Dynamical charge density waves rule the phase diagram of cuprates

S. Caprara\textsuperscript{1,2}, C. Di Castro\textsuperscript{1,2}, G. Seibold\textsuperscript{3}, and M. Grilli\textsuperscript{1,2}

\textit{1} Dipartimento di Fisica, Università di Roma “La Sapienza”, P.le Aldo Moro 5, 00185 Roma, Italy
\textit{2} ISC-CNR and Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia, Unità di Roma “Sapienza”
\textit{3} Institut für Physik, BTU Cottbus-Senftenberg - PBox 101344, D-03013 Cottbus, Germany

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In the last few years charge density waves (CDWs) have been ubiquitously observed in high-temperature superconducting cuprates and are now the most investigated among the competing orders in the still hot debate on these systems. A wealth of new experimental data raise several fundamental issues that challenge the various theoretical proposals. Here, we account for the complex experimental temperature vs. doping phase diagram and we provide a coherent scenario explaining why different CDW onset curves are observed by different experimental probes and seem to extrapolate at zero temperature into seemingly different quantum critical points (QCPs) in the intermediate and overdoped region. We also account for the pseudogap and its onset temperature \( T^*(p) \) on the basis of dynamically fluctuating CDWs. The nearly singular anisotropic scattering mediated by these fluctuations also account for the rapid changes of the Hall number seen in experiments and provides the first necessary step for a possible Fermi surface reconstruction fully establishing at lower doping. Finally we show that phase fluctuations of the CDWs, which are enhanced in the presence of strong correlations near the Mott insulating phase, naturally account for the disappearance of the CDWs at low doping with yet another QCP.

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\section*{INTRODUCTION}

The phase diagram of high-temperature superconducting cuprates (HTSC) is quite rich and indicates the coexistence of and competition between different physical mechanisms. First of all strong electron-electron correlations give rise to an antiferromagnetic (AF) Mott insulating phase when the CuO\textsubscript{2} planes are half-filled (one hole per unit cell). Although the AF phase is rapidly disrupted by doping, nearly critical spin fluctuations extend their action in the metallic phase. A major distinctive feature is then a pseudogap (PG) phase occurring below the doping-dependent temperature \( T^*(p) \) (in the prototypical HTSC family \( \text{YBa}_2\text{Cu}_3\text{O}_y \) (YBCO) \( T^* \sim 220 - 250 \) K at doping \( p \sim 0.1 - 0.12 \) and rapidly decreases merging with the SC \( T_c \) around optimal doping and seems to vanish at \( p \approx 0.19 \)). An intense debate is ongoing about the very nature of this PG phase with essentially two opposite points of view. Since the early times the idea was put forward (mostly by P. W. Anderson, \cite{1}) that these systems are strongly correlated doped Mott insulators, where the large electron-electron repulsion and the consequent short-range AF correlations, inside the low dimensional layered structure of the cuprates render these systems intrinsically different from standard metals ruled by the Landau Fermi liquid (FL) paradigm. In this framework many variants have been proposed ranging from the Luttinger liquid and the Resonating-Valence Bond paradigms \cite{2}, to the doped d-wave Mott state\cite{3} to the fractionalized Fermi liquid \cite{4}. The occurrence of this non-FL phase may imply a drastic rearrangement of the fermionic states: while far from the Mott state a FL is present with a large Fermi surface containing \( n_h = 1 + p \) holes per unit cell in the CuO\textsubscript{2} planes, approaching the Mott state the metallic character is given by just \( p \) carriers residing in four hole pockets in the so-called nodal regions \((\pi/2a)(\pm 1, \pm 1)\) of the Brillouin zone\cite{24}. In this context the PG phase is clearly related to the “Mottness” of the metallic state and, noticeably, \( T^*(p) \) marks a true phase transition towards the non-FL pseudogapped phase.

The opposite point of view is that in two dimensions strong correlations and the short-range AF correlations of doped Mott insulator are not enough \textit{per se} to spoil the Landau FL \cite{5} and the anomalous behavior of the metallic cuprates should be ascribed to the proximity to some form of instability ending at zero temperature into a second-order transition (quantum critical point, QCP). In this case the incipient order, which at low or zero temperature has an intrinsic quantum (and therefore dynamic) character produces strong long ranged and long lived fluctuations. In turn these mixed quantum-thermal fluctuations mediate strong scattering between the quasiparticles spoiling the FL character of (some of) the quasiparticles, possibly mediating a strong superconducting pairing. In this “quantum criticality” scenario a crucial role is obviously played by the type of order that the system would like to realize. Although many proposal have been put forward, the old evidences of charge density waves (CDW) \cite{6} have been strongly revived by the recent ubiquitous observations of charge density waves (CDWs) in all HTSC families.

The observed CDWs (see, e.g., \cite{9,21}) appear as a long-ranged phase under special circumstances only, like when high magnetic fields suppress superconductivity \cite{9,13}. Fig. \cite{1} reports the phase diagram of YBCO,
where the light-blue squares mark the onset of this static CDW order as detected by NMR and Hall experiments ([12] and references therein). Dynamical onset of CDWs, theoretically predicted long ago [6, 7, 24, 25], has been observed via X-ray spectroscopies [17, 18, 20] (green circles in Fig. 1). Recent Hall effect measurements indicate that a Fermi-surface reconstruction takes place in YBCO [12] and La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [26] at low temperature starting at doping $p'_c \approx 0.08$ and ending into a QCP at $p_c \approx 0.16$. On the other hand, the number of carriers changes rapidly between $p_c \approx 0.16$ and $p^* \approx 0.19$, where $T^*(p)$ extrapolates, with a clear connection to the above “Mottness” vs “quantum-criticality” issue discussed above. $p_c$ and $p^*$ are distinct and from...
the “Mottness” point of view one may argue that, while \( p^* \) marks the physical onset of a novel non-FL metallic phase, \( p_c \) is the start of the CDW phase, which is a mere “epiphenomenon” occurring “on top” of the more fundamental non-FL state. Conversely, supporters of the SC point of view may stress the close proximity of \( p_c \) and \( p^* \) claiming that CDW play the central role with their QCP at \( p_c = 0.16 \), while \( p^* \) is a crossover doping marking the region where strong CDW fluctuations appear before the QCP is met.

