

Phase diagram of cuprate superconductor: Evidence of universal properties?

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Abstract

In this essay, the phase diagram of cuprates superconductors is reviewed. The doping and magnetic field induced transitions are studied for finite temperature as well as for zero temperature and the two dimensional quantum superconductor to insulator and the three dimensional quantum superconducting to metal transitions are observed. Scaling predictions are performed and compared with experimental results.

1 Introduction

More than a decade and a half after the discovery of high-temperature superconductivity in ceramic compounds containing copper-oxyde planes, these material continue to puzzle condensed matter physicists. More than finding a reasonable argument that predicts the uniquely high values for the superconducting transition temperature in the cuprates, a theory of high temperature superconductivity would have to explain the unique and complex phase diagram exhibited by this class of materials. Depending on the temperature, the magnetic field and the level of doping, the cuprates can be insulators, metals or superconductors.

Before the mid-1980s, superconductivity had only been observed in metals and metallic alloys that had been cooled below 23 K. In 1986, high temperature superconductivity (high T_c) was discovered in barium doped lanthanum copper oxide with a transition teperature of 36 K. Similar materials with higher transition soon followed and more than 50 of them are now known. Amazingly, they are all variations of a single theme: lightly doped copper-oxide planes. Extensive research to find high temperature superconductivity in other families of materials has been singularly unsuccessful. The question is, what is so unique about the cuprates that enable them to challenge our fundamental understanding of electrons in a solid? Establishing and understanding their phase diagram would be a significant step towards the answer.

After sixteen years of reasearch on those material, there is enough experimental data available to build an empirical phase diagram. The key factors in creating and destroying the superconducting state have been identified to be the temperature and the magnetic field, as in the traditional superconductors but also the doping and substitution. In cuprates materials, superconductivity is derived from the insulating and antiferromagnetic parent compounds by by partial substitution of ions or by adding or removing oxygen. One property believed to be generic to cuprates superconductors is a phase transition line in the temperature-dopant concentration plane. The undoped compounds are not superconducting. As the dopant concentration x is increased, the compound passes the "underdoped limit" (x_u), i.e. minimum concentration with a superconducting phase transition at finite temperature. At that point adding dopant increases the transition temperature T_c until an optimal doping x_m is reached. With further increase of x , T_c decreases and finally vanishes in the overdoped limit (x_o). When the dopant concentration is lowered from the optimal value along the axis x , the compound undergoes at zero temperature a quantum phase transition at the underdoped limit. The resistivity takes an infinite value. It is a quantum superconductor to insulator (QSI) transition. On the other hand, if it is increased towards the overdoped limit, a quantum superconductor to normal metallic state (QSN) occurs. The doping has also been observed to change the anisotropy. In tetragonal cuprates, the anisotropy is defined to be the ratio $\gamma = \xi_{ab}/\xi_c$ of the correlation lengths parallel ξ_{ab} and perpendicular ξ_c to the CuO_2 layers (ab plane). In the superconducting state, it can also be expressed as the ratio $\gamma = \lambda_c/\lambda_{ab}$ of penetration depth of the supercurrents perpendicular and parallel to the ab planes. When approaching a nonsuperconducting to superconducting transition ξ diverges while in the superconductor to nonsuperconductor λ diverges. In both cases however, γ remains finite. There are two particular cases: $\gamma = 1$ means that the 2 correlations are

equal: it is the isotropic 3D case, and $\gamma = \infty$ when the perpendicular correlation vanishes: a 2D critical behavior. Experimentally, γ is obtained from resistivity ($\gamma = \xi_{ab}/\xi_b = \sqrt{\rho_{ab}/\rho c}$) and magnetic torque measurements for the normal state and from penetration depth and magnetic torque measurements in the superconducting state.

This paper aims to analyze the empirical phase diagram of cuprates superconductors and take a close look at various situation where the 2D-QSI to superconductor to 3D-QSN transition occur. Given the generic phase diagrams, the scaling theory of finite temperature and quantum critical phenomena leads to predictions, including the universal properties, which can be confronted with experiment. As it stands, the available data seem to be consistent with a single complex scalar order parameter, a doping tunned dimensional crossover and a doping, substitution, or magnetic field driven suppression of superconductivity due to the loss of phase coherence.

