

The separate role of pairing amplitude and phase in cuprates.

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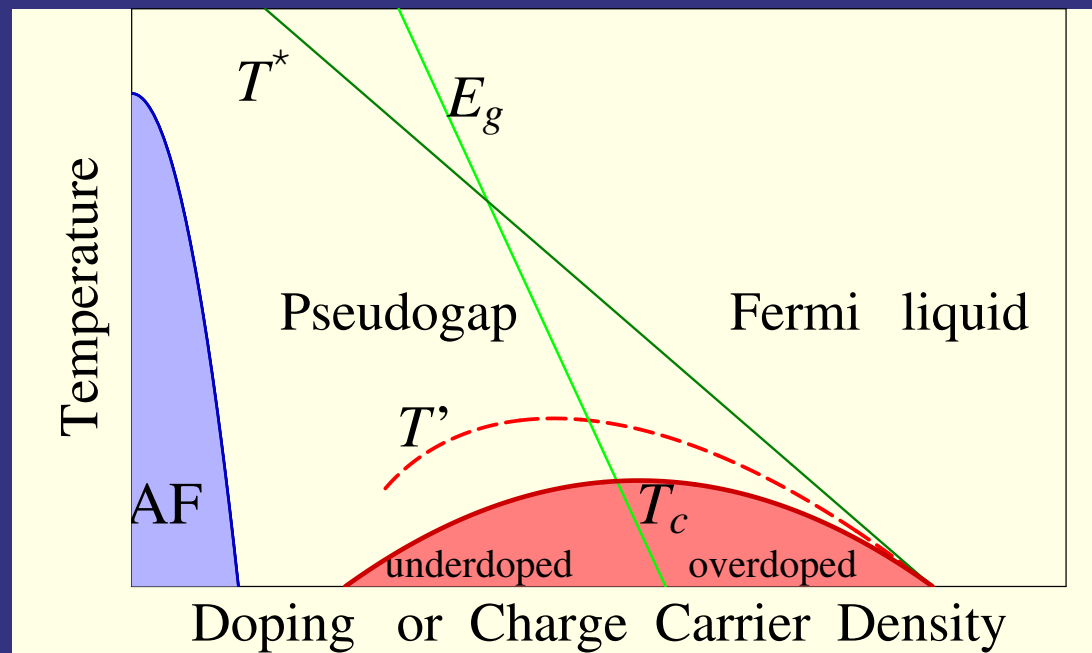
<http://www.philippecurty.ch>

outline

- What is the real phase diagram of cuprates?
- Why are phase and amplitude relevant?
- How is the pseudogap related to pairing and phase fluctuations?

