Charge and spin inhomogeneity as a key to the physics of the high $T_c$ cuprates

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Abstract

We present a coherent scenario for the physics of cuprate superconductors, which is based on a charge-driven inhomogeneity, i.e. the “stripe phase”. We show that spin and charge critical fluctuations near the stripe instability of strongly correlated electron systems provide an effective interaction between the quasiparticles, which is strongly momentum, frequency, temperature and doping dependent. This accounts for the various phenomena occurring in the overdoped, optimally and underdoped regimes both for the normal and the superconductive phase.

Key words: Superconductivity; Charge segregation; Incommensurate charge-density waves; Stripes; Pseudogap.

1. Introduction

A main issue in the cuprates is to clarify how these systems evolve from the antiferromagnetic (AF) insulator at very low doping to the superconductor and to the anomalous normal metal at higher doping. How does the repulsion characterizing the AF behavior evolve into an “effective attraction” necessary for superconductivity? Is this evolution connected with the anomalous properties of the normal phase? These anomalous properties manifest themselves with the linear-in-temperature behavior of the resistivity of the CuO$_2$ planes around optimum doping (doping at which for each cuprate family there is the maximum superconducting critical temperature $T_c$) and with the opening of pseudogaps both in the spin and charge channel in the underdoped materials. Is the strong pairing mechanism required to obtain the observed high superconducting temperatures related to these anomalous behaviors of the normal phase?

We will show that one way to accommodate the above puzzle into a coherent scenario is through charge segregation, which may manifest itself via local phase separation or incommensurate charge-density waves (ICDW) and stripe formation. In particular the formation of hole-poor regions and hole-rich regions enslaves and extends the AF correlations to doping values much larger than the doping at which the Néel temperature is zero, since AF correlations survive in the hole-poor regions of the segregated domains.
2. The charge-segregation scenario for the cuprates

Let us start with the understanding of the anomalous behavior of the normal phase at optimal doping. One possible explanation is that the low dimensionality of these highly anisotropic systems and their correlated nature are at the origin of the breakdown of the Fermi liquid. However, the proposal that the Luttinger liquid, the metallic state which is formed in one dimension, is also formed in two dimensions [1], has been strongly questioned.

The alternative attitude has been to accept the Landau theory of normal Fermi liquid as a starting point. The anomalous properties would then arise as a consequence of strong scattering processes at low energy between the quasiparticles.

One possibility, which we have been discussing along the years, is that a singular effective interaction between the quasiparticles is mediated by the critical fluctuations occurring near a charge instability. In particular, within a perturbative approach, it can be shown that near a gaussian critical point with dynamical critical index $z = 2$, the interaction has the form

$$\Gamma_{eff}(q, \omega) \approx \tilde{U} - \frac{V_c}{|q - Q_c|^2 + \kappa^2 - i\gamma \omega}$$  \hspace{1cm} (1)$$

where $\tilde{U}$ is the vestige of the strong bare local hole-hole repulsion characterizing the cuprates, $V_c$ is the strength of the static effective potential, $Q_c$ is the critical wavevector related to the ordering periodicity, $\kappa^2 \sim \xi^{-2}$ is a mass term which is related to the inverse of the correlation length and provides a measure of the distance from criticality. The characteristic time scale of the critical fluctuations is $\gamma$. We elaborate here on the proposal that the relevant instability is controlled by an incommensurate charge-density-wave (ICDW) quantum critical point (QCP) [2,3]. If the onset of this instability, i.e. the QCP where $\kappa^2 = 0$, is located around optimal doping, then in this region no other energy scale would be present besides the temperature $T$, as suggested by the in-plane resistivity experiments. The presence of the QCP near optimal doping naturally divides the phase diagram according to the general scheme of criticality into a nearly ordered, a quantum critical, and a quantum disordered region, which correspond to the underdoped, optimally doped, and overdoped regions respectively. The nearly ordered region is related to the occurrence of a phase with spatially modulated charge distribution (stripe phase) in the underdoped region of the cuprates, where the charge ordering becomes more pronounced and mixes with spin degrees of freedom, which are AF correlated in the hole-poor regions. Owing to this connection, we shall indifferently use the ICDW- or Stripe-QCP terminology.

