Implications of 3D xy Critical Point Universality for the Properties of High-T_c Cuprates

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It is shown that the available experimental data on the intriguing doping dependence of specific heat singularity and of the magnetic penetration depth, as well as the relation between transition temperature and magnetic penetration depth can be understood in terms of three-dimensional xy critical point universality supplemented by the empirical phase transition line.

Considerable debate has arisen over the doping dependence of the transition temperature T_c [1,2], magnetic penetration depth λ [3–8] and specific heat singularity [9] of cuprate superconductors as well as the resulting correlation between these properties. As thermal fluctuations are essential in these extreme type II materials and because these fluctuations are known to mediate universal behavior [10,11], we sketch in this Letter the implications of three-dimensional (3D)-xy critical point universality, supplemented by the experimental phase transition line, and its effect on the intriguing doping dependence of the magnetic penetration depth λ and of specific heat singularity, as well as the relationship between these properties.

The paper is organized as follows. First, we outline the experimental evidence that cuprate superconductors and uncharged superfluids like ^{4}He share universal 3D-xy properties in the fluctuation dominated regime. Then we explain how the universal relations between critical amplitudes and T_c, supplemented by the empirical phase diagram (doping dependence of T_c) imply unconventional behavior of the penetration depth in the overdoped regime in agreement with recent kinetic induction measurements of high-quality $La_{2-x}Sr_xCuO_4$ films [12] and μSR data [3,7,8]. The remainder of the paper addresses the implications of these findings.

Measurements of various properties, including specific heat [9,13–15] and magnetic penetration depth [13,16], strongly suggest that in the Meissner phase and close to the transition temperature the fluctuations of the order parameter are essentially those of a neutral superfluid or 3D-xy model. The associated complex scalar order parameter field $\Psi(\vec{r}) = |\Psi(\vec{r})| \exp(i\varphi(\vec{r}))$ represents in a superconductor the macroscopic wave function of singlet pairs of charge $2e$ where $|\Psi(\vec{r})|$ is the local pair density and $\varphi(\vec{r})$ denotes the phase. Introducing the magnetic penetration depth λ and the correlation length ξ, which describes the decay of the fluctuations in the modulus $|\Psi(\vec{r})|$ of the order parameter, the uncharged behavior of the cuprates can be understood in terms of the dimensionless charge, $\tilde{e} = 1/\kappa = \xi/\lambda$ [15,17]. In cuprate superconductors, this charge is small, because $\lambda \gg \xi$ [15]. Close to the 3D-xy critical point the specific heat diverges as $C^{\pm} = (A^{\pm}/\alpha)\ |t|^{-\alpha} + B^{\pm}$, where $t = 1 - T/T_c$, $A^+ \approx A^-$ and $\alpha \approx 0$ [11]. The parameter $B^{\pm}$ accounts for the background. Consistency with this 3D-xy critical behavior has been established for $DyBa_2Cu_3O_{7-x}$ [14], $YBa_2Cu_3O_7$, $Tl_2Ca_2Ba_2Cu_3O_{10}$ and $Bi_{1.8}Pb_{0.2}Sr_2CaCu_2O_{10-\delta}$ [15]. The resulting estimates for $A^+ \approx A^-$ can now be used to determine the correlation volumes of phase $\left((\xi^{\varphi}_{\|0})^2\xi^{\varphi}_{\perp 0}\right)$ and amplitude $\left((\xi_{\|0})^2\xi_{\perp 0}\right)$ fluctuations via the universal relations [11] extended to systems with uniaxial effective mass anisotropy [14]

$$R^3_{\varphi} = A^-(\xi^{\varphi}_{\|0})^2\xi^{\varphi}_{\perp 0} \quad , \qquad R^3 = A^+(\xi_{\|0})^2\xi_{\perp 0} \qquad (1)$$

with $R_{\varphi} \approx 0.8$ and $R \approx 0.3$ [11]. The index $\|$ denotes a direction parallel and $\perp$ perpendicular to the layers; the correlation lengths diverge as $\xi = \xi_0 \mathrm{t}^{-v}$ with $\nu \approx 2/3$. The length scales and effective pair mass anisotropy are related by [14]

$$\frac{\xi^{\varphi}_{\|0}}{\xi^{\varphi}_{\perp 0}} = \left(\frac{\lambda_{\|0}}{\lambda_{\perp 0}}\right)^2 = \frac{M_{\|}}{M_{\perp}} \quad , \qquad \frac{\xi_{\|0}}{\xi_{\perp 0}} = \sqrt{\frac{M_{\perp}}{M_{\|}}} \quad . \qquad (2)$$