phase diagram of cuprates

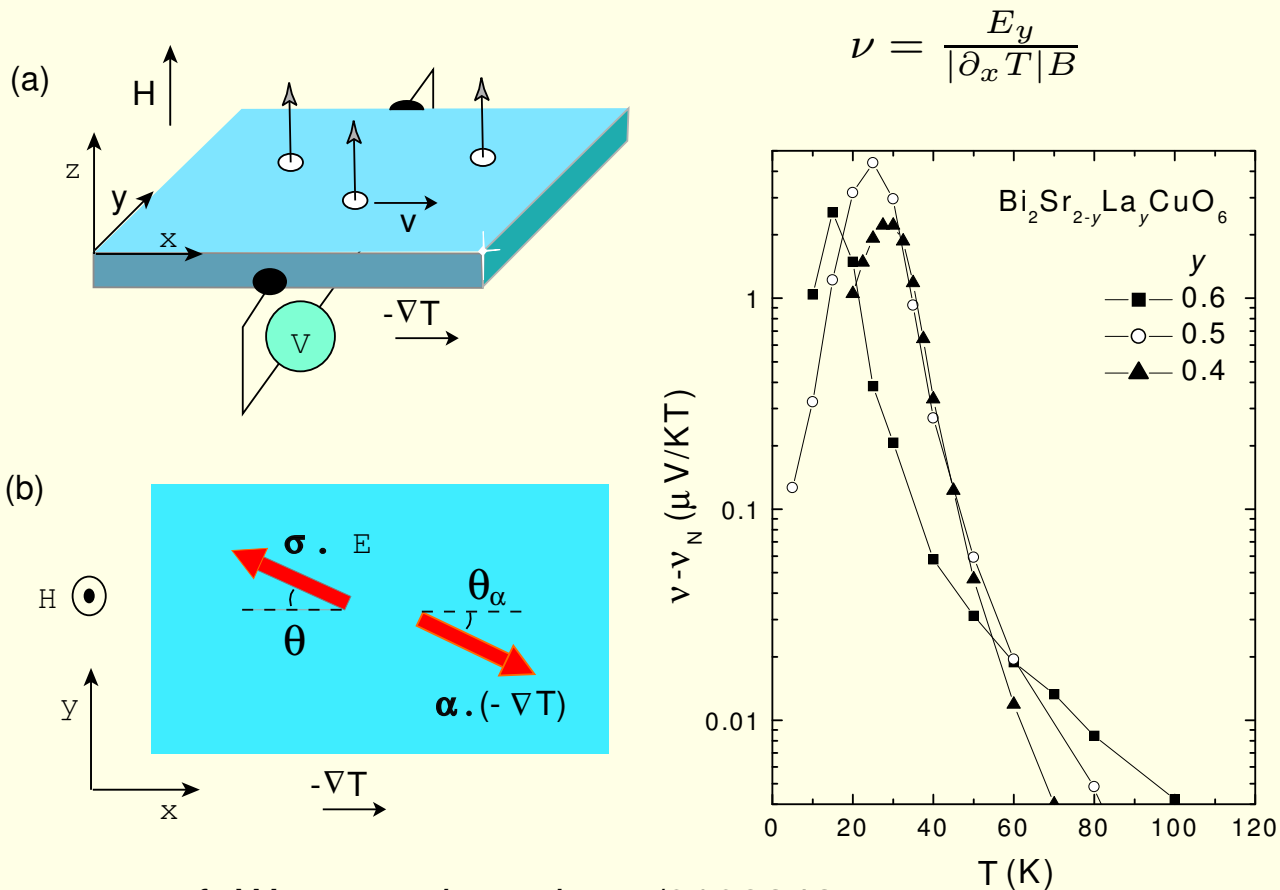
pseudogap: two or four regimes?



T' : Nernst effect, Hall effect, specific heat.

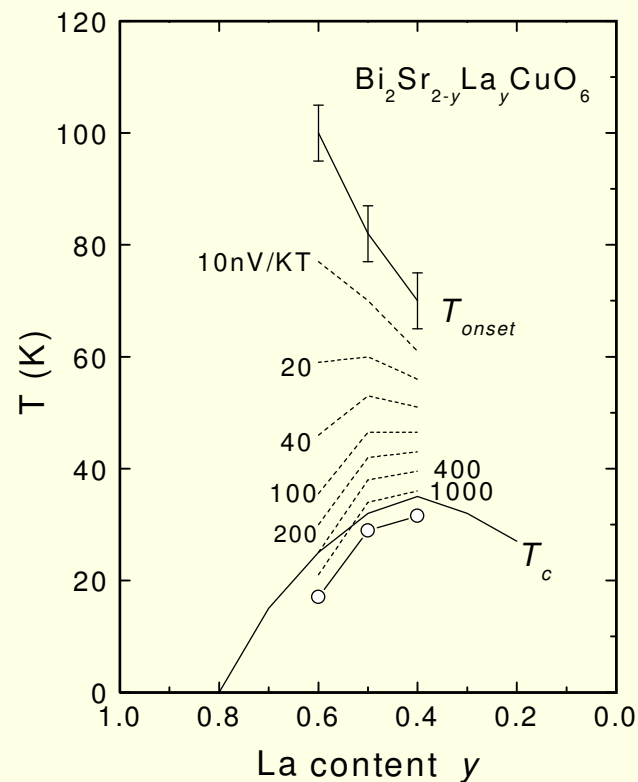
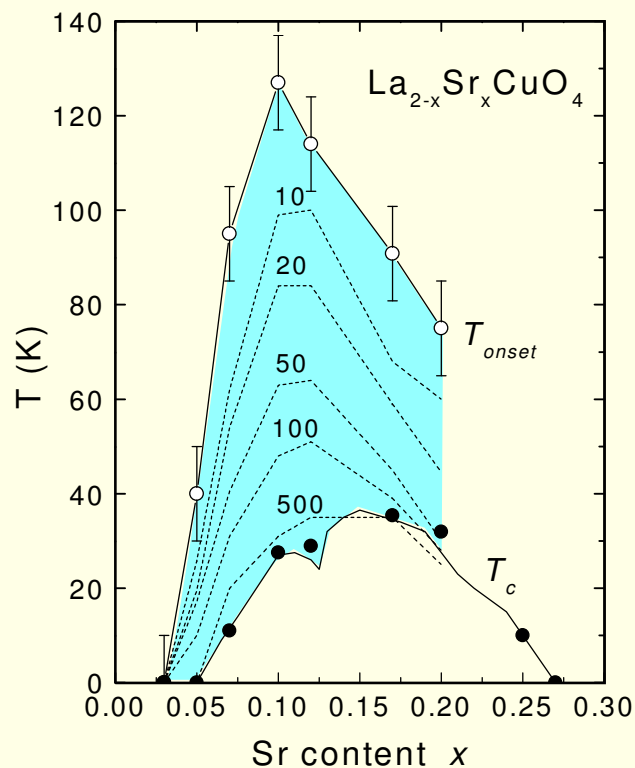
E_g : specific heat, spin susceptibility, ARPES,...