2 Phase diagrams

There are very few compounds for which the dopant concentration can be varied continuously throughout the entire doping range. One of them is $La_{2-x}Sr_xCuO_4$, obtained by doping La_2CuO_4 with Sr , an alkaline-earth ion. Its empirical phase diagram in the temperature-dopant concentration plane is showed on fig.1.

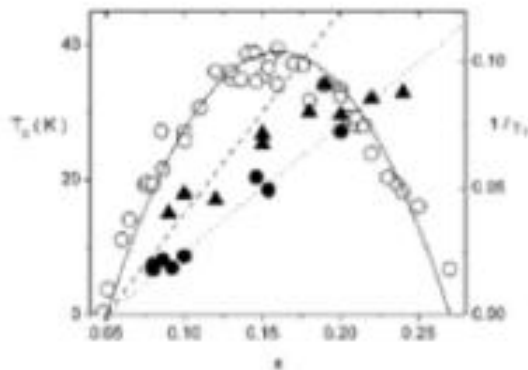


Figure 1: Variation of T_c (open circles) and $1/\gamma_T$ with x for $La_{2-x}Sr_xCuO_4$. Filled circles correspond to $1/\gamma_{T_c}$ and filled triangles to $1/\gamma_{T=0}$. The solid curve is Eq. (1) with $T_c^m = 39K$. The dashed and dotted lines follow from Eq.(2) with $\gamma_0, T_c = 2$ and $\gamma T_c = 1.63$. From [1]

The underdoped limit is $x_u = 0.047$, the optimal doping is $x = 0.16$ and the overdoped limit is $x = 0.273$. This phase transition line obeys the empirical relation:

$$T_c(x) = T_c(x_m) \left(1 - 2 \left(\frac{x}{x_m} - 1 \right)^2 \right) = \frac{2T_c(x_m)}{x_m^2} (x - x_u)(x_0 - x). \quad (1)$$

The doping dependance of $1/\gamma_T$ evaluated at $T_c(\gamma_{T_c})$ and $T = 0$ ($\gamma_{T=0}$) is also shown. As the dopant concentration is reduced, γ_{T_c} and $\gamma_{T=0}$ increase systematically, and tend to diverge

in the underdoped limit. Thus, increasing the anisotropy seem to shrink the range where superconductivity occurs in the underdoped regime. This competition between anisotropy and superconductivity raises serious doubts whether 2D mechanisms and models corresponding to the limit $\gamma T = \infty$ can explain the essential observations of superconductivity in the cuprates. A fitting of the graph shows that $\gamma T(x)$ is well described by

$$\gamma T(x) = \frac{\gamma_{T,0}}{x - x_u}, \quad (2)$$

which gives in terms of T_c :

$$\frac{T_c}{T_c(x_m)} = 1 - \left(\frac{\gamma_T(x_m)}{\gamma_T} - 1 \right)^2. \quad (3)$$

For eqs (1), (2) to be of interest, it is necessary to verify their validity on other materials to ensure that we are not looking at a feature particular to $La_{2-x}Sr_xCuO_4$. In practice however, there is a lack of experimental results due to the difficulty of varying the doping continuously. An alternative way of performing a check is to use the fact that the substitution of magnetic and non-magnetic impurities depress T_c of the cuprates superconductors very effectively. If Eq.(3) is satisfied for a wide range of compounds, the two other equations can be considered valid. The comparison is done on fig. 2.

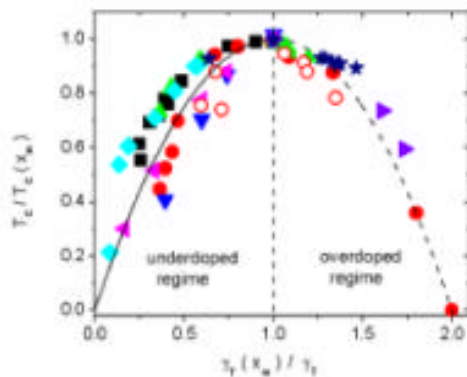


Figure 2: $T/T_c(x_m)$ versus $\gamma_T(x_m)/\gamma_T$ for 8 different cuprates. The solid and dashed curves are marking the flow from the maximum T_c to QSI and QSN criticality, respectively. [1]

There is a fairly good agreement between the experimental results and the parabola representing eq. (3).

