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A quantum phase transition driven by the electron lattice interaction gives high T_C superconductivity

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Abstract

We identify for the first time the quantum phase transition (QPT) as a function of the electron lattice interaction for charge localization in stripes with local lattice distortions in cuprate perovskites at metallic densities. The electron lattice interaction $\lambda(\eta)$ is triggered at the localization limit by the strain η of the CuO_2 plane due to the chemical pressure generated by the mismatch between the copper oxide and the rocksalt layers. The strain of the CuO_2 plane has been directly measured by Cu K-edge EXAFS. The critical point for the charge localization in striped lattice domains coexisting with itinerant carriers is at $\eta_c = 0.04 \pm 0.005$ and $\delta_c = 0.16 \pm 0.03$. We report a 2D plot $T_C(\delta,\eta)$ for the doped perovskites, where δ is the doping. The plot $T_C(\eta)$, for δ=constant, shows the highest T_C at the critical point $\eta_c = 0.04 \pm 0.01$. The attractive pseudo Jahn–Teller (pJT) interaction and the particular critical charge and spin fluctuations driven by critical ordering of cooperative pJT local lattice distortions, forming a superlattice of quantum stripes tuned at a 'shape resonance' near this quantum critical point, provide a possible solution for two long standing mysteries: the phase diagram and the pairing mechanism in cuprate superconductors.

Keywords: High T_C superconductors; Phase diagram; Pairing mechanism; Critical point; Stripes; Cooperative pseudo Jahn–Teller local lattice distortions; Incommensurate charge density wave; Intermediate coupling

The low temperature phase transitions in strongly correlated electron systems remain only partially understood. An increasing number of systems are coming to light such as heavy fermion and cuprate superconductors where the Fermi liquid regime is suppressed due to their proximity to quantum phase transitions.

A quantum phase transition (QPT) is a zero temperature generically continuous transition tuned by a parameter in the Hamiltonian. Near this transition quantum fluctuations take the system between two distinct ground states. Examples of QPT include the metal-to-insulator transition in disordered alloys, the integer and fractional Quantum–Hall transitions, magnetic transitions in heavy Fermion alloys, the superconducting-to-insulator transition in granular superconductors [1]. The unconventional normal state can be described in terms of fluctuations of the local order parameter. For example if the magnetic ordering temperature in heavy Fermions is suppressed to absolute zero these fluctuations soften leading to strong enhancement of quasiparticle scattering rate and potentially to a breakdown of the Fermi liquid description in its simplest form [2–4]

The presence of non-conventional pairing mechanisms in superconductivity near a QPT is well established in several exotic materials [5]. In several organic materials and heavy Fermions, $CePd_2Si_2$ [6], $CeNi_2Ge_2$ [7] and $CeRh_2Si_2$ [8–10] the superconducting phase appears by increasing the pressure above a critical value. The superconducting phase is in the regime of quantum fluctuations near a QPT from a metal to a spin ordered phase [11].

In barium bismuthates ($Ba_{1-x}K_xBiO_3$ and $Ba_{1-x}Pb_xBiO_3$) the exotic superconducting phase is near QPT to a charge ordered phase (CDW) due to valence skipping ($Bi^{4+} -> Bi^{3+} + Bi^{5+}$) [12]]. The superconducting phase with a short coherence length in these materials has clear similarities with high T_C superconductors (HTcS).

The non Fermi liquid behavior of transport properties in HTcS is an indication of the proximity to some unknown QPT. Several proposal have been presented for the presence of a QCP at some critical value of the doping.

It has been proposed that the critical point is due to the doping of the 2D AF Mott–Hubbard insulator, in fact a