We exploit the recent experimental data to shape a coherent scenario based on the “quantum critical” point of view, which rationalizes the following issues: a) How the different CDW onset curves and corresponding seemingly different QCPs are related to one another? b) Are the CDWs related or unrelated to the pseudogap and to its different QCPs related to one another? c) Can CDWs account for the rapid changes of the Hall number seen in experiments? d) Which is the mechanism leading to the disappearance of the CDWs at low doping with yet another QCP located at \( p_c' \approx 0.08 \)? We concentrate our analysis on YBCO, for which the most complete set of experiments has been collected. Our results in comparison with experiments are summarized in the phase diagram of Fig.1.

Our paper is organized as follows: Section II initially revisits the frustrated phase separation mechanism underlying the formation of incommensurate CDW in strongly correlated systems. From this starting point a new analysis is carried out explaining why the strong correlations of HTSC favor the occurrence of CDW along the observed directions of the Cu-O bonds. The dynamical character of the CDW fluctuations is then analyzed to explain why probes with different characteristic timescales may detect different CDW onset temperatures. Section III provides a possible explanation for the rapid change in carrier density observed by Hall experiments based on the strongly anisotropic scattering induced by CDW fluctuations. In Section IV, again starting form the strongly correlated character of cuprates, we propose a mechanism to explain why CDW tend to weaken and disappear in the low-doping region of the phase diagram. In Section V we discuss our findings and we present our concluding remarks.

THE OPTIMAL/OVERDOPED PHASE DIAGRAM: DYNAMICAL CDW CROSSEVERS AND CDW TRANSITION

Before addressing the above a)-d) issues, we revisit the frustrated phase separation mechanism, which was proposed long ago \cite{27,28} as the formation mechanism of CDW, giving rise to a QCP around optimal doping \cite{24}. The region around optimal doping is naturally described within a Fermi-liquid picture and CDWs occur as a second-order instability. The correlated character of the Fermi liquid is described within a standard Slave-boson/Gutzwiller approach, where the residual interaction among the quasiparticles \( V(q) = U(q) - \lambda + V_c(q) \) arises from three distinct contributions (see Appendix A): \( U(q) \) is a short-range residual repulsion stemming from the large repulsion of a one-band Hubbard model, \( \lambda \) is a local short-range attraction triggering charge segregation, due to a local phonon \cite{24}, to the instantaneous magnetic interaction present in doped antiferromagnets \cite{29}, or to both mechanisms, and \( V_c(q) \) is the long-range part of the Coulomb repulsion. Notice that even if phonons are involved in \( \lambda \), they are not directly related with pairing. The screening processes are described by the Lindhard polarization bubble \( \Pi(q,\omega_n) \) for quasi-particles having a renormalized band structure fitting the dispersion obtained from angle resolved photoemission spectroscopy (ARPES) experiments. The CDW instability is found as a divergence of the density-density correlation function, when \( 1 + V(q)\Pi(q,\omega_n) = 0 \) at \( \omega_n = 0 \) and \( q = q_c \). \cite{0,24,25} For its pictorial representation see Fig.2.

In our mechanisms strong correlations favor the CDW instability along the (1,0) or (0,1) Cu-O bond directions, in agreement with hard X-ray experiments \cite{24}. Indeed, these are the directions along which the short-range repulsion (see Fig.2(a) and Appendix A) is smaller, making the instability of the frustrated phase separation due to the local effective attraction \( \lambda \) easier. This shows that the frustrated phase separation mechanism naturally exploits the strongly correlated nature of HTSC to account for the occurrence of CDW along the ubiquitously observed (1,0) or (0,1) directions.

Expanding \( V(q) \) and \( \Pi(q,\omega_n) \) around \( q = q_c \) and \( \omega_n = 0 \) one obtains the standard quantum-critical charge-fluctuation propagator (see Appendix A)

\[
D(q,\omega_n) = \left[ m_0 + \nu(q) + |\omega_n| + \omega_n^2/\Lambda \right]^{-1},
\]

where \( m_0 \propto \xi_0^{-2} \propto 1 + V(q_c)\Pi(q_c,0) \) is the mean-field mass of the fluctuations, \( \xi_0 \) is the mean-field CDW correlation length, \( \nu(q) \approx \tilde{\nu}/|q - q_c|^2 \), \( \tilde{\nu} \) is an electronic energy scale (we work with dimensionless momenta, measured in inverse lattice spacings \( 1/a \)), and \( \Omega \) is a frequency cutoff. The mean-field instability line \( T_{\rm CDW}^0(p) \) (magenta solid line in Fig.1) is characterized by a vanishing \( m_0 \). This is the well-known frustrated-phase-separation instability \cite{27,25} underlying the formation of CDWs near optimal doping \cite{0,24,25}. We notice that, although \( \lambda \) might have a magnetic contribution, the present mechanism of CDW formation, contrary to other proposals \cite{30,33}, does not require the proximity to a magnetic QCP. The same CDW-mediated interactions are also active in the Cooper channel, providing a high-temperature \( d \)-wave pairing mechanism \cite{34}. Therefore, this region of the phase diagram is characterized also by the gradual onset of CDW-mediated pairing fluctuations, with reducing temperature and/or doping.
The fluctuation suppression of the mean-field critical line $T_{CDW}^0(p)$ is obtained by the self-consistent evaluation of the correction to the mean-field mass $m_0$, due to the fluctuator Eq. (1) (see Methods, Fig. [3]).