Another aspect that have been investigated experimentally is the substitution of some of the Cu content of the compound by magnetic or nonmagnetic metals. Empirical results show that T_c is suppressed in the same manner in both cases. The phase diagram of $La_{2-x}Sr_xCu_{1-y}Zn_yO_4$ is given to illustrate what happens.

Apparently, the substituent axis (y) extends the complexity and richness of the phase diagram considerably. The overall critical temperature is reduced. An additional line of

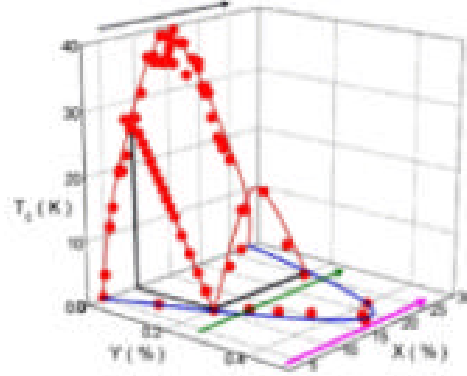


Figure 3: Phase diagram of $La_{2-x}Sr_xCu_{1-y}Zn_yO_4$. The blue solid curve corresponds to $y_c(x)$, a line of quantum phase transitions. The pink arrow marks the dopng tuned insulator to metal crossover and the green arrow marks a path where a QSI and QSN transition occurs. [3]

quantum phase transition is given by $y_c(x)$. At the underdoped limit, substitution has no effect. As x increases, larger values of y are allowed before the transition. y reaches a maximum, start decreasing and eventually vanish at x_o . More experimental results show that isotope substitution(fig.4) does the same thing less effectively. This suggest that substitution, rather than magnetism, is the important factor. For $y > y_c(x)$ superconductivity is suppressed due to the destruction of phase coherence.

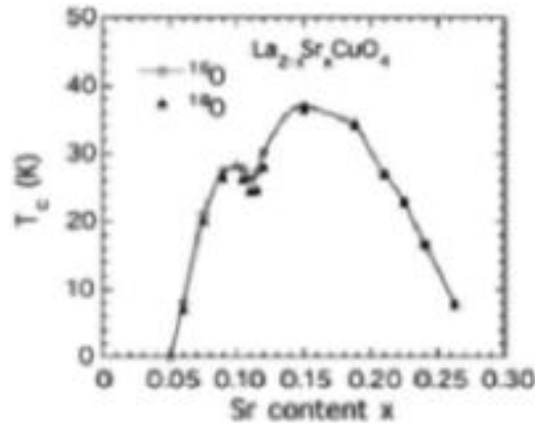


Figure 4: $T_c(^{16}O)$ and $T_c(^{18}O)$ versus x for $La_{2-x}Sr_xCuO_4$. [1]

One last aspect of the study of the phase diagram is adding the magnetic field to the picture. The phase diagram is sketched on fig. 5.

Close to the $t-x$ plane, thermal fluctuations are believed to be responsible for a first order vortex melting transition in a clean cuprates. Adding disorder to the system will destroy the long range of the vortex lattice and the vortex solid becomes a glass. Since a sufficiently