From the theoretical point of view this charge instability is the natural outcome of the generic tendency of models of strongly correlated electrons with short-range interactions to phase separate (PS) into hole-rich and hole-poor regions. This instability is turned into a frustrated PS or in an ICDW instability when long-range Coulomb forces are taken into account to guarantee large-scale neutrality [2,4–6]. The physics of the ICDW-QCP was first derived within an infinite-$U$ Hubbard model extended by a Holstein electron-phonon interaction and a long-range Coulomb potential [2,7]. With realistic values of the parameters, the instability was indeed located around optimal doping and the form (1) for the effective interaction both in the particle-hole and in the particle-particle channels was derived. Another proposal [5] for the mechanism of phase separation is the magnetic interaction. We believe that the specific mechanism producing phase separation is rather immaterial, since the strong correlations are the basic ingredient leading to a charge segregation, whatever residual interaction (magnetic, phononic, repulsion between holes on neighbor Cu and O ions,...) is considered. The relative role of these additional interactions might quite naturally depend on doping. The stripe phase continuously connects the low and intermediate doping regimes were the expulsion of holes from the AF background and the ICDW instability (where non-magnetic effects...
may cooperate) are respectively dominant.

...From the experimental point of view, the existence of charge-controlled inhomogeneities in some underdoped or optimally doped cuprates is now established. There is also compelling evidence for a QCP at sizable doping as provided by magneto-resistivity measurements in La$_{2-x}$Sr$_x$CuO$_4$: An insulator-to-metal transition is found when the SC phase is suppressed by means of a pulsed magnetic field [8]. A clear indication that this insulator-to-metal transition is driven by some spatial charge ordering is provided by its occurrence at a much higher temperature in samples near the “magic” filling 1/8, where commensurability effects have repeatedly been reported in related compounds. When extrapolated to $T = 0$ the transition takes place near optimum doping. The QCP itself is directly observable only when SC is suppressed. Therefore it would be more appropriate to refer to a “hidden” QCP.

The stripe-QCP scenario is schematically summarized in Fig. 1, where the underdoped, optimally and overdoped regions are apparent.

At large doping the crossover between the quantum critical and quantum disordered regime takes place, marking a different temperature and doping dependence of the CDW correlation length, $\xi^{-2} \sim T$ in the QC region and $\xi^{-2} \sim (x - x_c)$ in the QD one. The effective interaction (1) due to the fluctuations mediate strong pairing giving rise to (d-wave) gap formation in the Cooper channel. The doping and temperature dependence of the mass term in the pairing potential gives rise to a critical temperature, which strongly depends on doping in the overdoped regime and saturates around optimal doping [9]. Around this latter point the same effective interaction in the particle-hole channel disrupts the Fermi-liquid behavior accounting for the absence of any energy scale besides $T$. In the underdoped region, the $T^*$ crossover temperature marks the proximity to the nearly charge-ordered phase. Near and below this temperature the strong critical CDW fluctuations tend to open pseudogaps in the quasiparticle spectra due to the strong scattering in the particle-hole channel [10].

We emphasize here that the most prominent consequence of the presence of a critical line ending in a QCP near optimal doping is this strongly singular effective interaction mediated by the critical charge fluctuations. This is a distinguished feature of the present scenario, which provides a more two-dimensional mechanism both for the pair formation and for the disruption of the Fermi liquid with respect to other scenarios, also based on stripe formation, which rely on the strongly one-dimensional character of the stripes. The singular interaction here described has remarkable fea-

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**Fig. 1.** Schematic phase diagram of the cuprates including the stripe-QCP.
tured: i) It is strongly momentum dependent being peaked around the ordering wavevector related to the specific ordering taking place in the system (which may vary from system to system and is not related to the nesting of the Fermi surface); ii) it depends strongly on temperature and/or on doping via the mass term determined by the correlation length. In particular, around optimal doping it leaves the temperature as the only relevant energy scale, whereas in the underdoped regime it introduces the new scale of energy $T_{CDW}$. iii) It affects the properties of the system both in the particle-hole and the particle-particle channels.

In the following we will present some of the main effects arising from the singular effective interaction besides those already generically outlined above. We will first report the main consequences in the particle-hole channel and afterwards in the particle-particle channel.

3. Stripe fluctuations in the metallic regime: Effects on the one-particle spectra

The electronic structure should be directly affected by the appearance of the anomalous properties described above. We therefore investigate the effects of stripes on the electronic spectra in the metallic phase. Within our approach, we start from a tight-binding model suitable to describe the quasiparticles in the cuprates. The quasiparticles interact with the collective (nearly critical) charge and spin fluctuations. In the over and optimally doped regimes, this interaction can be dealt with perturbatively, whereas in the underdoped phase, where stripes fluctuations are more pronounced, requires a different approach, which at the moment is only partially devised [10]. We consider an effective interaction between quasiparticles of the form (1), which now contains both the charge and the (enslaved) spin channels 

$$\Gamma_{eff}(q, \omega) = -\sum_{i=c,s} V_i/\left[\kappa_i^2 + \eta_{q-Q_i} - i\gamma_i \omega\right],$$

where $\eta_Q = 2 - (\cos q_x + \cos q_y)$, which is mediated by both charge (c) and spin (s) fluctuations. The $q$ dependence reproduces the $(q - Q_i)^2$ behavior for $q \approx Q_i$ while maintaining the lattice periodicity. The direction of the critical wavevector $Q_c$ is still debated and can be material dependent.