Nernst effect: experiment



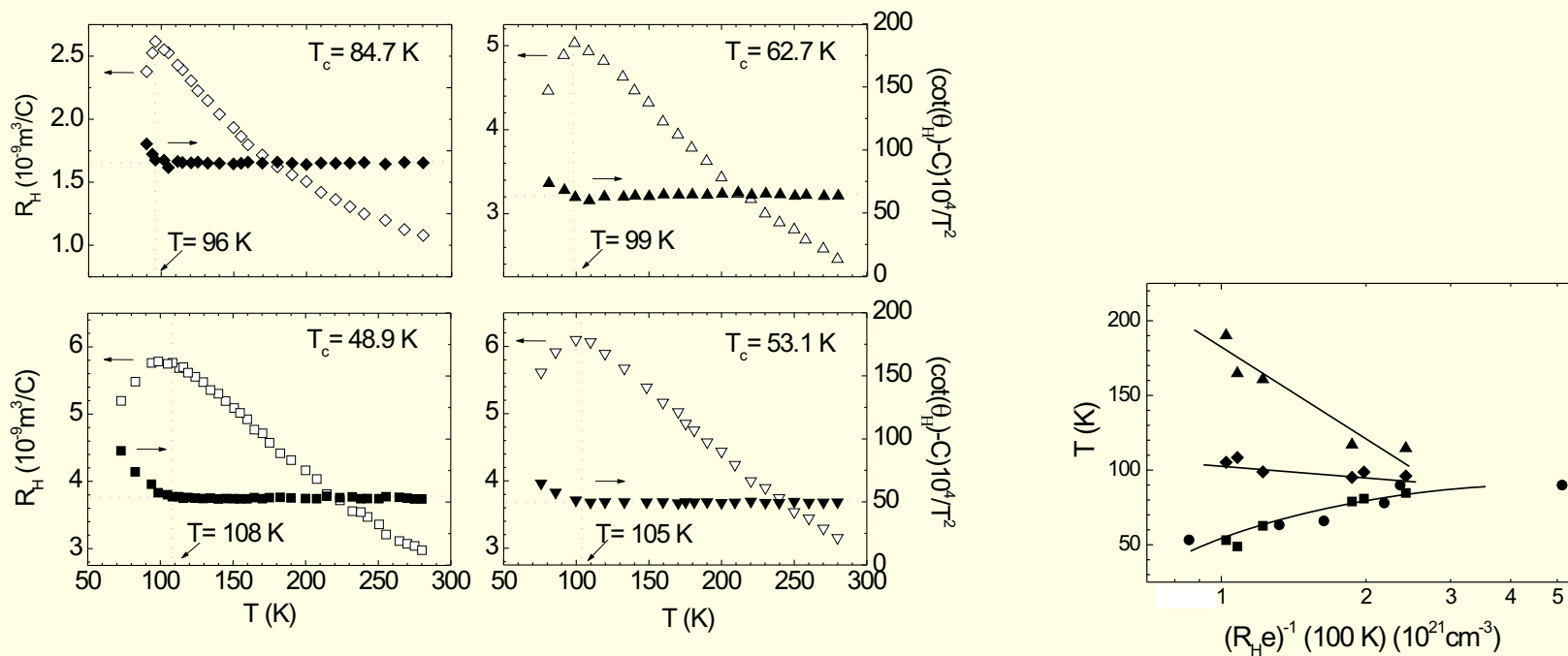
ref: Wang *et al*, cond-mat/0108242
 Wang *et al*, PRL 88, 257003 (2002)