\[
m = m_0 + uT \sum_n \int_0^{\Lambda} d\nu \frac{N(\nu)}{m + \nu + |\omega_n| + \omega_n^2 / \Omega},
\]

where $u$ is the strength of the coupling between CDW fluctuations, $N(\nu)$ is the density of states corresponding to the dispersion law $\nu(q)$ and $\Lambda$ is an ultraviolet cutoff, corresponding to a momentum cutoff $\bar{q} \sim 1/a$.

One can numerically solve the self-consistent expression (2), finding the conditions for the instability $m = 0$ and the dependence of $m$ on temperature and doping. In a two-dimensional system, as a single CuO$_2$ plane of cuprates, $N(\nu)$ is constant for $\nu \to 0$. This leads to a finite shift of the two-dimensional QCP at $T = 0$, but the correction to the critical line at finite $T$ is divergent, consistently with the absence of long-range order in two dimensions for a two-component order parameter (as in the incommensurate CDW case). However, cuprates are layered systems and the planes are weakly coupled. This allows for an ordering at finite temperature $T_{CDW}(p)$, which arises in the solution of Eq. (2) for $m = 0$, provided $N(\nu)$ assumes a three-dimensional form $N(\nu) \sim \sqrt{\nu}$ below some energy scale $\nu_\perp$ related to the inter-plane coupling (see Methods). $T_{CDW}(p)$ is so reduced (see Fig. [1]) with respect to the mean-field line $T_{CDW}^0(p)$ that it occurs below the superconducting dome. Superconductivity therefore appears as the stabilizing phase against CDW long-range order. This explains why the experimental data corresponding to long-range CDWs are only detected for magnetic fields large enough to weaken the superconducting phase [4]. These experiments also allow to estimate $\nu_\perp$. Fig. [4] displays the $m(T_{CDW}) = 0$ blue line obtained with $\nu_\perp = 10$ K.

We now address the issue a) of why different probes identify different CDW onset temperatures. The key point is the dynamical character of the CDW fluctuations. A probe with long characteristic timescale (like, e.g., NMR or NQR) will only detect static order, otherwise the fluctuating CDWs average to zero during the probing time. This is why these probes identify a true phase-transition line $m(T_{CDW}^0(p) = 0$ at high magnetic field (of course, if in real systems pinning intervenes to create locally a static order, this can be detected by local static probes even at larger temperatures and low magnetic fields. This seems to be the case in recent NMR experiments [14]). On the other hand, a fast probe with a short probing time $\tau_{pr}$ takes a fast snapshot of the fluctuating system and finds a seemingly higher transition temperature when the CDW order is still dynamical, as long as the CDW characteristic timescale $\tau_{CDW} \propto \xi^2 \propto m^{-1}$ is longer than $\tau_{pr}$, thus acting as an infrared cut-off and diminishing the reduction effect of the fluctuations on the onset temperature. We identify the dynamical onset line as the line where $m \approx \omega_{pr} = \tau_{pr}^{-1}$. The green solid line in Fig. [1] represents the dynamical onset of CDWs observed with X-ray spectroscopy with a mass $m \approx \omega_{pr} = 50$ K, thus solving the experimental puzzle a).
**CDW-QCP INTERPRETATION OF HALL TRANSPORT**

According to issue c), recent Hall experiments [12] show a rapid increase of the Hall number in a narrow doping range from \( n_H = p \) at \( p \approx 0.16 \) up to \( n_H = 1 + p \) for doping larger than the pseudogap zero temperature onset point \( p^* \). Such crossover has been attributed to a large Fermi surface at \( p > p^* \) as observed with ARPES and the formation of hole pockets for \( p < p^* \) due to either the establishment of a new metallic phase like a d-wave Mott insulator [3, 55] or a 'topological metal' [56], or some more conventional kind of order as e.g. a spin spiral [37]. In all these scenarios \( p^* \) is completely unrelated to CDWs whose QCP is then placed at the lower doping value \( p_c \).

Here, instead, we keep a minimal framework showing that the crossover behavior of the Hall number can be explained by the increasingly strong fluctuations starting below \( T^*(p) \) and approaching the nearby CDW-QCP. In particular, we exploit the strong momentum dependence of the effective quasiparticle interaction mediated by the CDW propagator Eq. (1) which naturally splits the Fermi surface in hot and cold regions: The quasiparticles in the hot regions (\( \phi = 0, \pi/2 \)) are connected by \( \mathbf{q} \sim \mathbf{q}_c \) and interact strongly, while the scattering in the cold regions stays weak. This results in a marked anisotropy of the quasiparticle scattering rate [38]

\[
\Gamma(\phi) = \{ \Gamma_{max}^{-1} + [\Gamma_0 + \Gamma_\Sigma(\phi)]^{-1} \}^{-1},
\]

with

\[
\Gamma_\Sigma(\phi) = \text{Im} \frac{2 T \Gamma_2(\phi)}{1 + \sqrt{1 - i \frac{2 T}{\Gamma_2(\phi)}}},
\]

