two most important parameters characterizing SDW liquid, $\kappa^2 = 1 - |J_{\mathbf{Q}}|\chi^0(\mathbf{Q}, 0)$ describing a "proximity" to the SDW instability and $\Gamma_{\mathbf{Q}} = \kappa^2/C(0)$ describing a relaxation energy, behave in a reentrant way in increasing T: κ^2 decreases (slightly) with T until $T^*_{\mathrm{Re}}(\delta)$ and $\Gamma_{\mathbf{Q}}$ decreases (strongly) until $T^*_{\mathrm{Re}}(\delta) < T^*_{\Gamma} < T^*_{\mathrm{Im}}(\delta)$ as if the system would move towards an ordered phase. However, it does not reach it; the reentrancy stops and the system passes to the regime II of a minimum disorder above which a standard disordered state behavior is restored (regime III). On the other hand, the quantum SDW liquid state in the regime I is practically *frozen in doping* due to the very weak dependence of κ^2 on doping. As a result the disordered metal state in the regime $\delta < \delta_c$ keeps a strong memory of the ordered SDW phase (and therefore develops strong critical SDW fluctuations) very far in doping and in temperature. On the contrary, in the regime $\delta > \delta_c$ the memory of SDW instability and the corresponding fluctuations disappear rapidly due to the sharp decrease of $\chi^0(\mathbf{q}, 0)$ with increasing $\delta - \delta_c$ and T. The same is valid in both regimes $\delta > \delta_c$ and $\delta < \delta_c$, for SC fluctuations due to the above discussed behavior of SC RF as a function of T and $|Z|$. Therefore, although the SDW phase itself is energetically unfavorable with respect to the SC phase (except in the case of very high J/t), the metal state above T_{SC} in the underdoped regime is a precursor of the SDW phase rather than of the SC phase.

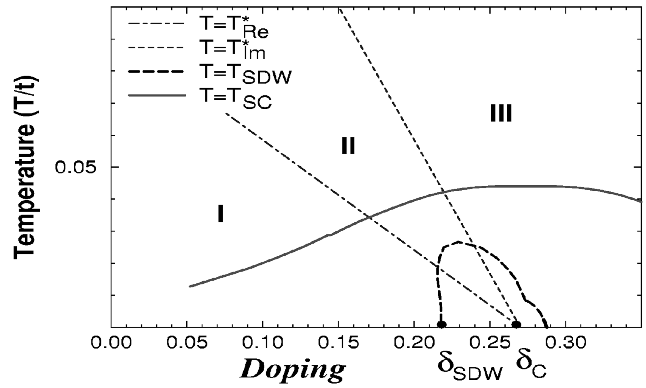

FIG. 3. Phase diagram with the lines of SDW and d-wave SC instabilities and the lines $T^*_{\mathrm{Re}}(\delta)$, $T^*_{\mathrm{Im}}(\delta)$ ($t'/t = -0.3$, $t/J = 1.9$). We consider only the metallic part of the phase diagram (for a discussion about a passage from the AF localized-spin state at low doping to the metallic state with large FS for intermediate doping, see Ref. [8]).

The lines $T^*_{\mathrm{Re}}(\delta)$ and $T^*_{\mathrm{Im}}(\delta)$ are basic lines for anomalies in the disordered metallic state. To demonstrate how the anomalies appear for different properties we consider some examples. In Fig. 4a we show calculated quasistatic magnetic characteristics corresponding to these measured by NMR $1/T_1T$ and $1/T_{2G}$ on copper as functions of T. The physical reason for a slight increase of $1/T_{2G}$, extending until $\approx T^*_{\mathrm{Re}}$, and a much stronger increase of $1/T_1T$, extending until $T \approx T^*_{\Gamma}$, is the reentrant behavior of κ^2 and $\Gamma_{\mathbf{Q}}$ with T discussed above. The theoretical behavior is very close to that observed experimentally (Fig. 4b) and explains it in fact for the first time.

In Fig. 5 we show an electron spectrum calculated for the ordered SDW phase (a) and for the disordered metal state (namely, for the regime II) (b). For the ordered

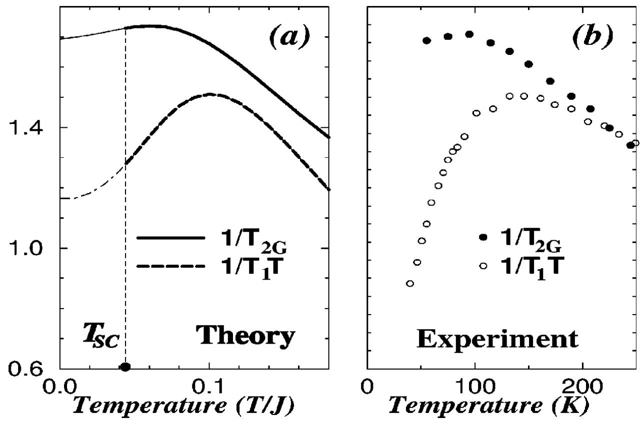

FIG. 4. $1/T_1T$ and $1/T_{2G}$ (a) calculated for $\delta = 0.15$ ($t'/t = -0.3$, $t/J = 1.9$) (should be considered only above T_{SC}) and (b) taken from NMR for $YBCO_{6.6}$ [2].

