Why there is a difference between optimal doping for maximal $T_c$ and critical doping for highest $\rho_s$ in cuprate superconductors?

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A long-standing puzzle is why there is a difference between the optimal doping $\delta_{\text{optimal}} \approx 0.15$ for the maximal superconducting (SC) transition temperature $T_c$ and the critical doping $\delta_{\text{critical}} \approx 0.19$ for the highest superfluid density $\rho_s$ in cuprate superconductors? This puzzle is calling for an explanation. Within the kinetic energy driven SC mechanism, it is shown that except the quasiparticle coherence, $\rho_s$ is dominated by the bare pair gap, while $T_c$ is set by the effective pair gap. By calculation of the ratio of the effective and the bare pair gaps, it is shown that the coupling strength decreases with increasing doping. This doping dependence of the coupling strength induces a shift from the critical doping for the maximal value of the bare pair gap parameter to the optimal doping for the maximal value of the effective pair gap parameter, which leads to a difference between the optimal doping for the maximal $T_c$ and the critical doping for the highest $\rho_s$.

In this paper, we try to answer this question. Experimentally, the measured energy gap $\Delta(k)$ is an effective energy gap $\Delta_{\text{eff}}$, which incorporates both the coupling strength and the bare energy gap $\Delta(k)$. Theoretically, the kinetic energy driven SC mechanism has been developed$^{12}$, where $T_c$ is controlled by both the effective charge carrier pair gap and the quasiparticle coherence. Within this kinetic energy driven SC mechanism, we calculate the doping dependence of the coupling strength $V_{\text{eff}}$, and the result shows that $V_{\text{eff}}$ smoothly decreases upon increasing doping from a strong-coupling case in the underdoped regime to a weak-coupling side in the overdoped regime. Our results also show that the maximal value of the bare charge carrier pair gap parameter appears around the critical doping $\delta_{\text{critical}} \approx 0.19$, then as a natural consequence, the highest $\rho_s$ occurs around this same critical doping. However, the special doping dependence of $V_{\text{eff}}$ shifts this critical doping for the maximal value of the bare charge carrier pair gap parameter to the optimal doping $\delta_{\text{optimal}} \approx 0.15$ for the maximal value of the effective charge carrier pair gap parameter, which leads to that $T_c$ exhibits a maximum around the optimal doping.

Cuprate superconductors have a layered structure consisting of the two-dimensional CuO$_2$ planes separated by insulating layers$^2$. The single common feature is the presence of the CuO$_2$ plane, and it seems evident that the unusual behaviors of cuprate superconductors are dominated by this CuO$_2$ plane$^2$. In this case, it has been argued that the essential physics of the doped CuO$_2$ plane is properly accounted by the $t$-$J$ model on a square lattice$^{13}$. However, for discussions of the difference between the optimal doping for the maximal $T_c$ and the critical doping for the highest $\rho_s$, the $t$-$J$ model can be...