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phenomenological model for the low energy spin dynamics in the normal state shows that these systems are close to a QPT [13,14]. However in this case the predicted maximum T_C is expected at the critical point for disappearing of AF order in the range $0.02<\delta<0.06$ [15] in disagreement with the experiments. Other authors have considered a case of QPT near a metal to insulating CDW phase transition in the strong local electron–lattice interaction regime [16–18] and in the weak coupling Hubbard–Holstein model [19,20]. The first experimental evidence for a CDW with its associated modulation of local lattice distortions (LLD) was found by joint X-ray diffraction and extended X-ray absorption fine structure (EXAFS) [21–40]. It was shown that the charge localization in the correlated 2D electron gas is driven by cooperative pseudo Jahn–Teller (pJT) electron lattice interaction in the intermediate coupling regime (ICR). In the Bi2212 case the one-dimensional (1D) ordering of LLD form stripes that co-exist with itinerant carriers. The resulting scenario of superconducting stripes in high T_C superconductors where 'the free charges move mainly in one direction, like the water running in the grooves of a corrugated iron foil', was first introduced in 1992 at Erice [21–23]. The 1D incommensurate CDW that co-exists with the superconducting phase is made of stripes of distorted lattice due to the freezing of pseudo Jahn–Teller Q_2 modes of the CuO_4 square lattice (LTT-like) [41] that are separated by domain walls of undistorted lattice stripes (LTO-like). The size of the domain of cooperative local lattice distortions where the localized electrons are trapped was found to be 5 Å [34] in agreement with an intermediate coupling regime. In Bi2212 with $T_C=80$ K the charge ordering temperature was found to be 120 K. By changing the doping in Bi2212 the system remain always in the coexistence regime (localized charges in the CDW and itinerant electrons) but is was never possible to find a critical density for the onset of CDW, i.e. a QCP for CDW.

Quantum spin density wave fluctuations near an electronic topological transition [42], i.e. by tuning the chemical potential at a van Hove singularity was ruled out by the fact that the van Hove singularity is located at doping 0.25 [43].

Recently some experiments have provided further compelling evidence for quantum critical fluctuations in high T_C superconductors [44,45]. Therefore the key problem to be solved to understand the pairing mechanism and phase diagram in HTcS is the actual nature of the QPT and the location of the quantum critical point (QCP).

All available experimental data show that in the anomalous metallic phase of cuprates we are in a regime of coexistence of localized and itinerant carriers [46,47]. The standard plots $T_C(\delta)$ of La214 and Bi2212 do not cross the quantum critical point. The electron lattice interaction giving the CDW is well established by the isotope effect experiments [48] observed also for the stripe formation temperature [49]. It provides a second variable to describe the phase diagram of doped cuprate perovskites. Therefore we have looked and found the QCP for the onset of the coexistence phase of polaronic stripes and itinerant carriers in the intermediate coupling regime studying the physical properties at constant doping as a function of the electron lattice coupling.

The pseudo Jahn–Teller electron–lattice interaction λ in cuprate families is driven by the strain η of the CuO_2 plane. High T_C superconductors are heterogeneous materials made of alternated layers of metallic bcc CuO_2 layers and insulating rocksalt fcc AO layers [50,51]. The bond-length mismatch across a block-layer interface is given by the Goldschmidt tolerance factor $t=[r(\text{A–O})]/\sqrt{2}[r(\text{Cu–O})]$, where $[r(\text{A–O})]$ and $[r(\text{Cu–O})]$ are the respective bond lengths in homogeneous isolated parent materials A–O and CuO_2 [52,53]. The hole doped cuprate perovskite heterostructures are stable in the range $0>t>0.9$ that corresponds to a mismatch $1-t$ of $0<1-t<10\%$. The CuO_2 sheets are under compression and (AO) layers under tension in the hole doped cuprates showing high T_C.

The electron–lattice interaction of the pseudo JT type is given by $\lambda=g(Q)\ f(\Delta_{JT})\ h(\beta)$, where Q is the conformational parameter for the distortions of the CuO_4 square, like the LTT-type tilting and its rhombic distortion; β is the dimpling angle that measures the displacement of the Cu ion from the plane of oxygens; and Δ_{JT} is the JT splitting that is modulated by the Cu–O (apical) bonds. Q and/or β increase with the increasing strain η of the CuO_2 plane due to the mismatch. Therefore the pseudo JT polaronic electron lattice interaction is a function $\lambda(\eta)$. For small variations of η, in all cuprate perovskites $0.02<\eta<0.08$, we can assume a proportionality between λ and η.

We have directly measured the strain of the CuO_2 lattice by measuring the Cu–O distances by in plane polarized Cu K-edge EXAFS. The 3D lattice structure has been solved by X-ray diffraction. The anomalous X-ray diffraction at the Cu K edge has been used to measure directly the diffraction due to only the Cu lattice. The 1D ordering of charge and local lattice distortions has been detected by diffuse X-ray scattering using synchrotron radiation. The strain $\eta=2(1-\langle\text{Cu–O}\rangle/d)$ for each sample has been obtained from the measured average $\langle\text{Cu–O}\rangle$ bond by EXAFS where $d=1.97$ Å is the Cu–O equilibrium distance with no lattice mismatch $1-t\sim\eta$.