and \( \Gamma_2(\phi) = \Gamma_2[1 + \alpha \cos^2(2\phi)] \). The expression of \( \Gamma_\Sigma(\phi) \) is derived from the quasiparticle self-energy near hot spots in models with spin [39] or charge [38] nearly critical fluctuations. Here, \( M(\phi) = m(T) + \nu \sin^2(2\phi) \) is the energy scale below which the quasiparticles have a Fermi-liquid behavior and is minimal at the hot spots. The anisotropy of \( \Gamma(\phi) \) is enhanced by approaching the CDW criticality, where \( n_H \) vanishes. The resulting fits of \( R_H \) as a function of temperature are reported in Fig. 3(a), while the related hole densities are reported in Fig. 3(b) by the blue circles, in good agreement with the experimental values (red squares) [12]. Interestingly, we also find a good agreement with the resistivity curves [see Fig. 7 in Methods] in contrast to a similar analysis in Ref. [12]. The inset of Fig. 3(a) also shows that the anisotropic component of scattering strongly increases with approaching \( p_c \approx 0.16 \) so that the dominating contribution to \( n_H \) is coming from the nodal regions.

The anomalous singular scattering is a general consequence of the CDW-QCP and it must occur when this

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**FIG. 3.** Analysis of Hall constant and hole density within the CDW-QCP scenario. (a) Fits of \( R_H \) vs. \( T \) of the low-field (empty circles) and high-field (filled circles) measures at various dopings (data taken from Ref. [12]) using the anisotropic scattering model of Eqs. (3) and (4). The anisotropy parameter \( \alpha \Gamma_2 \) is reported in the inset. (b) (Adapted from Ref. [12]) Doping evolution of the hole density extracted from \( R_H \) measurements in Ref. [12]. The experimental points in the range \( 0.16 \leq p \leq 0.205 \) are the red rectangles with error bars, while the blue circles are the values of \( n_H \) extracted from the fits based on the microscopic anisotropic scattering model. The Fermi surfaces in the various doping regimes are schematically depicted above: (from left to right) hole pockets in the strongly correlated region near the Mott transition, Fermi surface reconstruction with electron pockets in the CDW region; large Fermi surface for \( p > p_c \approx 0.16 \) with dashed (hot) regions where for \( T < T_{\text{cdw}} \) the anisotropic CDW scattering suppresses the quasiparticle states; for \( T < T_{\text{pair}} \) this suppression is enhanced by CDW-mediated pairing fluctuations leading to the formation of Fermi arc features; large Fermi surface in the region far from the CDW-QCP, where CDW scattering is weak and the Fermi-surface states are cold.
is approached, as it has indeed been measured by quantum oscillations in [40], and corresponds to the region of Fermi surface reconstruction and of anomalous behavior of the Hall number. Hence, coming from high temperatures our CDW-QCP scenario predicts a significant increase of $R_H$ upon crossing the pseudogap critical temperature when the CDW scattering starts to deplete spectral weight from the antinodal Fermi surface states $T_{cdw}$ in agreement with ARPES experiments [41]. However, it is important to note that our analysis does not incorporate pairing fluctuations which have been shown [42] to be relevant in a certain temperature window $T_c < T < T_{pair} < T_{cdw}$ and which would further increase the anisotropic scattering via the formation of antinodal gaps in the electronic spectrum (the relevant interplay of CDW and pair fluctuations has already been noticed, e.g. in Ref. [43]). In particular, if long-range superconducting order is suppressed by strong magnetic fields these fluctuations extend down to $T = 0$ in contrast to the anisotropic scattering from Eq. (1) which vanishes in this limit (even though the vanishing of $m(T)$ tempers this reduction). Therefore, upon lowering temperature the increasing contribution of pairing fluctuations will counteract the decrease in the CDW anisotropic quasiparticle scattering and thus eliminate the downturn of the $R_H$ curves in Fig. 3 in the limit $T \to 0$ as is observed in Nd-codoped LSCO [44] where $R_H$ can be measured to much lower temperatures than in YBCO where the measures end at $T = 40$ K.

THE UNDERDOPED PHASE DIAGRAM: THE ROLE OF CDW PHASE FLUCTUATIONS

In all the models proposed so far (including ours), were it not for the competing superconducting phase, the critical line for static CDWs monotonically increases with underdoping and saturates to a finite value at low doping (see Fig. 1 and Fig. 4 below the solid blue line). This is at odds with the experiments, where CDWs appear below a dome-shaped critical line ending into a QCP at low doping $p_c^* = 0.08$ [45]. In our model we solve this inconsistency taking into account the role of the dynamical fluctuations of the phase $\theta$ of the CDW order parameter $\Psi(r) = |\Psi(r)|e^{i\theta(r)}$ at low doping.

A well-known feature of CDWs [16] is that their phase stiffness is proportional to the strength of the metallic character (like, e.g., high Fermi velocity, high quasiparticle DOS, etc.), which is strongly reduced in the proximity of the Mott transition. Thus the experimentally observed reduction of the CDW critical (or onset) temperatures in the underdoped region appears as a crossover from a transition ruled by the vanishing of the amplitude of the CDW order parameter $\langle \Psi \rangle = \langle |\Psi(r)| \rangle = 0$ to a transition controlled by the suppression of the stiffness, due to fluctuations of the phase $\theta$. In this region (below the solid blue line and above the dashed blue line in Fig. 4) the translational symmetry is restored by the sliding motion of the CDW, with the sliding CDW possibly oriented along the a or b direction of the CuO$_2$ planes, thereby marking a nematic breaking of the $C_4$ symmetry of the lattice. This situation is reminiscent of the so-called vestigial charge order [47, 48], obtained in a different context.