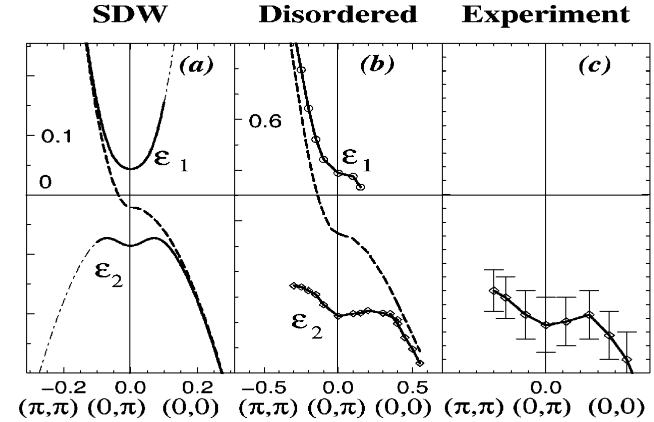

FIG. 5. Electron spectrum $\varepsilon(\mathbf{k})/t$ along Γ-X symmetry lines, (a) in SDW phase [$Z/t = 0.03$ ($\delta = 0.25$), $T = 0$], (b) in the metallic state above T_{SC} [$Z/t = 0.3$ ($\delta = 0.1$), $T/t = 0.15$], (c) ARPES data [10] for underdoped $Bi_2Sr_2CaCu_2O_{8+5}$ above T_{SC}. The dashed lines correspond to the bare spectrum, and the thin line in (a) corresponds to the spectrum with the spectral weight less than 0.1. $t'/t = -0.3$, $t/J = 1.8$; wave vectors are taken in units of π.

phase the spectrum is given by $\varepsilon_{1,2} = (\epsilon_A + \epsilon_B)/2 \pm \sqrt{[(\epsilon_A - \epsilon_B)/2]^2 + \Delta^2}$ $[\epsilon_A(\mathbf{k}) \equiv \epsilon(\mathbf{k}), \epsilon_B(\mathbf{k}) \equiv \epsilon(\mathbf{k} + \mathbf{Q})]$ with the gap Δ determined self-consistently in the usual way. For the disordered state the "spectrum" is obtained from the maxima of electron spectral functions strongly renormalized due to the interaction with the above described SDW fluctuations. The characteristic form of the spectrum in both cases is a result of a hybridization of two parts of the bare spectrum in the vicinity of two different SP's $(0, \pi)$ and $(\pi, 0)$. The hybridization is static for the ordered SDW phase and is dynamic for the disordered state. (Details about the pseudogap opening in the disordered state and its behavior with T and δ will be the subject of a separate paper.) The spectrum is in excellent agreement with ARPES data (see Fig. 5c) (ARPES measures only the part corresponding to $\epsilon < 0$). The effect of splitting into two branches, and of the pseudogap, disappears quite rapidly in the regime $\delta > \delta_c$ due to the rapid weakening of SDW fluctuations. It disappears roughly above $T^*_{\mathrm{Im}}(\delta)$ for the same reason. Both facts agree with experiments for the cuprates.

We will now discuss the behavior of $\mathrm{Im}\,\chi(\mathbf{q}, \omega)$, the characteristics measured by inelastic neutron scattering (INS). As follows from the previous analysis, below T^*_{Im} it has a maximum at $\omega = \omega_0 \propto \kappa^2$ (being peaked at $\mathbf{q} = \mathbf{Q}$). Since κ^2 almost does not change with δ, the position of the peak does not as well. This agrees with INS data and explains (for the first time) the existence of the characteristic energy ($\sim$30 MeV) above T_{SC} for all δ; see, e.g., the summarizing picture in Fig. 25 in [11]. As was emphasized before, strong SDW fluctuations disappear in the overdoped regime $\delta > \delta_c$. In the underdoped regime they disappear (or strongly diminish) above $T^*_{\mathrm{Im}}(\delta)$. Both facts are in good agreement with INS.

Summarizing, the simple picture arising from the effect of ETT in a 2D electron system on a square lattice gives a unified vision of normal state anomalies in the underdoped high-T_c cuprates for both magnetic and electronic properties. We succeed in explaining the temperature anomalies in $1/T_1T$ and $1/T_{2G}$ NMR characteristics, some crucial features of INS in the normal state, the disappearance of magnetic fluctuations in the overdoped regime, an opening of a pseudogap in the electron spectrum, the shape of the latter in a vicinity of $(0, \pi)$, and the disappearance of the pseudogap in the overdoped regime. All of these are most nontrivial experimental results. Regarding that the theory does not use any external phenomenological hypothesis and only two microscopical parameters t'/t and t/J, the similarity between the theoretical results and experiments seems quite remarkable. We emphasize that the effect exists for any t'/t, $t''/t, \ldots$, except for two limit cases: (i) isotropic $a = b$ in Eq. (2) ($t' = t'' = \ldots = 0$) and (ii) extreme anisotropic one $a = 0$ or $b = 0$. Although ETT exists in both cases, the corresponding QCP's belong to different classes of universality. For $a = b$ (nesting) the behavior is symmetrical in Z, the anomalous regime discussed in this paper disappears.

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