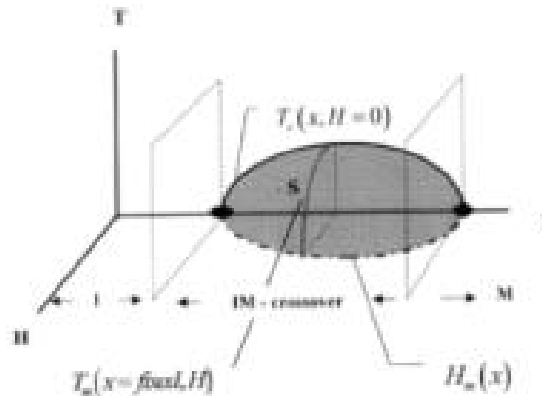


Figure 5: Schematic (x, H, T) -phase diagram. There is the superconducting phase (S) bounded by the zero field transition line, $T_c(x, H = 0)$, the critical lines of the vortex melting or vortex glass to vortex fluid transitions, $T_m(x = fixed, H)$ and the line of quantum critical points, $H_m(x, T = 0)$. Along this line superconductivity is suppressed and the critical endpoints coincide with the 2D-QSI and 3D-QSN critical points at x_u and x_o respectively.[1]

large magnetic field destroys superconductivity, there is a line in the $x - H$ plane ($H_m(x)$) connecting zero field QSI and QSN transitions. Recent experiments have shown that besides destroying superconductivity, strong magnetic fields mediate a metal to insulator crossover.

A number of conclusions come from the above empirical phase diagrams:

1. The superconducting phase seem to occur in a regime that would correspond at higher temperatures to an insulator to metal crossover. At low enough temperature, the transition becomes insulator to superconductor to metal as doping is increased.

2. Substituting magnetic and nonmagnetic impurities seem to have the same effect on the superconducting state.

3. The $H(x)_{T=0}$ graph roughly look like the $T(x)_{H=0}$ graph. Here, the transition goes as vortex lattice in the superconducting state to thermal fluctuation induced vortex melting in the absence of disorder and to vortex glass in the presence of disorder. If the field is above the critical value, an insulator to metal transition is observed once again.

3 Universal properties.

The theoretical method used to predict empirical results is the scaling theory for critical phenomena and the related concept of universality. Hohenberg et al. summarized the concept behind the theory in a very succinct way in the introduction of their 1975 paper[2]:

“The phenomenological theory of scaling has been extremely useful for understanding critical phenomena in model systems and real materials. A related concept, formulated as the hypothesis of universality greatly reduces the variety of different types of critical behavior by dividing all systems into a small number of equivalence classes. Within each class, the

exponent and the equation of state will be the same, provided one fixes the scale of the order parameter and its conjugate field appropriately. Thus, apart from two scale factors which will differ from system to system, the thermodynamic functions of all elements in the same class will be the same, sufficiently close to the critical point. The scaling hypothesis extended to time independent correlations of the order parameter in the earliest formulations, and it was found that the correlation exponents are simply related to the thermodynamic ones. (...) This hypothesis [two-scale factor universality for correlation functions] states that the correlation function for a system is fully determined near the critical point once the two independent thermodynamic scales have been chosen. This means that the length scale is not independent, but is universally related to the thermodynamic scales. ”

In other words, scaling consist in a few steps:

1. Find the dimensions of the dependent and independent variables. The usual choice for a length scale is the correlation length;

2. Find a combination of the independent variable and the correlation length that does not change under scale transformation; That quantity is universal for a certain group of systems and does not depend on the variables of the system.

Before applying this theory on the finite temperature and quantum critical behavior, a number of difficulties specific to the problem have to be taken care of. The universality class to which the cuprates belongs is characterized by its critical exponents and various critical-point amplitude combinations that are functions of the transition temperature, critical amplitude of the specific heat, correlation length and penetration depth.

3.1 Scaling predictions for finite temperature critical behavior

The superconducting state order parameter is a complex scalar that can be represented by a two component vector (XY). Sufficiently close to the phase transition line, 3D-XY fluctuations dominate. The scaling form of the singular part of the bulk energy density has the form[1, 2]:

$$f_s = -k_B T Q_3^\pm (\xi_x^\pm \xi_y^\pm \xi_z^\pm)^{-1}; \quad (4)$$

where ξ_i^\pm is the correlation length in the i direction and $\pm = \text{sign}(t)$, $t = \frac{T-T_c}{T_c}$ and Q_3^\pm are universal constants. In superconductors, the pairs carry a non zero charge in addition to their mass and the gradient term of the Ginzburg-Landau Hamiltonian couples that charge to the electromagnetic field. However, it seems that inhomogeneities in cuprates superconductors prevent these fluctuations from driving the system close to a charged critical point. The vector potential fluctuations can therefore be neglected and the critical properties at finite temperature are those of the 3D-XY-model, similar to the lambda transition in superfluid helium, extended to take the anisotropy into account.