Since pronounced fluctuation effects are tied to small correlation volumes, the estimates for $(\xi^{\varphi}_{\|0})^2\xi^{\varphi}_{\perp 0}$, 579 Å^3 in $DyBa_2Cu_3O_7$, 916 Å^3 in $YBa_2Cu_3O_7$ and those for $(\xi_{\|0})^2\xi_{\perp 0}$, 30 Å^3 in $DyBa_2Cu_3O_7$ and 48 Å^3 in $YBa_2Cu_3O_7$) [3,13] clearly reveal the importance of fluctuations, because these volumes are comparable to those in superfluid helium, $(\xi^{\varphi}_{\|0})^2\xi^{\varphi}_{\perp 0} \approx 307$ Å^3, $(\xi_{\|0})^2\xi_{\perp 0} \approx 16.7$ Å^3 [3,11] and of the order of the unit cell volume. Thus, analogous to ^{4}He, fluctuation effects that expose the universal 3D-xy critical point behavior are essential, experimentally accessible and invalidate mean-field treatments.

Another quantity of interest is the magnetic penetration depth. Indeed, the Meissner effect occurs if an external magnetic field is expelled, except for a penetration depth λ. In extreme type II superconductors with short correlation length amplitudes, λ is simply related to the helicity modulus Y [18] in terms of $Y_{\|,\perp} = (\hbar^2/M_{\|,\perp})n_s = (\Phi_0^2/16\pi^3)\lambda^{-2}_{\|,\perp} = (\Phi_0^2/16\pi^3)\lambda^{-2}_{\|,0\perp}t^{-\nu}$. Here, Φ_0 is the flux quantum and n_s denotes the number density of the superfluid pairs which tends to zero as $n_s \propto t^{\nu}$ with $\nu \approx 2/3$ [10,11] by approaching the 3D-xy critical point from below. This behavior is nicely confirmed by recent penetration depth measurements on $YBa_2Cu_3O_7$ [16], which yield $\nu \approx 2/3$ and $\lambda_{\|}(T=0)/\lambda_{\|0} \approx 1.22$. In this context it is important to recognize that at the 3D-xy critical point, transition temperature, phase correlation length, specific heat and superfluid number density or, equivalently, London penetration depth, are not independent of one another. Indeed, there is also the universal relation [11,13,15]:

$$k_B T_c = \frac{\Phi_0^2}{16\pi^3}\frac{\xi^{\varphi}_{\|,\perp 0}}{\lambda^2_{\|,\perp 0}} = \frac{\Phi_0^2}{16\pi^3}\left(\frac{M_{\|}}{A^- M_{\perp}}\right)^{1/3}\frac{1}{\lambda^2_{\|0}} \quad , \qquad (3)$$

which connects T_c with the amplitudes of penetration depth $\lambda_{\|0}$ and phase correlation length $\xi^{\varphi}_{\|,\perp 0}$, or specific heat A^-. To obtain the latter expression we used Eqs. (1) and (2). Because A^-, $M_{\perp}/M_{\|}$ and $\lambda_{\|0}$ can be measured independently, relation (3) provides a consistency check for critical amplitude estimates. As an example, we evaluate $\xi^{\varphi}_{\|0}$ with the aid of Eq. (3) and compare it with the value derived from the specific heat anomaly (Eq. (1)). The penetration depth measurements yield $\lambda_{\|0} \approx 0.82\lambda_{\|}(T=0)$. Using $T_c \approx 92.4$ K [16], $\lambda_{\|}(T=0) = 1817$ Å [19] and relation (3) we find

$\xi^{\varphi}_{\|0} \approx 3.24$ Å, which is close to 3.3 Å, the estimate derived from the specific heat data ($(\xi^{\varphi}_{\|0})^2\xi^{\varphi}_{\perp 0} \approx 579$ Å^3 with $M_\perp/M_\| \approx 25$ [13]). Thus, the evidence of 3D-xy critical point behavior is not restricted to the asymptotic temperature dependence, but includes the universal relations for the critical amplitudes. Furthermore, there is consistency with the universal scaling properties of specific heat and magnetization as a function of magnetic field and temperature [20,21]. As of yet, however, no study of the implications of critical point universality along the phase transition line has been made.