Nernst effect: phase diagram



ref: Wang *et al*, cond-mat/0108242
Wang *et al*, PRL 88, 257003 (2002)

Hall effect

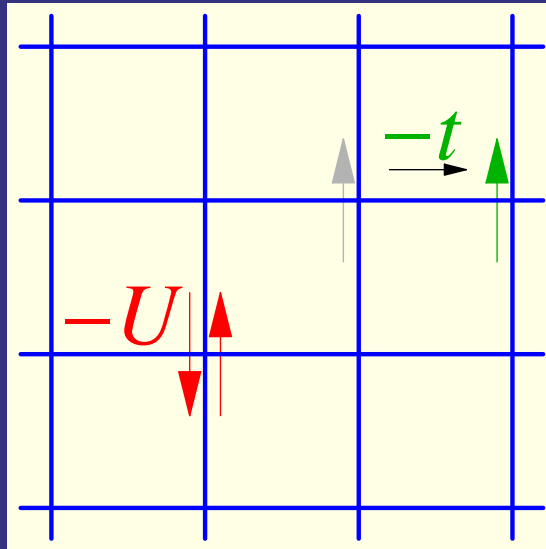


ref: Matthey *et al*, PRB 64, 24513 (2001)

model

Experiments show d -wave (s -wave) pairing
 \Rightarrow attractive d -wave Hubbard model:

$$H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow}$$



introducing phase and amplitude

Hubbard-Stratonovich transformation:

$$e^{-Un_{i\uparrow}n_{i\downarrow}} = cst \int d\psi d\psi^* e^{-\frac{|\psi|^2}{U} + \psi n_{i\uparrow} + \psi^* n_{i\downarrow}}$$

$$\psi \rightarrow |\psi|e^{i\phi}$$

- Universality class of superconductors is 2DXY or 3DXY \Rightarrow phases are relevant!
- The amplitude $|\psi|$ is the energy scale. ($|\psi|_{T=0} = \Delta_0$).

effective action

Integrate fermionic operators \Rightarrow standard action:

$$S[\psi] = S_0(|\psi|) + S_\phi(\vec{\nabla}\psi)$$

$S_0 = F_{BCS}$ for a fixed $|\psi|$.

$S_\phi = \int dV |\nabla\psi|^2$ is the phase part.

The free energy is

$$F(T) = -\frac{1}{\beta} \log \int d\psi_1 \cdots d\psi_N e^{-\beta S[\psi]}$$

Two parameters: T_0 and V_0 .

goal and method

What is the influence of the pairing field ψ on thermodynamics?