At long wavelength in the superconducting phase, the transverse fluctuations of the order parameter dominates and the correlation does not decay exponentially. The usual definition of ξ cannot be used but a phase coherence length can be defined in terms of the helicity modulus, which is a measure of the response of the system to a phase-twisting field. In the presence of a phase twist, a universal relation can then be derived in terms of the phase

coherence length, also called transverse correlation length:

$$k_B T_c = \frac{\Phi_0^2}{16\pi^3} \frac{\xi_{ab,0}^-}{\lambda_{ab,0}^2 \gamma T_c}; \quad (5)$$

where $\Phi_0 = hc/2e$ and γ is the anisotropy. Even though some terms in this expression depend on the dopant concentration, universality implies that this relation holds at any finite temperature, irrespective of the doping level and the material, except at the critical endpoints of the 3D-XY critical line. In the presence of a magnetic field, the scaling form is defined as a function of a universal scaling function. When the non-universal critical amplitudes of the correlation length and the scaling functions are known, universal properties such as specific heat, magnetic torque, diamagnetic susceptibility, melting line,... can be derived from the singular part of the free energy close to the zero field transition.

Does the theory match with experimental results? One thing to bear in mind when comparing the theory with experiment is that in practice, cuprates are only homogeneous over a finite length L only. The correlation length $\xi(t)$ proportional to $t^{-\nu}$ cannot grow beyond L as $t \rightarrow 0$, and the transition appears rounded. Fig 6. shows experimental results of specific heat in YBCO. C/T is plotted versus $\log_{10}|t|$. The straight lines correspond to the

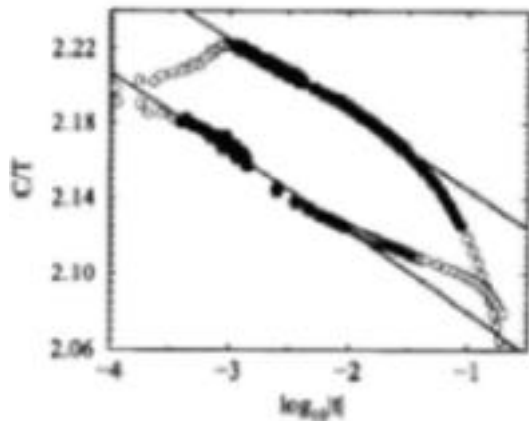


Figure 6: Specific heat coefficient $C/T(mJ/(gK^2))$ versus $\log_{10}|t|$ for $YBa_2Cu_3O_7$ for $T_c=92.12$. [4]

scaling predictions for homogeneous system, the circles are experimental results (data from sample YBCO3 in [4], graph from [1]). The full circles are the points in agreement with the theory and the open circles correspond to finite-size affected region. The upper branch is for $T < T_c$ and the lower one for $T > T_c$. Further from T_c , the temperature dependence of the background becomes significant.

The high anisotropy of most cuprate also contribute in making the 3D-XY behavior difficult to observe. Even though the strength of the thermal fluctuations increase with increasing γ , they become essentially 2D away from T_c .

3.2 Quantum critical phenomena.

At zero temperature, the thermodynamics and the dynamics of the systems are inextricably mixed. In order to apply the scaling theory for quantum phase transitions, the path integral formulation of quantum mechanics is used to change the statistical mechanics of a D -dimensional system at $T = 0$ and with dynamical degrees of freedom into a $D + z$ dimensional classical system with a fake temperature which is some measure of the dynamics with critical exponent z .

