Charge-ordering quantum criticality in the phase diagram of the cuprates

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Abstract. We discuss how the quantum-critical-point scenario for high-$T_c$ superconductors with density-driven charge order or stripe formation finds support from recent EXAFS experiments. Our phase diagram has the interesting feature, which is also suggested by the EXAFS experiments, that some cuprates may not show well-formed stripe phase. We also consider the extensions of the scenario to include the interesting possibility of first-order transitions which call for further experimental and theoretical investigation.

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There are by now several evidences of the existence of a Quantum Critical Point (QCP) around the optimal doping of the cuprates\cite{1,2,3,4,5}. The issue we address here is to interpret the recent experimental results of Ref. \cite{7} as further evidence for the QCP scenario for high $T_c$ cuprates, that we have been proposing along the years\cite{6}. This scenario found one of its possible realizations within a model of strongly correlated electrons interacting with phonons, i.e. the simple one-band Hubbard-Holstein model in the presence of long-range Coulombic forces\cite{8,9}. Starting from the comparison with the recent experiments, we here also propose possible extensions of this model. The simplifications with respect to models taking into account the complex structure of the cuprates was adopted for two main reasons: first of all it makes the model manageable despite the formal complications related to the treatment of strong e-e correlations via the slave-boson large-N expansion formalism. Moreover it allows to concentrate on the relevant aspects providing both a non-Fermi-liquid behavior and a strong pairing mechanism. Although the relevant features related to quantum criticality should be generic, different cuprates should of course show different aspects related to their specific structure.

Two major results were obtained within the Hubbard-Holstein model\cite{8,9}: i) Charge collective fluctuations mediate a doping- and temperature-dependent singular scattering among the quasiparticles, and ii) the $T = 0$ phase diagram here reported in Fig. 1 with a line of the electron-phonon (e-ph) coupling $g$ as a function of the doping $\delta$. This line marks a second-order transition for the onset of charge ordering (CO) characterized by an order parameter $\rho_{q_c}$ representing the microscopic charge modulation at a wavevector $q_c$\cite{8}. The low-doping region is only indicative since the magnetic effects have not been considered. The separation between the homogeneous phase and the CO phase is marked by a line having a minimum $g = g_{\text{min}}$ controlling the transition. For $g < g_{\text{min}}$ no CO (or stripes) could be formed as a static phase. Of course strong quantum fluctuations mediating pairing and non-Fermi-liquid behavior in the normal phase would be present both above and below the quantum critical line. For each value of $g_c(\delta_c)$ there is a QCP, which is the $T = 0$ end-point of a critical line $T_{\text{CO}}(\delta)$. This line extends to finite temperature the effective scattering mediated by the critical fluctuations. A recent analysis\cite{10} has shown that $T_{\text{CO}}$ is of the order of the observed pseudogap crossover temperature $T^*$. Indeed, within the CO-QCP scenario, the pseudogap temperature $T^*$ arises because the quasiparticles feel an increasingly strong attractive interaction by approaching the critical line $T_{\text{CO}}(\delta)$. In the particle-hole channel, this interaction can produce a gap due to the incipient CO\cite{11}. At the same time in the particle-particle channel, the strong attraction can lead to the formation of Cooper pairs even in the absence of phase coherence, which is only established at a lower temperature $T_c$\cite{12}. Therefore $T^*$ closely tracks the underlying transition line $T_{\text{CO}}(\delta)$, and merges with $T_c$.

\* In the framework of Ref. \cite{9} the charge ordering instability is a second-order transition leading to a gradual increase of the charge modulation. It is only when one enters deeply inside the (locally) ordered phase that anharmonic distortions of the charge profile may arise from the enhanced interactions with the spin and the lattice degrees of freedom. This may lead to the stripe formation.
around optimal doping, when the opening of the pseudogap and the phase coherence occur simultaneously.