The superconducting critical temperature $T_C(\delta,\eta)$ of many cuprate perovskites as a function of doping δ and the CuO_2 strain η is plotted in Fig. 1. The cuprates ($La_{1-x}Ba_xCuO_4$, $La_2CuO_{4+\delta}$, $La_{0.6}Nd_{0.4}La_{1-x}Sr_xCuO_4$) with strain $0.08>\eta>\eta_0$ larger than the strain $\eta_0=0.07$ occupy the upper region of Fig. 1 while those in the weaker electron–lattice interaction regime $0.02<\eta<\eta_0$ show quantum fluctuations of pJT LLD near the critical strain $\eta_c=0.04$. The maximum $T_C=135$ K appears in the circle centered at the QCP at $\eta=\eta_c$. The high T_C superconductivity is suppressed around the black dots where the commensurate polaron crystal (CPC) at $\delta=0.125$ appears

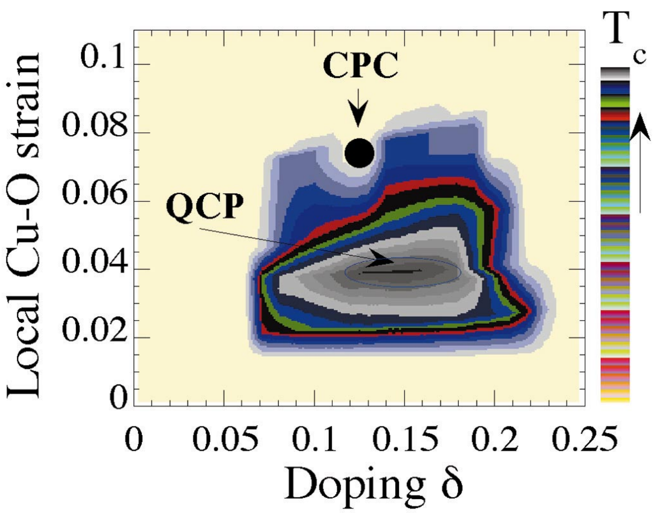

Fig. 1. The experimental superconducting critical temperature T_C (δ,η) of different superconducting cuprates as a function of strain η and doping δ of the CuO_2 plane. The elliptical blue area indicates the location of the QCP at the critical strain $\eta_c = 0.04$.

in compounds with $\eta > 0.07$. This point P_0 where the CPC appears with the minimum electron lattice interaction in the families of $La_{1-x}Ba_xCuO_4$ and oxygen doped $La_2CuO_{4+\delta}$ at the doping $\delta_0 = 1/8$ is identified by the black dot.

Fig. 2 shows the plot $T_C(\eta)$ at constant doping, $\delta = 0.16$, i.e. for optimally doped samples, following the second vertical dashed line in Fig. 1. The plot $T_C(\eta)$ shows a quantum critical point $\eta_c \sim 0.04$. In this regime the superconducting phase extends well beyond the critical point for $\eta > \eta_c$ indicating that the particular superlattice of polaron stripes due to quantum LLD fluctuations can coexist and amplify the critical temperature in agreement with the well established 'shape resonance' amplification of the critical temperature for this particular ICDW [25,26,29].

In Fig. 3 we have reported the value of the critical temperature as a function of the lattice strain $T_C(\eta)$ at a fixed doping, $\delta = \delta_0$, (i.e. along the vertical dashed line passing across the black dot in Fig. 1). The superconducting phase appears below T_C in the green area. It is evident that the critical temperature reaches a maximum value near the critical value $\eta_c = 0.04$ that is the quantum critical point (QCP) shown in Fig. 1. The line separating the quantum fluctuation regime from the phase where local lattice distortions appear (A+B and A) is the experimentally observed charge ordering temperature T_{co} for the oxygen doped La124 and Bi2212 systems at $\delta = 0.125$. This line separates the non Fermi liquid or quantum fluctuating regime from the co-existence region A+B (polaronic 1D ICDW and free carriers, and the pJT polaron commensurate crystal phase A at larger strain. The critical strain $\eta_c = 0.04$ is the critical point for the onset of the polaron stripes which is associated with the critical point for spin ordering SDW. The quantum critical point at $\eta_c = 0.04$ gives the highest superconducting transition temperature as expected. The superconducting phase is rapidly suppressed by the formation of the CPC that competes with the superconducting order. The anomalous metallic phase in a quantum critical regime is expected at $\eta \sim \eta_c$ as shown by many experiments.