In the case of quantum critical phenomena ($T = 0$), two kind of correlation length are needed close to quantum criticality: spatial and temporal correlation length. Scaling theory leads to a universal expression:

$$k_b T_c = \frac{\bar{y}_c}{\xi_{\tau,0}^-} \delta^{z\bar{\nu}}, \quad (6)$$

where y_c is the universal value of the scaling function argument at which the scaling function exhibit a singularity at finite temperature and δ is a parameter introduced to measure the relative distance from quantum critical points.

The zero temperature critical amplitudes are given by

$$\lambda_c(0) = \Omega_s (\sigma_c^{DC}(T_c^+))^{-(2+z)/4}, \quad (7)$$

and

$$\Omega_s = \gamma_{0,0} \lambda_{ab,0}(0) \left(\frac{4e^2 \sigma_0}{h \lambda_{T_c,0}^2} \right)^{(2+z)/4}, \quad (8)$$

where

$$\gamma_T = \gamma_{T,0} \delta^{-\bar{\nu}}, \quad (9)$$

and

$$\lambda_{ab,0}(0) = \lambda_{ab,0}(0) \delta^{-z\bar{\nu}/2}. \quad (10)$$

The universality classes emerging from the empirical relations are characterized by the critical exponents:

$$2D - QSI : z = 1, \bar{\nu} = 1, 3D - QSN : z\bar{\nu} = 1. \quad (11)$$

The 2D-QSI exponent agree with the theory of bosonic disordered system in 2D with long range Coulomb interaction. The loss of superfluidity is due to the localisation of the pairs which causes the transition. A possible explanation for the 3D-QSN transition is the Ginzburg-Landau theory for a disordered d-wave superconductor to metal transition at weak coupling and is characterized by the critical exponents $z = 2$ and $\bar{\nu} = 1/2$, except in an exponentially narrow region.

In order to confirm the occurrence of the 2D-QSI transition, the scaling prediction are compared to resistivity measurements near criticality. Eq. (6) together with the definition:

$$\frac{\sigma_c^{DC}}{\sigma_{ab}^{DC}} = \left(\frac{\xi_c}{\xi_{ab}} \right)^2 = \left(\frac{1}{\gamma_{T_c}} \right), \quad (12)$$

yield $\rho_c/\rho_{ab} = \gamma_{T_c}^2 \propto \delta^{-2\bar{\nu}} \propto T_c^{2/z}$. The corresponding experimental data plotted on Fig. 7. is in agreement with the prediction. Inedeed, the anisotropy increases by approaching the

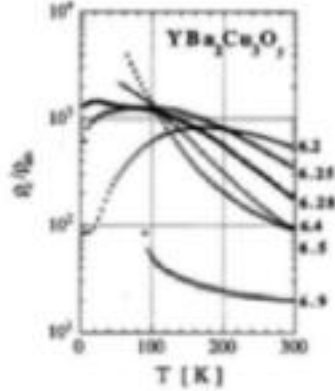


Figure 7: ρ_c/ρ_{ab} versus T of underdoped $YBa_2Cu_3O_y$

2D-QSI transition.

4 Results and discussion

The phase diagram of cuprate superconductor have been established in the temperature-dopant concentration-magnetic field space. There are temperature induced phase transition at finite temperature and quantum phase transitions induced by fluctuations at $T = 0$. In both cases, the material goes from insulator below the underdoped limit to superconductor to normal metal beyond the overdoped limit. As the dopant concentration is decreased, the anisotropy at T_c and at $T = 0$ increases and tend to diverge at the underdoped limit. That seems contradictory with a possibility of 2D superconductivity as suggested by some models. In the presence of a magnetic field larger than the critical value, a doping induced metal-insulator transition is observed. This part of the paper was essentially a compilation of experimental results used to draw an empirical phase diagram.

In the second part of the review, the authors derived a scaling theory and universal properties for finite temperature and quantum critical phenomena. The results were compared to experiments.

Even if the experimental results seem to be consistent with the scaling predictions, it usually take a lot more data for a critical exponent or a universal property to be recognized.

This theory in compatible with microscopic models relying on competing order parameters. Here, it is assumed that in the doping regime where superconductivity occurs, competing fluctuations, including antiferromagnetic and charge fluctuations can be integrated out.

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