Here we reveal these implications in terms of the universal relations (1) and (3) and the experimentally given doping dependence of T_c. For this purpose it is sufficient to describe the phase transition line by the simple interpolation formula [1,2]

$$\bar{T}_c = \frac{T_c}{T_c^m} = 1 - \beta(x - x_c)^2 = 4\rho(1-\rho) \quad , \tag{4}$$

with $x_c \approx 0.16$, $\beta \approx 82.6$ and $2\rho = 1 \pm \sqrt{\beta}(x - x_c)$ and where x is the number of holes per CuO_2 unit in the CuO_2 layer, estimated from bond-valence sums. The parameter ρ denotes the corresponding fraction of mobile holes introduced by doping, while T_c^m is the transition temperature at optimum doping ($x = x_c$, $\rho = 1/2$). There is considerable evidence that this relation provides an approximate description of the phase transition line of all hole doped superconducting cuprates. Considering homogeneous phases only, we can appeal to 3D-xy critical point universality along this phase transition line. In the underdoped ($\rho \to 0$) and overdoped limit ($\rho \to 1$), T_c tends to zero and the system approaches the 3D quantum xy critical point or, equivalently, the 3+1=4D classical xy critical point [22] where the mean field treatment becomes exact up to logarithmic corrections, and $A^\pm$ vanishes. Thus, $A^\pm$ is expected to decrease as T_c tends to zero in the underdoped ($\rho \to 0$) and overdoped ($\rho \to 1$) limits. Experimental evidence of this behavior comes from the specific heat measurements on underdoped $YBa_2Cu_3O_{7-x}$ [9] and overdoped $Tl_2Ba_2CuO_{6+\delta}$ [23]. Guided by the experimental data for $YBa_2Cu_3O_{7-x}$, covering $0.27 \leq \rho \leq 0.5$, we describe the reduction of $A^\pm$ with the ansatz

$$\bar{A}^- = \frac{A^-}{A_m^-} \approx (\bar{T}_c)^6 \quad , \tag{5}$$

which interpolates between the limits $\rho \to 0$ and 1 and describes the empirical data well. Combining Eqs. (3) and (4) with this ansatz we find

$$\bar{T}_c \approx \left(\frac{\bar{M}_\|}{\bar{M}_\perp}\right)^{1/9} \left(\bar{\lambda}^2_{\|0}\right)^{-1/3} \approx 4\rho(1-\rho) \quad , \tag{6}$$

where $\bar{M}_{\|,\perp} = M_{\|,\perp}/M^m_{\|,\perp}$ and $\bar{\lambda}_{\|,\perp} = \lambda_{\|,\perp}/\lambda^m_{\|,\perp}$. The index m refers to the respective values for optimum doping ($x = x_c$, $\rho = 1/2$). In this context it is important to emphasize that 3D-xy critical point behavior along the phase transition line also implies that $\bar{M}_\perp/\bar{M}_\|$ remains finite in the full doping range ($0 \leq \rho \leq 1$), because in the limit $\bar{M}_\perp/\bar{M}_\| \to \infty$ the system is strictly two-dimensional. For this reason Eq. (6), rewritten in the form

$$\bar{\lambda}^2_{\|0} \approx \left(\frac{\bar{M}_\|}{\bar{M}_\perp}\right)^{1/3} (4\rho(1-\rho))^{-3} \quad , \tag{7}$$

also exposes the dominant doping dependence of the penetration depth in terms of $\rho(1-\rho)$. Thus, 3D-xy universality, supplemented by the experimental phase transition line (Eq. (4)), also implies intriguing behavior concerning both the doping dependence of $\lambda_\|$ and relationship between T_c and $1/\lambda^2_{\|0}$. In contrast to the standard picture λ^2 is no longer inversely proportional to ρ, the fraction of mobile holes. Indeed, according to Eq. (7), $\bar{\lambda}^2_{\|0}$ reaches a minimum at optimum doping and increases again in the overdoped regime ($\rho > 1/2$). This behavior is well confirmed by recent kinetic induction measurements on high-quality $La_{2-x}Sr_xCuO_4$ films [12]. The data covering both the underdoped and overdoped regimes is depicted in Fig. 1 in terms of $\lambda_{\|0}$ versus ρ. The solid curve is a fit to Eq. (7) with $(\bar{M}_\|/\bar{M}_\perp)^{1/3} \approx 1$, because $\bar{M}_\perp/\bar{M}_\| \leq 3$ [24]. According to Eq. (6), the doping dependence of λ and T_c also leads to a definite relation between T_c and $1/\lambda^2_{\|0}$ depicted in Fig. 2 by the solid line for $\bar{M}_\|/\bar{M}_\perp \approx 1$. The arrows denote the evolution of a system as ρ increases from the underdoped ($\uparrow, 0 \leq \rho \leq 1/2$) to the overdoped ($\downarrow, 1/2 \leq \rho \leq 1$) regimes. Apparently, this behavior is consistent with the available μSR data plotted in terms of T_c versus $\bar{\sigma}_\|(T=0) \propto 1/\bar{\lambda}^2_\|(T=0)$. Here $1/\bar{\lambda}^2_\|(T=0)$ is taken as a measure for $1/\bar{\lambda}^2_{\|0}$. The parameter σ is the μSR relaxation rate which is proportional to the square of the inverse penetration depth. Deviations from this behavior are not unexpected in the low-T_c regime, because the interpolation formula (5) is only qualitatively correct in the limits $\rho \to 0, 1$, and because the effective mass ratio $\bar{M}_\|/\bar{M}_\perp$ might depend on doping. Better agreement requires $\bar{M}_\perp/\bar{M}_\|$ to increase with decreasing T_c, as observed in underdoped $YBa_2Cu_3O_{7-\delta}$ [25]. More importantly, the experimental points of overdoped $Tl_2Ba_2CuO_{6+\delta}$ [7,8] and $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$ [26] confirm the essential implication of Eq. (6), namely, reversed evolution of underdoped ($\uparrow$) and overdoped ($\downarrow$) systems. The dashed lines in Fig. 2, which resemble the outline of a fly's wing, are a guide to the eye and illustrate the effect of a doping-dependent anisotropy, $\bar{M}_\|/\bar{M}_\perp$. The upper part of the outline describes underdoped and the lower one overdoped systems. Indeed, the experimental points of overdoped $Tl_2Ba_2CuO_{6+\delta}$ and $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$ are close to the outline of the lower part of the wing, while the remaining data, referring to underdoped and mildly overdoped materials, is close to the upper branch.