Finally Fig. 4 shows a generic phase diagram in the intermediate coupling regime as a function of electron lattice coupling and doping. The cuprates are at the critical point for the formation of local lattice distortions and the

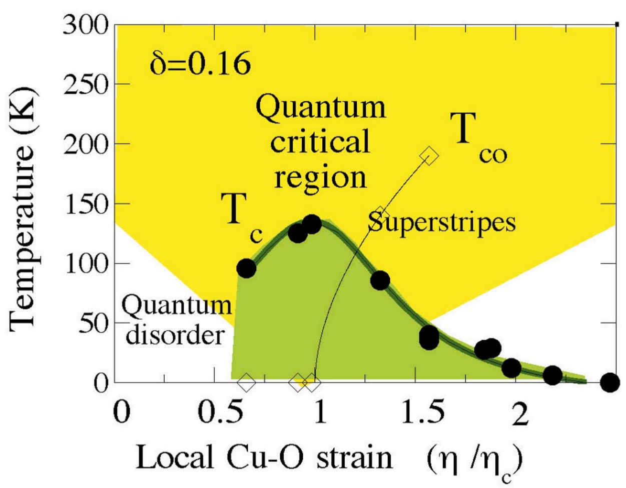

Fig. 2. The superconducting critical temperature $T_C(\eta)$ (circles) as a function of the lattice strain η. The critical temperatures $T_{co}(\eta)$ for polaron stripe formation in oxygen doped La214 and Bi2212 are shown by open squares at fixed doping $\delta = 0.16$. The superconducting critical temperature reaches a maximum at the critical strain η_c ~0.04. The critical point is the onset of the inhomogeneous phase, where pseudo JT polaron stripes and conducting carriers co-exist.

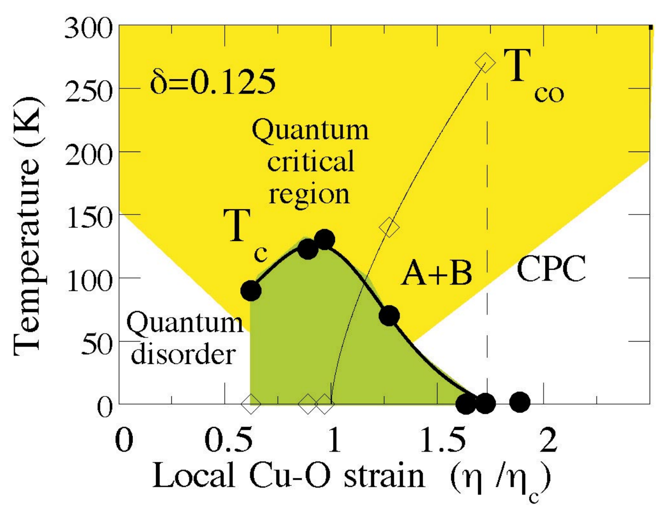

Fig. 3. The superconducting critical temperature $T_C(\eta)$ (circles) as a function of the lattice strain η at $\delta_0 = 0.125$. The superconducting critical temperature reaches a maximum at the critical mismatch $\eta_c = 0.04$. The critical point is the onset of the coexistence phase, where JT polaron stripes (phase A) and itinerant carriers (phase B) co-exist. The CPC (or the pure phase A) competes and suppresses the critical temperature for $\eta > 0.07$.