The first-order in perturbation theory yields an electron self-energy [11], which customarily provides the broadening of the quasiparticle peaks, the effective mass renormalization, and the appearance of incoherent parts in the single-particle spectra.

The resulting changes of the quasiparticle dispersions, together with the appearance of (incoherent) dispersing shadow peaks leads to strong modifications of the spectral densities and of the Fermi surface, which are in agreement with the observed ARPES spectra [12].

More recently this analysis was extended [13] by considering the more realistic bilayer structure of the Bi2212 compound, where a wealth of ARPES experiments is available. In particular, the following issue was addressed: Although the interplane hopping, as obtained from band calculations, is sizable ($t_\perp \sim 50meV$), the splitting between the two bands arising from the hybridization between the two planes in the unit cell, which should be particularly strong near the M [i.e. $(0, \pm \pi)$ and $(\pm \pi, 0)$] points, is not observed. Even taking into account the reduction of $t_\perp$ due to the strong electron-electron interaction characterizing the cuprates, the bilayer splitting should still be observable around the M points. Turning on a moderate coupling between the quasiparticles and the charge and spin critical fluctuations rapidly dresses and drastically reduces the effective interplane hopping, thus washing out any band-splitting effect and strongly modifying the Fermi surface shape. This indicates that the puzzling absence of the band splitting in ARPES spectra of bilayer materials can be due to the stripe fluctuations driving the proliferation of charge and spin collective modes scattering the quasiparticles. This analysis accounts for the good agreement between the single-layer calculations of the spectra referred above with the experimental results on the (two-layer) Bi2212.
4. Two-gap features

We want now to explore in more detail how the singular interactions related to the stripe formation affect the particle-particle channel. The simultaneous presence in Eq. (1) of a weak momentum independent repulsion together with a strong attraction at small or intermediate wavevectors has been shown to favor $d$-wave superconductivity [9,14] within direct calculations in the BCS approximation. Already within this simplified approach, some non-trivial features of the superconducting gap were found and the specific shape of the gap along the fermi surface was not simply given by the pure $d$-wave form $\Delta(k) = \Delta_0[\cos(k_x) - \cos(k_y)]$. In particular, the gap flattens around the (1,1) or (1,-1) directions when the parameters in Eq. (1) are chosen such that the effective interaction is strongly peaked around $Q_c$. Moreover, the gap presents local maxima around the k-points on the Fermi surface, which are connected by the critical wavevectors (hot spots). Both these features have possibly been identified in underdoped cuprates.

Despite these intriguing features of the gap determined in BCS approximation, some interesting peculiarities of the pairing effects due to the effective interaction near the stripe singularity line could have been missed in this approach. In particular, the strong momentum dependence of the effective interaction gives rise to regions around the hot-spots, where the time-reversed “hot” states form nearly local pairs which are tightly bound, but strongly fluctuating in phase due to the low velocity of the hot points. These paired states, together with the particle-hole stripe scattering described in the previous sections can be responsible for the pseudogaps arising in the underdoped cuprates below $T^*$. On the other hand, “cold” states far from the hot spots interact more weakly and preserve a propagating quasiparticle character. For these states alone a standard BCS approach would be appropriate and would likely provide a coherent superconducting state, but at a temperature much lower than $T^*$. We believe that the interplay between these states can provide a description of the pseudogap phenomena in the underdoped regime.

To explore in detail this possibility, a toy model has been recently investigated [15], where two bands, say 1 and 2, are present, with a large and small Fermi surface respectively [16]. While the electrons in the band 1 represent the cold particles of the cuprates and interact weakly via a constant attractive interaction $g_{11}$, the hot particles are represented by the hot electrons in the band 2, which interact strongly via $g_{22}$. In this way we schematize electrons in the same band interacting with a strongly $q$-dependent potential via electrons in two different bands interacting with different coupling constants. In a BCS mean field approximation the hot electrons in band 2 would have a high superconducting critical temperature $T^*_{c2}$, but the smallness of their Fermi surface leads to a small stiffness $\eta_2$ of the fluctuations, which strongly reduce the critical temperature. These fluctuations, instead do not affect the cold electrons in band 1 having a large Fermi surface and, therefore, a large stiffness $\eta_1$ (but a low $T^*_{c1}$). It is remarkable that, turning on an interband coupling $g_{12}$, the stiffness of the hot-pair fluctuations is increased, but it becomes sizable (of the order of $\eta_1$) only approaching $T^*_{c1}$.