The parent compounds of cuprate superconductors are Mott insulators with an antiferromagnetic long-range order (AFLRO)$^2$. However, this AFLRO is suppressed by doped charge carriers, then superconductivity arises from the binding of charge carriers into Cooper pairs$^3$, thereby forming a superfluid with a superconducting (SC) energy gap $\Delta(k)$ in the single-particle excitation spectrum. This energy gap is corresponding to the energy for breaking a Cooper pair of the charge carriers and creating two excited states$^4$, while the superfluid density $\rho_s$ is proportional to the squared amplitude of the macroscopic wave function$^5$, and therefore describes the SC charge carriers. In this case, both $\Delta(k)$ and $\rho_s$ are thus two fundamental parameters whose variation as a function of doping and temperature provides important information crucial to understanding the details of the SC state$^2$. After intensive investigations over more than two decades, some essential features of the evolution of the SC state in cuprate superconductors with doping have been experimentally established$^{5-11}$: where the measured energy gap parameter $\bar{\Delta}$ and the SC transition temperature $T_c$ show a domelike shape doping dependence, i.e., the maximal $\bar{\Delta}$ and $T_c$ occur around the optimal doping $\delta_{\text{optimal}} \approx 0.15$, and then decrease in both the underdoped and the overdoped regimes$^5$. Moreover, the experimental measurements$^6$ throughout the SC dome show that the superfluid density $\rho_s$ appears from the starting point of the SC dome, and then increases with increasing doping in the lower doped regime. However, this $\rho_s$ reaches its highest value around the critical doping $\delta_{\text{critical}} \approx 0.19$, and then decreases at the higher doped regime, eventually disappearing together with $\bar{\Delta}$ at the end of the SC dome. In particular, it has been shown$^5$ that the maximal $T_c$ around the optimal doping and the peak of $\rho_s$ around the critical doping is a common feature of cuprate superconductors. Since $\bar{\Delta}$ measures the strength of the binding of charge carriers into Cooper pairs$^5$, while $\rho_s$ is a measure of the phase stiffness$^5$, therefore $\bar{\Delta}$ and $\rho_s$ separately describe the different aspects of the same SC charge carriers. In this case, a long-standing...
extended by including the exponential Peierls factors as,
\[ H = -t \sum_{\langle \ell \ell' \rangle} P_{\ell \eta} C_{\ell \sigma}^{\dagger} C_{\ell' \sigma} + t' \sum_{\langle \ell \ell' \rangle} P_{\ell' \eta'} C_{\ell \sigma}^{\dagger} C_{\ell' \sigma} + \mu \sum_{\ell} C_{\ell \sigma}^{\dagger} C_{\ell \sigma} + J \sum_{\ell} S_{\ell} \cdot S_{\ell + \eta}, \]  
(1)

supplemented by an important on-site local constraint \( \sum_{\sigma} C_{\ell \sigma}^{\dagger} C_{\ell \sigma} \leq 1 \) to remove the double occupancy, where the summation is over all sites \( \ell \), and for each \( \ell \), over its nearest-neighbors (NNN) \( \eta \) or the next nearest-neighbors (NNN) \( \eta' \), \( C_{\ell \sigma}^{\dagger} \) and \( C_{\ell \sigma} \) are electron operators that respectively create and annihilate electrons with spin \( \sigma \), \( S_{\ell} = (S_{\ell}^{x}, S_{\ell}^{y}, S_{\ell}^{z}) \) are spin operators, and \( \mu \) is the chemical potential. The exponential Peierls factors \( P_{\ell \eta} = e^{-i/(\varepsilon_{\ell}(h)A(t)\eta)} \) and \( P_{\ell' \eta'} = e^{-i/(\varepsilon_{\ell'}(h)A(t)\eta')} \) account for the coupling of electrons to an external magnetic field in terms of the vector potential \( A(t) \). To incorporate the electron single occupancy local constraint in the \( t-J \) model [1], the charge-spin separation (CSS) fermion-spin theory [2,16] has been proposed, where a spin-up annihilation (spin-down annihilation) operator for the physical electron is given by a composite operator as \( C_{\ell \sigma} = h_{\ell \sigma}^{\dagger} S_{\ell}^{z} \) (\( C_{\ell \sigma} = h_{\ell \sigma}^{\dagger} S_{\ell}^{+} \)), with the spinful fermion operator \( h_{\ell \sigma} = e^{-i/\varepsilon_{\ell}(h)} h_{\ell} \) that describes the charge degree of freedom of the electron together with some effects of spin configuration rearrangements due to the presence of the doped hole itself (charge carrier), while the spin operator \( S_{\ell} \) represents the spin degree of freedom of the electron, then the electron single occupancy local constraint is satisfied in analytical calculations. In this CSS fermion-spin representation, the \( t-J \) model [1] can be rewritten as,
\[ H = t \sum_{\ell \eta} P_{\ell \eta} (h_{\ell + \eta}^{\dagger} h_{\ell \eta} h_{\ell + \eta \eta}^{\dagger} S_{\ell + \eta \eta}^{z} + h_{\ell + \eta \eta}^{\dagger} h_{\ell \eta} h_{\ell + \eta \eta}^{\dagger} S_{\ell + \eta \eta}^{z}) - t' \sum_{\ell \eta'} P_{\ell \eta'} (h_{\ell + \eta}^{\dagger} h_{\ell \eta'} h_{\ell + \eta \eta'}^{\dagger} S_{\ell + \eta \eta'}^{z} + h_{\ell + \eta \eta'}^{\dagger} h_{\ell \eta'} h_{\ell + \eta \eta'}^{\dagger} S_{\ell + \eta \eta'}^{z}) - \mu \sum_{\ell} h_{\ell \sigma}^{\dagger} h_{\ell \sigma} + J_{\text{eff}} \sum_{\ell} S_{\ell} \cdot S_{\ell + \eta}, \]  
(2)

where \( J_{\text{eff}} = (1 - \delta)^{2} J \), and \( \delta = \langle h_{\ell \sigma}^{\dagger} h_{\ell \sigma} \rangle / \langle h_{\ell \sigma}^{\dagger} h_{\ell \sigma} \rangle \) is the doping concentration. 