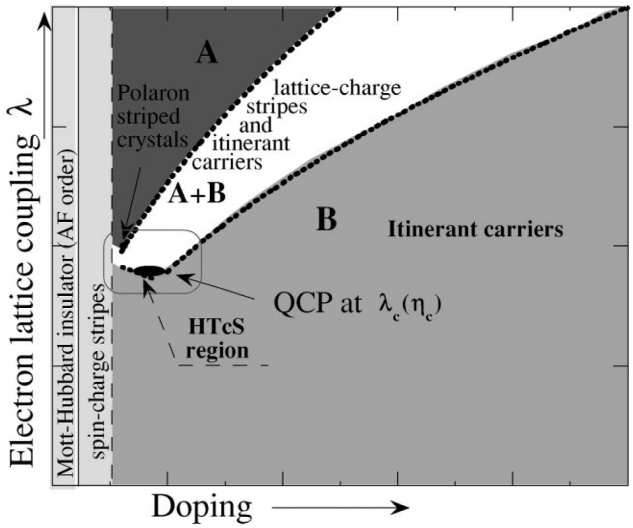

Fig. 4. The generic phase diagram of the electronic phases formed in doped perovskites in the intermediate electron lattice coupling regime. Beyond the charge transfer Mott–Hubbard insulator there is a region of phase separation of a glassy phase (G) of an electron glass in the localization regime $k_F l<1$ where spin-charge stripes can occur. The homogeneous phase of itinerant carriers (phase B) appears for a weak electron lattice interaction and high doping. The phase of commensurate polaron crystals (CPC), region A, appear at strong λ and low doping. The region of coexistence of itinerant carriers and carriers trapped in local lattice interactions (generalized polarons), phase A+B, shows a critical point, QCP, at $\lambda=\lambda_c$, indicated by a blue ellipse. The rectangle around the QCP indicate the region spanned by the electron lattice coupling $\lambda(\eta)$ in the cuprates by changing the lattice strain that is shown in Fig. 1.

onset of co-existence of localized charges trapped in LLD and itinerant carriers [52,53], i.e. in the intermediate electron–lattice coupling regime [54]. In this regime between the strong coupling regime where all charges are trapped by local lattice distortions at metallic densities (small polarons of radius between 5 and 2 Å), phase A and the phase B of itinerant charges in the weak coupling regime and high densities there is regime of coexistence of two phases: the A+B phase. It is well established that for the single polaron (doping $\delta \sim 0$) there is cross over from the localized to itinerant polaron. On the contrary at metallic densities there is critical value of the electron–lattice interaction indicated by the ellipse for the onset of coexistence of localized and itinerant charge carriers [54]. Commensurate polaron crystals (CPC) appear in the phase A where all carriers are trapped in the distorted local domains, the black dots is the commensurate crystal appearing at $P_0(\delta_0,\eta_0)$ the lowest possible density δ_0 and electron lattice interaction $\eta_0>\eta_c$. The region of high T_C superconductivity in Fig. 1 spans the small gray rectangle around the QCP at $\lambda=\lambda_c$ in Fig. 4. The rectangle around the QCP indicate the region spanned by the electron lattice coupling $\lambda(\eta)$ in the cuprates by changing the strain of the CuO_2 plane that was plotted in Fig. 1 reaching λ_c at critical η_c.

In conclusion, we have shown that high T_C superconductivity occurs at the critical point of the electron lattice interaction for the formation of local lattice distortions at metallic density. The electron–lattice interaction is driven at this critical point by the strain of the CuO_2 plane η controlled by the lattice mismatch between the metallic layers and the intercalated block layers.

The maximum T_C occurs at the critical point for the transition from a homogeneous metallic phase to an inhomogeneous metallic phase with coexisting polaron stripes and free carriers at $\eta_c=0.04$. For $0.04<\eta<0.07$, by decreasing the temperature the materials exhibit a transition at T_{co} from the homogeneous to the inhomogeneous phase that can be defined as the temperature for the polaron stripe formation.

We can understand now the complex phenomenology of cuprates showing quite different superconducting and normal phases in the under-doped to over-doped regime. For $\eta>0.07$, at $\delta=0.125$, the high T_C superconductivity is suppressed by the formation of the CPC. On the contrary the high T_C superconductivity co-exists with the ICDW.

In the underdoped regime at doping $\delta \sim 0.09$, and at a 2D electron density parameter $r_s \sim 12$, the highest T_C appears in a low density inhomogeneous phase (A+B) where the number of free carriers is smaller than that of charges trapped in LLD (generalized polarons in a intermediate density 2D electron gas $r_s \sim 12$). In this regime superconductivity is formed by local pairs with anomalous large $2\Delta/T_C$ ratio [41,42]. In the optimum doping regime $\delta \sim 0.16$, $r_s \sim 6$–8, the density of itinerant carries is larger than that of localized carriers.

In conclusion, we have deduced a phase diagram for the superconducting phases where T_C depends from both doping δ and lattice strain η of the CuO_2 layers. The anomalous normal phase of cuprate superconductors is determined by an inhomogeneous phases with co-existing stripes of charges trapped in LLD (generalized polarons) and itinerant carriers that appears for an electron lattice interaction larger than a critical value λ_c. Lattice-charge stripes or polaron stripes appear in this critical fluctuation regime. The lattice mismatch η drives the electron lattice interaction to a QCP of a quantum phase transition. The plot $T_C(\eta)$ crosses the critical point and the highest superconducting critical temperature occurs at $\eta=\eta_c$. These results show that the particular spin and charge critical fluctuations in the inhomogeneous phase of polaron stripes and itinerant carriers favor the superconducting pairing.

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