Two methods

- variational: the free energy is minimal with respect to $|\psi|$. (amplitude correlations are neglected)
- average value: expand the energy around the average amplitude $\langle |\psi| \rangle$.

variational method

Polar coordinates:

$$\int d^2\psi = \int_0^\infty d|\psi| |\psi| \int_0^{2\pi} d\phi$$

Fix the amplitude to a constant $|\bar{\psi}|$. The free energy is:

$$F = -\frac{1}{\beta} \log \int_0^{2\pi} D\phi e^{-\beta(S_0(\bar{\psi}) - \log(|\bar{\psi}|)V/\beta + S_\phi)}$$

equation of the variational method

Minimize:

$$\frac{\partial F}{\partial |\bar{\psi}|} = 0$$

\Rightarrow

$$\underbrace{\frac{\partial S_0(|\bar{\psi}|)}{\partial |\bar{\psi}|}}_{\text{amplitude part}} - \underbrace{\frac{1}{\beta |\bar{\psi}|}}_{\text{Jacobian term}} + \underbrace{c |\bar{\psi}| \langle S_\phi \rangle_{S_\phi}}_{\text{phase fluctuations}} = 0.$$

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\Downarrow (*static*)

BCS

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\Downarrow (*static*)

BCS

\Downarrow ($|\psi| = \text{cst}$)

XY model

solving the variational equation

$$\frac{\partial S_0(|\bar{\psi}|)}{\partial |\bar{\psi}|} - \frac{1}{\beta |\bar{\psi}|} + c |\bar{\psi}| \langle S_\phi \rangle_{S_\phi} = 0.$$

solving the variational equation

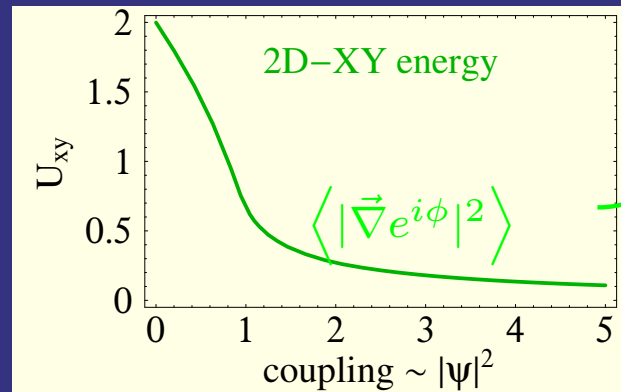
$$\frac{\partial S_0(|\bar{\psi}|)}{\partial |\bar{\psi}|} - \frac{1}{\beta |\bar{\psi}|} + c |\bar{\psi}| \langle S_\phi \rangle_{S_\phi} = 0.$$

$$\frac{|\bar{\psi}|^2}{U} - \frac{|\bar{\psi}|^2}{W} \int_{-\mu}^{W-\mu} d\xi \frac{\tanh \left[\sqrt{\xi^2 + |\bar{\psi}|^2} / (2T) \right]}{\sqrt{\xi^2 + |\bar{\psi}|^2}} - \frac{\bar{\psi}_0^2}{\beta} + |\bar{\psi}|^2 \langle |\nabla e^{i\phi}|^2 \rangle_{S_\phi} = 0.$$

solving the variational equation

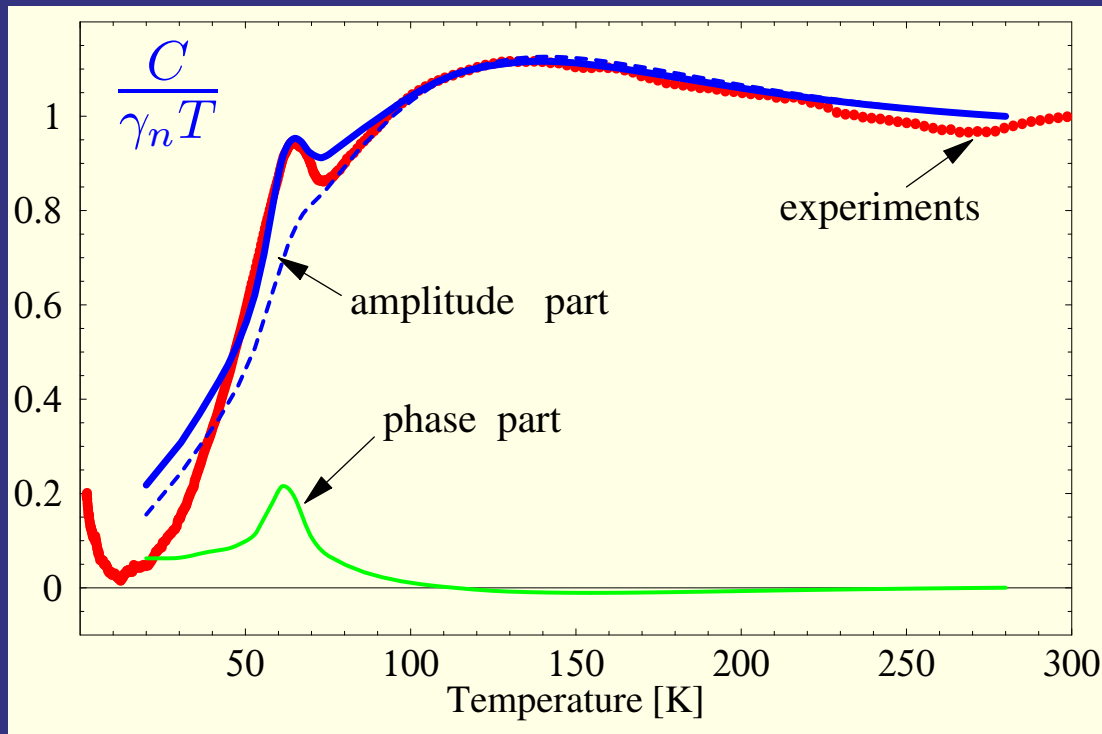
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variational method: specific heat