Since the experimental measurements [2] have shown that in the real space the gap function and the pairing force have a range of one lattice spacing, the bare energy gap parameter can be expressed as \( \Delta = \langle C_{\ell \sigma}^{\dagger} C_{\ell \sigma} \rangle = \langle h_{\ell \sigma}^{\dagger} h_{\ell \sigma} \rangle \). In the doped regime without AFLRO, the spin correlation functions \( \langle S_{\ell}^{z} S_{\ell + \eta}^{z} \rangle = \chi_{1} \), and then the bare energy gap parameter can be rewritten as \( \Delta = -\chi_{1} \Delta_{h} \), with the bare charge carrier pair gap parameter \( \Delta_{h} = \langle h_{\ell + \eta \eta}^{\dagger} h_{\ell + \eta \eta} - h_{\ell + \eta \eta}^{\dagger} h_{\ell \eta} \rangle \), which shows that the bare energy gap is closely related to the bare charge carrier pair gap, therefore the essential physics in the SC state is dominated by the corresponding one in the charge carrier pairing state. For a microscopic description of the SC state in cuprate superconductors, the kinetic energy driven SC mechanism has been developed [12] based on the \( t-J \) model [1], where the charge carrier interaction directly from the kinetic energy by exchanging spin excitations induces a d-wave charge carrier pairing state, and then their condensation reveals the SC ground-state. Moreover, this SC state is controlled by both the effective energy gap and the quasiparticle coherence. Within this kinetic energy driven SC mechanism, the full charge carrier Green’s function in the zero magnetic field case has been obtained explicitly in the Nambu representation as [15,16],
\[ G(k, \omega_{n}) = \frac{\omega_{n} \tau_{0} + \xi_{k} \tau_{3} - \Delta_{h}(k) \tau_{1}}{(\omega_{n}^{2} - E_{hk}^{2})^{2}}, \]  
(3)

where \( \tau_{0} \) is the unit matrix, \( \tau_{1} \) and \( \tau_{3} \) are Pauli matrices, the renormalized charge carrier excitation spectrum \( \xi_{k} = Z_{hf}(\xi_{k}) \), with the mean-field charge carrier excitation spectrum \( \xi_{k} = Z_{hf}(\xi_{k}) \), where the charge carrier interaction directly from the kinetic energy by exchanging spin excitations induces a d-wave charge carrier pairing state, and then their condensation reveals the SC ground-state. Moreover, this SC state is controlled by both the effective energy gap and the quasiparticle coherence. Within this kinetic energy driven SC mechanism, the full charge carrier Green’s function in the zero magnetic field case has been obtained explicitly in the Nambu representation as [15,16],
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where \( \tau_{0} \) is the unit matrix, \( \tau_{1} \) and \( \tau_{3} \) are Pauli matrices, the renormalized charge carrier excitation spectrum \( \xi_{k} = Z_{hf}(\xi_{k}) \), with the mean-field charge carrier excitation spectrum \( \xi_{k} = Z_{hf}(\xi_{k}) \), while the quasiparticle coherent weight \( Z_{hf} \) is directly associated with the self-energy \( \Sigma_{\text{hs}}^{(k, \omega)}(k, \omega) \) in the particle-hole channel as \( Z_{hf}^{-1} = 1 - \text{Re} \Sigma_{\text{hs}}^{(k, \omega)}(k, \omega) \), with the antisymmetric part of \( \Sigma_{\text{hs}}^{(k, \omega)}(k, \omega) \), where the self-energies \( \Sigma_{\text{hs}}^{(k, \omega)}(k, \omega) \) and \( \Sigma_{\text{hs}}^{(k, \omega)}(k, \omega) \) have been given in Refs. [16,18]. In this case, the effective charge carrier pair gap parameter \( \Delta_{h} \), \( Z_{hf} \), and all the other order parameters have been determined by the self-consistent calculation [16,18]. For a convenience in the following discussions, the self-consistently calculated result [18] of \( \Delta_{h} \) versus doping for temperature \( T = 0.002J \) with parameters \( t/J = 2.5 \) and \( t'/t = 0.3 \) is replotted in Fig. [1], where the maximal \( \Delta_{h} \) occurs around the optimal doping \( \delta_{\text{optimal}} \approx 0.15 \), and then decreases in both the underdoped and the overdoped regimes. 