The effect of the phase fluctuations on the CDW dy-
namics is customarily described by the \( S_{XY} \) like action
\[
S_{XY} = \frac{1}{8} \sum_{\mathbf{q}, \omega_m} \left[ D\omega^2 + \chi\omega_m^2 \right] \theta(\mathbf{q}, \omega_m) \theta(-\mathbf{q}, \omega_m),
\]
where \( D \) is the bare stiffness, and the coefficient \( \chi \) deter-
mines the speed \( c_0 = \sqrt{Dn/\chi} \) of the phase fluctuations.
As long as the CDW critical temperature is larger than the interplane coupling (\( \approx 10 \text{ K} \) in the optimal doping region), we can make this transition to be of the Berezinski-Kosterlitz-Thouless (BKT) type. According to the above arguments, the phase stiffness \( D \propto p \) and therefore the bare critical temperature of the BKT transition obtained from the usual condition \( T^0_{\text{CDW}} = \frac{\pi}{2} D_0 \) (see magenta line in the inset of Fig. 4) is also proportional to doping \( T^0_{\text{CDW}} \approx T^0 p \) (magenta dashed line in Fig. 4).

However, similarly to what happens on the high-doping side to the mean-field critical temperature, whatever is the bare \( T^0_{\text{CDW}} \), this is reduced by the quantum and thermal phase fluctuations. Within the XY model with sound-like phase fluctuation modes one obtains the perturbative expression of the depleted stiffness \( D \)
\[
D = D_0 - \frac{nq_c q_0}{2\pi\Lambda_0} \int_0^\Lambda_0 dq q^2 \left[ 1 + b(q_c q_0) \right]
\] (5)
where \( \Lambda_0 \approx 1/a \) is a momentum cutoff (hereafter we take \( \Lambda_0 = 1 \)) and \( b(z) = \left[ e^{z/T^*} - 1 \right]^{-1} \) is the Bose function.

Starting from different \( D_0 \) at the different doping and calculating the perturbative corrections with a doping-independent coupling \( nq_c \), we reduce the bare BKT transition temperature to \( T_{\text{CDW}} = \frac{\pi}{2} D \), which vanishes at a value of \( p = p'_c \), thereby answering issue d) in the Introduction. The various physically relevant combinations of the microscopic parameters can be reduced to two effective parameters only (see Appendix C), the position of the QCP, which can be fixed by experiments at \( p'_c \approx 0.08 \) and the slope of the \( T_{\text{CDW}}(p) \) curve. Numerically solving Eq. 5 we obtain the dashed blue line in Fig. 4.

Above the static \( T_{\text{CDW}} \) the phase fluctuates dynamically and, similarly to what happened in the high-doping region, a fast probe may detect a seemingly ordered state. This occurs as long as the phase correlation time \( \tau_0 \) is longer than the characteristic timescale of the probe. Again, we mimic this effect with an infrared cutoff \( \omega_{pr} \), i.e., a lower limit \( \omega_{pr}/c_0 > 0 \) in the integral in Eq. 5.

The reduced effect of quantum and thermal fluctuations leads to a larger stiffness and, in turn, a CDW onset at a higher temperature. For \( \omega_{pr} = 50 \text{ K} \) we find the green dot-dashed line in Fig. 4 that matches with the same \( \omega_{pr} \), the analogous line found in the optimal/overdoped region. The joint onset line then accounts for the dome-shaped \( T_{\text{CDW}}(p) \) onset temperature found by X-ray scattering [issue a) in the Introduction].

The prediction of a low-doping CDW-QCP due to the vanishing of the CDW phase stiffness rises the obvious issue of a possible direct observation of the associated strong phase modes in the vicinity of the transition. Since the phasors are optically active [50], optical conductivity is a natural tool to this purpose, but the contribution to the planar optical conductivity from overdamped CDW modes has already been theoretically investigated [51] and it turns out that this contribution is likely overshadowed by the wealth of planar single particle excitations. On the other hand, the optical conductivity along the \( c \)-axis \( \sigma_c(\omega) \) could be much more suited to identify the effects. In fact, the observed resonance in bilayer (and three-layer) cuprates [52], which has been previously attributed to transverse (Josephson) plasma modes (TPM) [53] might also be associated with intralayer-coupled phason modes which generate a dipole moment along the c-direction [54]. The expected specific doping and temperature scaling properties [51] could be a useful test on the origin of this optical feature.

**DISCUSSION AND CONCLUSIONS**

We addressed several key issues of cuprates, and yet other issues remain open. First of all, the simplest single-band Hubbard model neglects the intra-cell CuO\(_2\) structure and therefore it makes it hard to address the interesting question of the internal d-wave structure of the CDW order parameter recently detected both in resonant X-ray scattering [55] and STM [16, 56] experiments.