As a consequence, the coupled 1-2 system acquires a critical temperature value, which is intermediate between $T^*_{c2}$ and $T^*_{c1}$. Thus the system takes advantage of the strong pairing between the hot electrons at $T^* \sim T^*_{c1}$, but the smallness of their Fermi surface leads to a small stiffness $\eta_2$ of the fluctuations, which strongly reduce the critical temperature. These fluctuations, instead do not affect the cold electrons in band 1 having a large Fermi surface and, therefore, a large stiffness $\eta_1$ (but a low $T^*_{c1}$). It is remarkable that, turning on an interband coupling $g_{12}$, the stiffness of the hot-pair fluctuations is increased, but it becomes sizable (of the order of $\eta_1$) only approaching $T^*_{c1}$.

As a consequence, the coupled 1-2 system acquires a critical temperature value, which is intermediate between $T^*_{c2}$ and $T^*_{c1}$. Thus the system takes advantage of the strong pairing between the hot electrons at $T^* \sim T^*_{c1}$, but reduces the phase fluctuation effects via their coupling to the colder electrons in band 1 at lower temperature $T_c$.

The above scheme, which we simply described by the introduction of two gaps finds some experimental support in the different behavior found for the gap around the M points and along the nodal directions [17–20].

In this scenario, the bifurcation of $T^*(x)$ and $T_c(x)$ below a doping value of the order of optimum doping and the pseudogap regime find their natural explanation: i) Around and above optimum doping the zero-temperature QCP provides the effective interaction which determines the disruption...
of Fermi liquid and the $d$-wave superconductivity; ii) In the underdoped regime, $T_{CDW}(x)$ is increasing by lowering $x$ and shifts to higher temperatures the effective singular potential, providing strong pairing and no coherence in the “hot” momentum regions and coherence via the “colder” holes.

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References

[1] P. W. Anderson, Science 235 (1987) 1196; Phys. Rev. Lett. 65 (1990) 2306.
[2] C. Castellani, C. Di Castro, M. Grilli, Phys. Rev. Lett. 75 (1995) 4650.
[3] C. Castellani, C. Di Castro, M. Grilli, Z. Phys. B 103 (1997) 137.
[4] S. Caprara, C. Castellani, C. Di Castro, M. Grilli, Physica C 235-240 (1994) 2155.
[5] V. J. Emery and S. A. Kivelson, Physica C 209 (1993) 597.
[6] U. L"ow, V. J. Emery, K. Fabricius, S. A. Kivelson, Phys. Rev. Lett. 72 (1994) 1918.
[7] For the occurrence of ICDW due to interplay between PS and long-range Coulomb forces in the three-band extended Hubbard model see the conclusions of R. Raimondi et al., Phys. Rev. B 47 (1993) 3331.
[8] G. S. Boebinger et al., Phys. Rev. Lett. 77 (1996) 5417.
[9] A. Perali et al., Phys. Rev. B 54 (1996) 16216.
[10] G. Seibold, F. Becca, F. Bucci, C. Castellani, C. Di Castro, M. Grilli, cond-mat/9906108, to appear in Eur. Phys. J. B.
[11] S. Caprara, M. Sulpizi, A. Bianconi, C. Di Castro, M. Grilli, Phys. Rev. B 59 (1999) 14980.
[12] N. L. Saini et al., Phys. Rev. Lett. 79 (1997) 3467.
[13] S. Caprara, C. Di Castro, M. Grilli, this conference.
[14] M. Grilli et al., Phys. Rev. Lett. 67 (1991) 259.
[15] A. Perali, E. Piegari, A. A. Varlamov, C. Castellani, C. Di Castro, M. Grilli, unpublished.
[16] Similar proposals of coexistence of strongly and weakly coupled pairs have been discussed in the literature. See e.g. J. Ranninger, J. M. Robin, M. Eschrig, Phys. Rev. Lett. 74 (1995) 4027; V. B. Geshkenbein, L. B. Ioffe, A. I. Larkin, Phys. Rev. B 55 (1997) 3173.
[17] C. Panagopoulos and T. Xiang, Phys. Rev. Lett. 81 (1998) 2336.
[18] J. Mesot et al., cond-mat/9812377.
[19] G. Deutscher, Nature 397 (1999) 410.
[20] J. Demsar et al., Phys. Rev. Lett. 82 (1999) 4918.