With the help of the Green’s function [13], the bare charge carrier pair gap parameter \( \Delta_{h} \) can be evaluated explicitly as,
\[ \Delta_{h} = \frac{1}{2N} \sum_{k} \text{Im} \langle \text{cos} k_{x} - \text{cos} k_{y} \rangle^{2} Z_{hf} \frac{\Delta_{h} \tau_{3}}{E_{hk}} \tan \frac{1}{2} \beta E_{hk}, \]  
(4)

Since the pairing force and this \( \Delta_{h} \) have been incorporated into the effective charge carrier pair gap parameter \( \Delta_{h} \), the strength \( V_{\text{eff}} \) of the attractive interaction mediated by spin excitations in the kinetic energy driven SC mechanism can therefore be obtained in terms of the ratio of \( \Delta_{h} \) and \( \Delta_{h} \) as,
\[ V_{\text{eff}} = \frac{\Delta_{h}}{\Delta_{h}}, \]  
(5)
is shown that $T_c$ increases with increasing doping in the underdoped regime, and exhibits a maximum around the optimal doping, then decreases with increasing doping in the overdoped regime, in good agreement with the experimental results of cuprate superconductors. In particular, $T_c$ that is set by the effective pair gap and the quasiparticle coherence has been observed experimentally in cuprate superconductors. We believe that this property may be a common feature for all superconductors, since in spite of the electron-phonon SC mechanism, $T_c$ in the conventional superconductors is also determined by the effective pair gap and the quasiparticle coherence.

Although both $\Delta_h$ and $\Delta_b$ measure the strength of the binding of charge carriers into charge carrier pairs, $\Delta_h$ is an experimentally measurable quantity, while $\Delta_b$ is not. In this case, we have calculated the doping dependence of $V_{\text{eff}}$ and $\Delta_h$, and the results of (a) $V_{\text{eff}}$ and (b) $\Delta_h$ as a function of doping for $T = 0.002J$ with parameters $t/J = 2.5$ and $t'/t = 0.3$. The essential physics of the domelike shape doping dependence of $T_c$ in cuprate superconductors can be attributed to a competition between the kinetic energy ($\delta t$) and magnetic energy ($J$). The parent compounds of cuprate superconductors are the Mott insulators, when charge carriers are doped into a Mott insulator, there is a gain in the kinetic energy per charge carrier proportional to $t$ due to hopping, however, at the same time, the magnetic energy is decreased, costing an energy of approximately $J$ per site. As a consequence, the strength of the spin excitation spectrum decreases with increasing doping, which leads to a decrease of the coupling strength $V_{\text{eff}}$ with increasing doping in the framework of the kinetic energy driven SC mechanism. Moreover, in the underdoped regime, the coupling strength $V_{\text{eff}}$ in Fig. 2(a) is very strong, this implies that the most doped charge carriers can be bound into the charge carrier pairs, then the number of the charge carrier pairs and $T_c$ increase with increasing doping. However, in the overdoped regime, the coupling strength $V_{\text{eff}}$ is relatively weak. In this case, not all doped charge carriers can be bound to form the charge carrier pairs by this weakly attractive interaction, and therefore the number of the charge carrier pairs and $T_c$ decrease with increasing doping. In particular, the optimal doping is a balance point, where the number of the charge carrier pairs and the coupling strength $V_{\text{eff}}$ are optimally matched. This is why the $T_c$ in cuprate superconductors exhibits a domelike shape doping dependence.
Now we turn to discuss the doping dependence of the superfluid density. The external magnetic field $\mathbf{B} = \text{rot} \mathbf{A}$ applied to the system usually represents a large perturbation, but the induced field generated by supercurrents cancels the external field over most of the volume of the sample. As a consequence, the net field acts only very near the surface on a scale of the magnetic field penetration depth, and then it can be treated as a weak perturbation on the system as a whole. In this case, the Meissner effect can be successfully studied within the linear response approach, where the response current density $J_\mu$ and the vector potential $A_\nu$ are related by a nonlocal kernel of the response function $K_{\mu\nu}$ as,

$$J_\mu(q, \omega) = - \sum_{\nu=1,2,3} K_{\mu\nu}(q, \omega) A_\nu(q, \omega). \quad (6)$$