The Hubbard-Holstein model is therefore able to describe a system with a (lattice-driven) electronic instability at $T = 0$ occurring below optimal doping, which divides the $T$ vs. $\delta$ phase diagram into a (nearly) ordered, quantum critical and a quantum disordered region naturally corresponding to the under-, optimal, and over-doped regions respectively. However, despite this gross correspondence, the model and its solution are too schematic to determine the relationship between the model parameters and the microscopic quantities of the real materials (in this sense the Hubbard-Holstein model can be regarded as the analog of the Ising model in critical phenomena: More involved models lead to different universality classes maintaining the main features related to scaling). In particular, the specific phonons involved, their coupling to the quasiparticles, the orbitals needed for a proper band description, are open issues presently under investigation. In this regard, experiments can provide crucial informations. In particular, recent EXAFS experiments \[7\] identified interesting features associated to the lattice structure. A microstrain of the Cu-O bonds was measured in terms of the deviation of the Cu-O distance with respect to a reference distance $d_0 = 1.985(\pm 0.05)\ \AA$

$$\varepsilon = 2 \left(1 - \frac{R_{\text{Cu-O}}}{d_0}\right),$$

(1)

which introduces a mismatch in the lattice between the CuO$_2$ layers and the rock-salt layers. In the $(\varepsilon, \delta)$ plane the experiments suggest a line separating a homogeneous phase from a “coexistence region of fluctuation bubbles of superconducting stripes” \[7\]. Actually, the published experimental data summarized in Fig. 7 of Ref. \[7\] leave various possibilities open: i) the above line could mark second-order transitions smoothly connecting the homogeneous and the “charge-ordered” phases, alternatively ii) it could
be a first-order line ending into a single QCP or into a finite segment of QCP’s, or, finally, iii) it could entirely be a line of first-order transitions. The experiments also suggest the remarkable possibility, that some cuprates may not show a stripe phase since their microstrain is lower than a critical value $\varepsilon_c$ estimated in Ref. 7 to be $\varepsilon_c \approx 0.045$ from the onset of local lattice distortions.

We address now the issue whether and how the experimental results presented in Ref. 7 can be connected with the above theoretical model and its extensions, both at the level of the calculated properties and of the open possibilities to be investigated with a further analysis. First of all one observes that the close resemblance between the experimental $(\varepsilon, \delta)$ and the theoretical $(g, \delta)$ phase diagrams is a clear indication that the Cu-O microstrain and the e-ph coupling $g$ of the simplified Hubbard-Holstein model are strictly related. From the microscopic point of view it is indeed quite natural that a lattice contraction in the CuO$_2$ planes can enhance the effective coupling between the electrons and the ions. Therefore the comparison between experiments and theory allows to draw the conclusion that a one-to-one monotonic relation $g = g(\varepsilon)$ is likely to exist.

Once this general framework is settled, one can move to identify more detailed possible scenarios. In particular the order of the homogeneous-metal to charge-ordered-metal transition is of obvious relevance. The simplest possibility is that in the real materials this transition is of the second order. In this case, at $T = 0$, the different microstrains determined by the rock-salt layers directly correspond to different e-ph couplings and are reflected in the similar phase diagrams. Of course this simple picture is not necessarily realized in the quite complex real materials where i) anharmonic effects and/or ii) additional non-ordering fields can partially or entirely transform the second-order transition into a first-order one. Both these possibilities can be considered within our Hubbard-Holstein scheme. The idea, which is standard in the theory of critical phenomena[13], is that both these mechanisms can change the sign of the quartic term $u|\rho_{q}|^4$ of an effective Ginzburg-Landau description of the free energy of the system. If this is the case a first-order transition is obtained and higher-order terms like $v|\rho_{q}|^6$ become important[13]. In case i) diagrams like in Fig. 2a, involving a coupling between a first and a second harmonic charge modulation $(\tilde{u}(\rho_{q, 2q} + c.c.)$, induce a negative correction to $u$.