We also ignored the effect of disorder, which may locally render the CDW fluctuations static [57] and therefore observable by NMR well above the true static transition line [14]. Nevertheless our scenario is a good starting point to address these remaining open issues since it provides a unified scheme based on a robust and generic frustrated phase-separation mechanism to explain all the a)-d) issues listed in the introduction. The direction of the critical CDW wavevector, which is a natural test on the validity of the various proposed CDW mechanisms, is determined here by the generic strong-correlation effect encoded in the residual interaction among the Fermi-liquid quasiparticles \( V(\mathbf{q}) \). At and above optimum doping the transition is ruled by quantum and thermal CDW fluctuations, whereas at low doping phase fluctuations control the reduction of the stiffness and determine the transition. Our main result is that only one \textit{bona fide} dome-shaped CDW transition line is present, ending into two CDW-QCPs. The low-doping one at \( p'_c \approx 0.08 \) marks the onset of a static CDW order as revealed by Fermi surface reconstruction with electron pockets. The CDW phase ends at higher doping \( p_c \approx 0.16 \), above which fluctuations destroy again the static order. The whole region below \( T^* \) (theoretically associated with the mean-field CD instability line) is characterized by increasingly stronger fluctuations for doping \( p_c < p < p^* \approx 0.19 \). Nonetheless, depending on the probe characteristic
timescale, fast probes, like X-rays, can detect different onset lines $T_{C-DW}(p)$, well accounted for within our dynamical CDW fluctuation approach. Extrapolating these lines to low temperature may erroneously lead to a misplacement of the real CDW-QCPs. This unifying picture is also supported by the fact that, although different experiments mark distinct onset lines, their in-plane modulation vector is observed [58] denoting their common origin. The experiment on the c-axis optical conductivity on multilayer systems, suggested in Section IV, could further support the relevance of CDW phase fluctuations in determining the low-doping transition line.

Within our scenario the effective quasiparticle interactions are strongly anisotropic as a result of the anisotropy of CDW fluctuations mediating them. Starting below $T^*(p)$, this scattering accounts for a progressive increase of $R_H$ as observed in Hall experiments. Although in YBCO the situation is not yet settled, this anisotropic scattering may be supported by other mechanisms (like pair fluctuations) to reconstruct the Fermi surface giving rise to arcs and pockets with effective hole number eventually tending to $p$ as it likely occurs in the other cuprate families [44]. The interplay between CDW fluctuations and pairing is an old issue [34], which might also explain how the superconducting dome splits in two smaller domes (see Fig. 4 b in Ref.59), showing that superconductivity survives longer in the critical regions associated to the two QCPs at $p_c' = 0.08$ and $p_c = 0.16$. This tight relationship between superconductivity and CDW criticality as it clearly emerges from this experiments further supports the central character of CDW quantum criticality in the cuprates phase diagram.

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**The microscopic model: mean-field and fluctuation corrected CDW instability**

We first obtain a mean-field phase diagram within the Random-Phase Approximation (RPA) for correlated single-band quasiparticles. Specifically, we assume that a strong Hubbard-like local repulsion $U$ can be treated with a standard slave-boson/Gutzwiller (SB/G) approach [41, 60], leading to a Fermi-liquid scheme where the quasiparticles are effectively described by the Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\mathbf{q}} V(\mathbf{q}) \rho_{\mathbf{q}} \rho_{-\mathbf{q}},$$

where $c^\dagger_{\mathbf{k},\sigma}$ ($c_{\mathbf{k},\sigma}$) creates (annihilates) a quasiparticle with momentum $\mathbf{k}$ and spin projection $\sigma$. The band takes a tight-binding form $E_{\mathbf{k}} = -2t (\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu$ (we take a unit lattice spacing $a = 1$ on the CuO$_2$ planes of the cuprates, so that momenta are dimensionless), with nearest (t) and next-to-nearest (t') neighbor hopping terms and $\mu$ is the chemical potential. $\rho_{\mathbf{q}} = \sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma}$ is the Fourier transform of the density operator, and $V(\mathbf{q})$ is the residual density-density interaction between the quasiparticles. In particular, we find that $V(\mathbf{q}) = U(\mathbf{q}) - \lambda + V_c(\mathbf{q})$ arises from three contributions, each with a clear physical meaning:

$$U(\mathbf{q}) = U_0 + U_1 (2 - \cos q_x - \cos q_y) + U_2 (1 - \cos q_x \cos q_y)$$

is a short-range residual repulsion between the quasiparticles; $\lambda$ is a generic local attraction that would drive a phase separation instability of the quasiparticles, were it not for the presence of a long-range Coulomb repulsion

$$V_c(\mathbf{q}) = \frac{\nu_c}{\sqrt{G^2_{\mathbf{q}} - 1}},$$

which is the Fourier transform of the long-range Coulomb interaction, projected onto a single CuO$_2$ plane, preventing phase separation of the charged electrons. The coupling constant is $\nu_c = e^2 d/(2\epsilon_\perp)$, and

$$G_{\mathbf{q}} = 1 + \frac{\epsilon_\parallel d^2}{\epsilon_\perp} (2 - \cos q_x - \cos q_y).$$

Here, $e$ is the electron charge, $d$ is the interlayer distance (in units of the lattice spacing on the CuO$_2$ planes), $\epsilon_\parallel$ and $\epsilon_\perp$ are the components of the dielectric tensor for a system with tetragonal symmetry, along the principal axes parallel and perpendicular to the CuO$_2$ planes, respectively. For the sake of definiteness we fix for YBCO, $\epsilon_\perp = 5$, $\epsilon_\parallel = 20$. As we shall see, the Coulomb repulsion changes the electronic phase-separation instability at $\mathbf{q} = 0$ into a CDW instability at some finite wavevector $\mathbf{q} = \mathbf{q}_c$.

Within a SB/G approach, the quasiparticle dispersion is suppressed by the hole doping $p$, i.e., $t = t_{\text{bare}} p$, $t' = p_{\text{bare}} (1 - p)$.
$t'_\text{bare} \, p$. For YBCO, suitable values are $t_{\text{bare}} = 0.3$ eV, $t'/t = -0.45$.

At a given doping $p$, the chemical potential $\mu$ is fixed by the equation

$$\frac{2}{N} \sum_k f(E_k) = 1 - p,$$

where $N$ is the number of $k$ vectors within the first Brillouin zone of the CuO$_2$ planes, and $f(z) = (1 + e^{-z/T})^{-1}$ is the Fermi distribution function at a temperature $T$. The parameters of the short-range repulsion are then found as $|U_0| = -4\mu/p$, $U_1 = \frac{4t'_{\text{bare}}}{pN} \sum_k (\cos k_x + \cos k_y) f(E_k)$, and $U_2 = \frac{4t'_{\text{bare}}}{pN} \sum_k \cos k_x \cos k_y f(E_k)$.