This kernel of the response function in Eq. (6) can be separated into two parts as $K_{\mu\nu}(q, \omega) = K^{(d)}_{\mu\nu}(q, \omega) + K^{(p)}_{\mu\nu}(q, \omega)$, where $K^{(d)}_{\mu\nu}$ and $K^{(p)}_{\mu\nu}$ are the corresponding diamagnetic and paramagnetic parts, respectively, and are closely related to the current-current correlation function. The vector potential $\mathbf{A}$ has been coupled to electrons, which are now represented by $C_{\uparrow} = h^\dagger_\uparrow S^-_\uparrow$ and $C_{\downarrow} = h^\dagger_\downarrow S^+_\downarrow$ in the CSS fermion-spin representation. In this case, the electron polarization operator is expressed as $\mathbf{P} = -e \sum_i \mathbf{R}_i C^\dagger_i \mathbf{C}_i = e \sum_i \mathbf{R}_i h^\dagger \mathbf{h}_i$, and then the current operator $\mathbf{j}$ in the presence of the vector potential $A_\nu$ is obtained by evaluating the time-derivative of this polarization operator. According to this current operator $\mathbf{j}$, the diamagnetic and paramagnetic parts of the response kernel have been evaluated as:

$$K^{(d)}_{\mu\nu}(q, 0) = -\frac{4e^2}{\hbar^2}(\chi_{\uparrow}\phi_1 t - 2\chi_2 \phi_2 t')\delta_{\mu\nu} = \frac{1}{\lambda^2_s}\delta_{\mu\nu}, \quad (7a)$$

$$K^{(p)}_{\mu\nu}(q, 0) = \frac{1}{N} \sum_k \gamma_{\mu\nu}(\mathbf{k} + \mathbf{q}, \mathbf{k}) \gamma^*_{\nu\mu}(\mathbf{k} + \mathbf{q}, \mathbf{k}) |L_1(k, q)| + L_2(k, q)] = K^{(p)}_{\mu\nu}(q, 0) \delta_{\mu\nu}, \quad (7b)$$

where the charge carrier particle-hole parameters $\phi_1 = (h^\dagger_{\uparrow+i\sigma} h_{\downarrow+i\sigma})$ and $\phi_2 = (h^\dagger_{\uparrow-i\sigma} h_{\downarrow-i\sigma})$, $\lambda^{-2}_s = -4e^2(\chi_{\uparrow}\phi_1 t - 2\chi_2 \phi_2 t')/\hbar^2$, while the functions $L_1(k, q, \omega)$ and $L_2(k, q, \omega)$ have been given in Ref. 22. In particular, we22 have shown that in the long wavelength limit, i.e., $|\mathbf{q}| \rightarrow 0$, $K^{(p)}_{\mu\nu}(q \rightarrow 0, 0) = 0$ at $T = 0$, reflecting that the long wavelength electromagnetic response is determined by the diamagnetic part of the kernel only. However, at $T = T_c$, $K^{(p)}_{\mu\nu}(q \rightarrow 0, 0) = -(1/\lambda^2_s)$, which exactly cancels the diamagnetic part of the response kernel (7a), and then the Meissner effect is obtained for all $T \leq T_c$. With the help of the response kernel in Eq. (7), the magnetic field penetration depth $\lambda(T)$ by taking into account the two-dimensional geometry of cuprate superconductors within the specular reflection model has been evaluated as:

$$\lambda(T) = \frac{1}{B} \int_0^\infty h_\uparrow(x) \, dx = \frac{2}{\pi} \int_0^\infty \frac{dq_\perp}{\mu_0 K_{yy}(q_\perp, 0) + q_\perp^2}, \quad (8)$$

then the superfluid density $\rho_s(T)$ is obtained as $\rho_s(T) = \lambda^{-2}(T)$.