Finally, we turn to the doping dependence of the helicity modulus $Y \propto 1/\lambda^2$ at zero temperature. The mapping on the (3+1)-D xy model validates a mean-field treatment around the critical points $\rho = 0$ and 1. Expansion of the mean-field order parameter around the critical points, supplemented by the effective mass enhancement in the intermediate regime, yields $Y_{\|}(T=0,\rho) \propto 1/\lambda_{\|}^2(0,\rho) \propto \left(\hbar^2/M_{\|}(\rho)\right)\rho \propto \rho(1-\rho)$, which interpolates in qualitative agreement with Eq. (7) between the mean-field behavior around the critical points. The enhancement of the effective pair mass, $M_{\|}(\rho) = M_{\|}(0)/(1-\rho)$, is a quantum effect arising from the repulsive pair interaction [27]. It then follows that the decrease of T_c and the associated intriguing behavior of specific heat singularity A^- and λ in the overdoped regime must be attributed to an enhanced effective pair mass.

In summary, we have shown that the available experimental data on the doping dependence of specific heat singularity and magnetic penetration depth as well as the relation between T_c and $1/\lambda_{\|}^2$ are fully consistent with 3D-xy critical point universality in pure materials, supplemented by the experimental phase transition line, and not merely an artifact of bad sample quality as proffered by Harshman and Fiory [5]. The fluctuation-mediated 3D-xy universality along the phase transition line not only provides relations between various properties in the Meissner state, which can also be used to test microscopic models, but also reveals essential information concerning the nature of the superconducting state.

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FIG. 1. Kinetic inductance estimates for $\lambda_{\parallel 0}$ in $La_{2-x}Sr_xCuO_4$ films plotted in terms of $\lambda_{\parallel 0}$ versus ρ taken from Ref. 12. The solid curve corresponds to Eq. (7) with $\bar{M}_{\parallel}/\bar{M}_{\perp} \approx 1$.

FIG. 2. $\bar{T}_c$ versus $\bar{\sigma}(T=0) = \left(\lambda_{\parallel}^{m}(T=0)\right)^2/\lambda_{\parallel}^{2}(T=0)$ taken from Refs. 3, 7, 8 and 26. The solid curve corresponds to Eq. (6) with $\bar{M}_{\parallel}/\bar{M}_{\perp} \approx 1$ and the arrows denote the underdoped $(\uparrow, 0 \leq \rho \leq 1/2)$ and overdoped $(\downarrow, 1/2 \leq \rho \leq 1)$ regimes. The dashed lines are a guide to the eye and sketch the effect of the doping dependence of the effective mass ratio $\bar{M}_{\parallel}/\bar{M}_{\perp}$.
$\square$: $Tl_2Ba_2Ca_2Cu_3O_{10}$, $Tl_{0.5}Pb_{0.5}Sr_2Ca_2Cu_3O_9$, $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{16}$,
$\diamond$: $Y_{1-x}Pr_xBa_2Cu_3O_{6.97}$, $\triangle$: $YBa_2Cu_3O_x$, $\bigtriangledown$: $La_{2-x}Sr_xCuO_4$,
$\star$: $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$, $\bigcirc$: $Tl_2Ba_2CuO_{6+\delta}$, : $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$