The Coulomb interaction prevents the segregation of charged quasiparticles on large scales, driven by $\lambda$, while leading to a finite-wavelength instability at $q = q_c$. These are the basic ingredients of the so-called frustrated-phase-separation mechanism [27, 28] underlying the formation of CDW near optimal doping. We notice that, while this model has been considered in the past to describe a phonon-mediated short-range attraction, $\lambda$ can well describe any short-ranged (i.e., weakly momentum dependent) attraction possibly arising from nearest-neighbor magnetic [61], Coulombic [62, 63] or/and phononic [24, 64] mechanisms. The in-plane longitudinal and transverse conductivities can be described by the standard quasiparticle Lindhard polarization bubble

$$\Pi(q, \omega_n) = -\sum_{k, \sigma} \frac{f(E_{k+q}) - f(E_k)}{E_{k+q} - E_k + \omega_n}, \quad \text{(6)}$$

where $\omega_n$ are bosonic Masubara frequencies. Electronic charge instabilities within the RPA approximation are found by imposing a divergent density-density response, i.e., a vanishing denominator $1 + V(q)\Pi(q, 0) = 0$ first occurring at some finite $q = q_c$. To find the RPA instability line we first adjust $\lambda$ and $V_c$ to match the instability point with the doping $p = p^* \approx 0.19$ at which the pseudogap crossover line $T^*(p)$ extracted from resistivity data extrapolates for $T \to 0$. Once the parameters of $V(q)$ are fixed, the instability is found at finite $T$ by considering the $T$ dependence of the polarization bubble Eq. (6) only. The resulting instability line is given by the magenta line in Fig. [4], remarkably fitting the entire experimental $T^*(p)$ line.

Expanding $V(q)$ and $\Pi(q, \omega_n)$ around $q_c$ and $\omega_n = 0$ one obtains the standard expression [1] for the quantum-critical charge fluctuation propagator [24, 51]. The frequency cutoff $\Pi$ is related to the characteristic energy scale of the short-range interaction mediators (e.g., for phonons of typical energy $\omega_0$, $\Omega \sim \omega_0^2/t \sim \omega_0/5 \sim 10 \text{meV}$ [51]). Above the mean-field QCP, the mass term $m_0 \propto \xi^{-2} \sim T^2$ increases, due to reduction of the correlation length $\xi$.

**Hall coefficient within the CDW-QCP model**

The in-plane longitudinal and transverse conductivities have been derived in Ref.[65] and read

$$\sigma_{xx} = \frac{e^2}{\pi^2 h \partial} \int d\phi \frac{k_F v_F \cos^2(\phi)}{\Gamma(\phi)} \quad \text{(7)}$$

$$\sigma_{xy} = \frac{e^2 H}{\pi^2 h^2 \partial} \int d\phi \frac{v_F \cos(\phi)}{\Gamma(\phi)} \frac{\partial v_F \sin(\phi)}{\partial \phi} \quad \text{(8)}$$

where $\Gamma(\phi)$ is the anisotropic scattering rate along the Fermi surface ($\phi$ denotes the angle between the in-plane momentum and its $x$-direction). Following the analysis of Ref.[12] we neglect the dependence of Fermi momentum $k_F$ and Fermi velocity $v_F$ on $\phi$ and evaluate these quantities from

$$v_F = \frac{\hbar k_F}{m^*},$$

$$k_F = \sqrt{\frac{2\pi (1 + p)}{\alpha}},$$

where $m^*$ is the effective mass.
with hole doping \( p \) and an effective mass \( m^* = 4.1 m_e \). The in-plane lattice constant for YBCO is taken as \( a = 3.85 \text{Å} \) and the distance between planes is \( d = 3.2 \text{Å} \). The Hall coefficient and longitudinal resistivity are then

\[
R_H = \frac{\sigma_{xy}}{\sqrt{\sigma_{xx}^2 + \sigma_{xy}^2}} \frac{1}{H},
\]

\[
\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}.
\]

As discussed in the main text, our model for the anisotropic scattering rate Eq. (5) is derived from the self-energy for quasiparticles subject to quantum critical fluctuations in the spin [39] or charge [38] channel. It is limited by a maximum scattering rate \( \Gamma_{\text{max}} = v_F/a \) and impurity scattering is considered via a (doping independent) elastic scattering rate which we fix to \( \Gamma_0 = 0.86 \text{THz} \). The specific form for the quantum critical scattering Eq. (4) comprises an anisotropic and doping dependent mass \( m(\phi) = m_0(T) + \nu \sin^2(2\phi) \) which is minimized at the hot spots for CDW scattering, i.e., around the antinodal points \( \phi = 0, \pi/2 \). The parameter \( \nu = 480 \text{K} \) is an electronic energy scale [51], whereas \( m_0(T) \) is obtained self-consistently by solving Eq. (2).