If the charge fluctuations around the second-harmonic $2q$ are large enough, this correction ($\propto -\tilde{u}^2$) can drive $u$ to negative values. The alternative possibility ii) is that the microstrain enhances the coupling of the electrons with an additional phonon field, in general not coupled à la Holstein, but, more likely, coupled to the Cu-O hopping like in Su-Schrieffer-Heeger models. At small values of this coupling the fluctuations of the additional phonon field weakly dress the electrons, which still undergo a second-order instability because of the coupling to the original phonon mode. However, for sufficiently large values of the microstrain, it could happen that the additional phonon field introduces a non-ordering field $\psi$, which is generically bilinear in the electronic variables. Within the Ginzburg-Landau approach, this generates a four-leg vertex of
the form $u' |\rho_{q_c}|^2 |\psi|^2$. Second-order processes ($\sim -u'^2$) involving the propagator of the new field $\psi$, like the one depicted in Fig. 2b, can also drive the $u|\rho_{q_c}|^4$ term negative and naturally transform partially or entirely the line of QCP’s in Fig. 1 into a line of first-order transition. According to the general discussion of density-driven first-order phase transitions in the presence of long-range forces [14], near the first-order line one expects in this case bubbles of stripes in the homogeneous metallic background.

We stress here that these two possible mechanisms to change the order of the CO transition naturally extend the simple second-order transition theoretically determined in Ref. [9]. In the previous work the technical large-$N$ scheme within the leading-order approximation and the consideration of a single phonon mode did not allow for the inclusion of processes like those exemplified in Fig. 2. Nevertheless, the above-mentioned resemblance of the experimental and the theoretical phase diagrams make it clear that the qualitative determination of the region where the instability takes place is already captured within the simplified scheme. Without qualitatively modifying the generic appearance of the phase diagram, the additional terms discussed above would simply shift the instability line and possibly replace partially or completely the second-order line with first-order coexistence regions.

We also notice that the reentrant behavior of the instability region at low doping is a consequence of the increased residual repulsion between the quasiparticles at finite wavelengths, when the large quasiparticle effective mass no longer allows for an effective screening of the large (actually infinite in our model) Hubbard repulsion between the electrons. This physically reasonable effect occurs regardless of magnetism, which is surely present in real systems at low doping, but is poorly described within out large-$N$ approach. Nevertheless, if the resemblance between our theoretical and the experimental phase diagrams is confirmed, this suggests that magnetic effects should become relevant at doping lower than the doping at which the reentrant behavior sets in.

Further experiments are needed to establish which of the above-mentioned
possibilities i)-iii) for the phase diagram is realized in the cuprates. However, in all
the three cases the implications of our QCP scenario maintain their full validity unless
the transition becomes strongly first-order. Indeed all the relevant observables mainly
depend on the deviation from criticality fixed by $\xi^{-2}(T, \delta - \delta_c)$, where $\xi$ is the correlation
length for the onset of charge ordering. The only difference is now that $\xi$ would acquire
an additional dependence on $\varepsilon - \varepsilon_c$. We stressed in several papers[6] that the actual
onset of a fully developed CO phase was competing with local or coherent pair formation,
which modifies the fermionic spectrum stabilizing the system against the electronic CO
transition. There is the complementary possibility that the CO state can never be
reached because $g$ is below $g_{\text{min}}$. The corresponding observable quantity identified by
the experiments in Ref. [7] is the critical microstrain $\varepsilon_c$, below which no stripe phase can
be observed. Therefore the cuprates can deviate from criticality not only by $\delta - \delta_c$ in the
(overdoped) quantum-disordered region, or by $T$ and $T - T_{\text{CO}}(\delta)$ in the quantum-critical
or underdoped region respectively, but also because $\varepsilon$ is smaller or larger than $\varepsilon_c$, thereby
tending to a homogeneous or an inhomogeneous phase respectively. As long as $\varepsilon - \varepsilon_c$ is
not too large and $T$ is finite, for $\delta \sim \delta_c$ we enter again the quantum-critical region with
strong dynamical fluctuations in both cases. According to the proposed mechanism of
pairing mediated by critical fluctuations, the stronger are these fluctuations and the
larger is $T_c$. Indeed in the experiment[7] the mercury compound Hg1212, having $\varepsilon \sim \varepsilon_c$, has the the largest $T_c$, while Hg1201 (with $\varepsilon < \varepsilon_c$) and Bi2212 or La214 (with $\varepsilon > \varepsilon_c$)
have a lower $T_c$. Moreover, since $\varepsilon < \varepsilon_c$ in Hg1201, we expect no $T_{\text{CO}}(\delta)$, and therefore
no $T^*$, for this material.

Acknowledgments

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