![FIG. 4: The superfluid density as a function of doping for temperature $T = 0.002J$ with parameters $t/J = 2.5$, $t'/t = 0.3$, and $J = 1000K$. Inset: the corresponding experimental results of cuprate superconductors taken from Ref. [10].](image)

In this case, for the discussions of the difference between the optimal doping for the maximal $T_c$ and the critical doping for the highest $\rho_s$, the result of $\rho_s$ as a function of doping at $T = 0.002J$ with $t/J = 2.5$, $t'/t = 0.3$, and $J = 1000K$ is replotted in Fig. 4 in comparison with the corresponding experimental data of cuprate superconductors (inset). The result in Fig. 4 shows clearly that $\rho_s$ increases with increasing doping in the lower doped regime, and reaches a maximum around the critical doping $\delta_{\text{critical}} \approx 0.195$, then decreases in the higher doped regime, in good agreement with the experimental results of cuprate superconductors. In particular, this anticipated value of the critical doping $\delta_{\text{critical}} \approx 0.195$ is very close to the critical doping $\delta_{\text{critical}} \approx 0.19$ obtained experimentally for different families of cuprate superconductors.
(d\lambda/d\delta)_{\delta=\delta_{\text{critical}}} = 0. In this case, (d\lambda/d\delta)_{\delta=\delta_{\text{critical}}} = 0 can be expressed in terms of Eq. (3) as,

$$\left[ \frac{d\lambda}{d\delta} \right]_{\delta=\delta_{\text{critical}}} = - \frac{2\mu_0}{\pi} \int_0^\infty dq_x \left[ \frac{1}{|\mu_0 K_{yy}(q_x, 0, 0) + q_\parallel^2|} \times \frac{dK_{yy}(q_x, 0, 0)}{d\delta} \right]_{\delta=\delta_{\text{critical}}} = 0,$$

(9)

then it is straightforward to obtain from Eq. (7) that when $(d\rho_s/d\delta)_{\delta=\delta_{\text{critical}}} = 0, (d\Delta_h/d\delta)_{\delta=\delta_{\text{critical}}} = 0$, which shows that the doping effects from the coupling strength $V_{\text{eff}}$ and all the other order parameters upon $\rho_s$ are canceled each other, then both the maximal $\Delta_h$ and the highest $\rho_s$ appear at the same critical doping. Moreover, both $\rho_s$ and $\Delta_h$ are the bare quantities and separately describe the different aspects of the same SC charge carriers. In this case, the domelike shape of the doping dependence of $\rho_s$ with the highest value appeared around the critical doping is a natural consequence of the domelike shape of the doping dependence of $\Delta_h$ with the maximal value appeared around the same critical doping within the kinetic energy driven SC mechanism. In other words, except the quasiparticle coherence, $\rho_s$ is dominated by the bare charge carrier pair gap parameter $\Delta_h$, while $T_c$ is set by the effective charge carrier pair gap parameter $\Delta_h$, this is why there is a difference between the optimal doping for the maximal $T_c$ and the critical doping for the highest $\rho_s$ in cuprate superconductors. Finally, we have noted that $\rho_s$ dominated by the bare energy gap parameter in cuprate superconductors has been observed from the photoemission experiments. Since in the SC state, the photoemission peak intensity as a function of doping scales with $\rho_s$, then a measurement of the coherent component in the quasiparticle excitation has been suggested as an indirect measure of the bare energy gap parameter in cuprate superconductors.

In conclusion, within the framework of the kinetic energy driven SC mechanism, we have discussed the origin of the difference between the optimal doping for the maximal $T_c$ and the critical doping for the highest $\rho_s$ in cuprate superconductors. By calculation of the ratio of the effective and bare charge carrier pair gap parameters, we have shown that the coupling strength decreases with increasing doping. This special doping dependence of the coupling strength induces an important shift from the critical doping $\delta_{\text{critical}} \approx 0.195$ for the maximal value of the bare charge carrier pair gap parameter to the optimal doping $\delta_{\text{optimal}} \approx 0.15$ for the maximal value of the effective charge carrier pair gap parameter, which leads to a difference between the optimal doping for the maximal $T_c$ and the critical doping for the highest $\rho_s$ in cuprate superconductors.

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