![FIG. 6. Dashed lines: Temperature dependence of the mass term \( m_0(T) \) as determined from Eq. (2) for the four doping values considered in the paper. Solid lines include a cutoff \( m_{\text{max}} = 255 \text{K} \) and \( m_{\text{min}} = 112 \text{K} \) for \( p = 0.19 \).](image)

The dashed lines in Fig. 6 report the temperature dependent mass for four doping values. However, since our theory is only valid in the quantum critical region we cutoff the mass at a value \( m_{\text{max}} = 255 \text{K} \), which yields the solid lines in Fig. 6. Moreover, for doping \( p = 0.19 \) we also cutoff the divergence at low temperature which is due to a reentrant behavior caused by the nearby van-Hove singularity. We want to stress that these cutoffs do not influence on our main conclusion, which is drawn from the significant doping dependent change of \( R_H \) at \( T = 50 \text{K} \), but allow us to fit \( R_H \) over a larger temperature interval as shown in Fig. 3 of the main text.

The only fit parameters for the four doping values are the overall coupling \( \Gamma_2 \) and the parameter \( \alpha \) (cf. Eq. 4) which governs the anisotropy of the coupling to the quantum critical CDW fluctuations. The doping dependence of these parameters is shown in the inset to Fig. 7. The anisotropy parameter \( \alpha \) strongly increases upon approaching the QCP and determines the total coupling as shown in the inset to Fig. 3 in the main text PAIR-ING. For the same parameter values Fig. 7 reports the temperature dependence of the longitudinal conductivity as compared to the high field normal state data from Ref. [12]. It should be noted that the QCP model yields resistivity curves much closer to the experimental data then the analysis of Ref. [12] which was based on a scattering model which anisotropy increases linear in temperature whereas at higher temperature a Fermi liquid type \( T^2 \) contribution dominates. In our model the low temperature regime is usually Fermi liquid like (except at the QCP) whereas the linear temperature regime is intermediate before crossing over to a \( \sqrt{T} \)-like behavior. Moreover, the scattering is anisotropic over the whole temperature range in contrast to the model in Ref. [12] where it is essentially confined to low temperatures.

As discussed in the main text, we disregard here the additional effect of pair fluctuations. While this will likely reduce the request of strong anisotropic CDW-mediated scattering (the parameter \( \alpha \) it naturally reduces the value of resistivity improving the agreement between calculated and experimental resistivity).

**CDW suppression by phase fluctuations**

We started from a bare CDW phase stiffness \( D_0 = A p \) linearly increasing with doping as a result of strong correlations near the Mott-Hubbard transition. In the absence of experimental indications on the value of \( A \), we took \( A = 5800 \text{K} \), which fixes \( D_0 = 580 \text{K} \) at \( p = 0.1 \). This choice is rather immaterial in the forthcoming discus-
sion, where we highlight the dependence of the outcomes of our calculations on quantities that can be accessed by experiments. Of course, any experimental determination of \(D_0\) is accommodated by a change of the other model parameters, so as to keep fixed the measurable quantities.

The reduction of the stiffness in Eq. (5) can be cast in a more convenient way by using the semiclassical approximation for the Bose function \(b(z) \approx T/z\) yielding

\[
D(T) = D_0 \left[ 1 - \frac{u_0 c_0 \Lambda_\theta}{6\pi D_0} \left( 1 + \frac{3T}{2c_0 \Lambda_\theta} \right) \right].
\]

The BKT transition is obtained when \(D = 2T/\pi\). We point out that, even if this transition were not ruled by the two-dimensional BKT physics, Eq. (5) nonetheless implies a transition at a temperature \(T_0\), where the \(D\) vanishes, (see blue dotted line in the inset of Fig. 4). \(T_0\) is obviously higher than \(T_{BKT}\), where \(D\) is still finite.

We define the dimensionless quantity \(\tilde{T} = 3T/(2c_0 \Lambda_\theta)\) and the dimensionless bare BKT temperature \(\tilde{T}_0 = 3T_0/(2c_0 \Lambda_\theta)\), using the characteristic energy scale of the phase mode \(c_0 \Lambda_\theta\) as an energy unit. Taking for the sake of convenience \(\tilde{u} = u_0/8\), we obtain from the above equation the condition for the BKT transition temperature suppressed by phase fluctuations, \(\tilde{T} = \tilde{T}_0 - \tilde{u} \left( 1 + \tilde{T} \right)\).

Within this approximation, the critical BKT line is then

\[
\tilde{T} = \frac{\tilde{T}_0 - \tilde{u}}{1 + \tilde{u}}
\]

while from the definition of \(\tilde{T}_0\) and \(c_0\), we find \(\tilde{T}_0 = \beta \sqrt{\tilde{p}}\) with \(\beta = 3\sqrt{\tilde{\Lambda} / (2\Lambda_\theta)}\). The condition for a QCP where the BKT transition temperature vanishes is then given by \(\tilde{T}_0 = \tilde{u}\), which also defines the critical doping \(\tilde{p}_c = 0.08\) fixed by experiments [12]. Expanding around this value, we find the equation for the critical line

\[
\tilde{T} = \frac{\tilde{u}}{2(1 + \tilde{u}) \sqrt{\tilde{p}_c}} (p - \tilde{p}_c)
\]

The slope of the physical \(T_{CDW}(p)\) line is obtained by reintroducing the characteristic energy scale \(c_0 \Lambda_\theta\)

\[
\frac{c_0 \Lambda_\theta \tilde{u}}{2(1 + \tilde{u}) \sqrt{\tilde{p}_c}}
\]

and is fixed by fitting the data (light-blue squares in Fig. 1). In this way, the various physically relevant combinations of the microscopic parameters have been reduced to two effective parameters only, the position of the QCP and the slope of the \(T_{CDW}(p)\) curve, which can be fixed by experiments. Specifically we obtain the dashed blue line in Fig. 1 with \(\tilde{u} = 4.5\), and the characteristic energy scale \(c_0 = 850\sqrt{\tilde{p}}\) K and numerically solving the full expression Eq. (5).

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