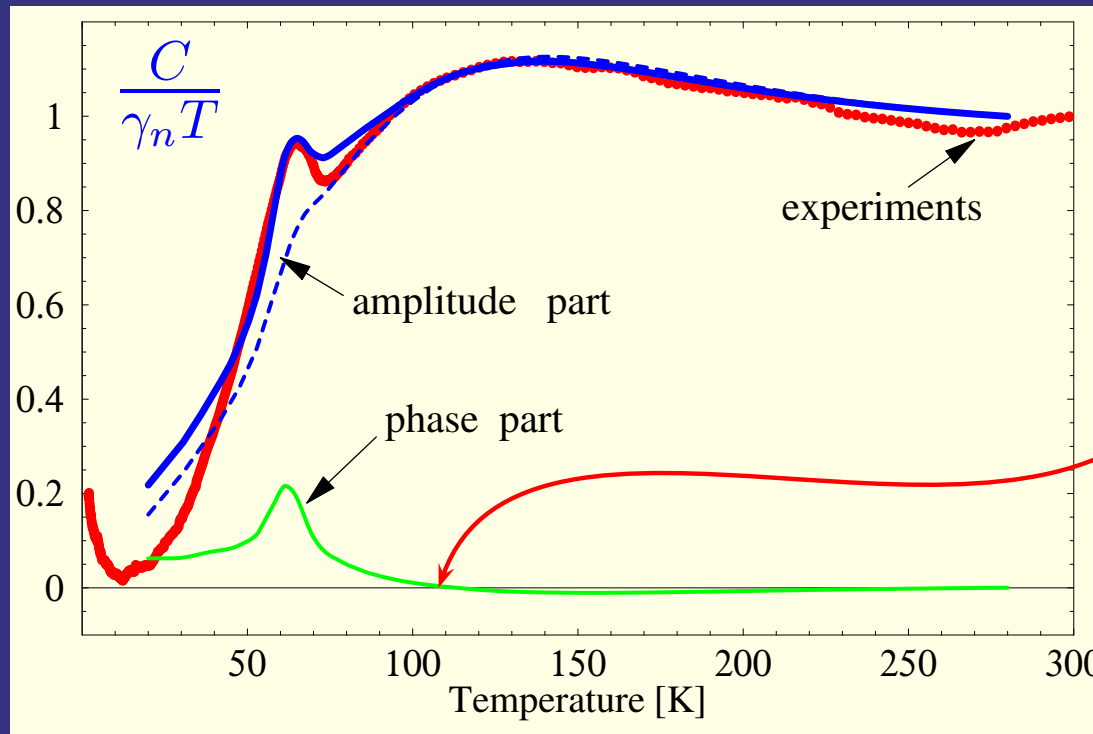
The specific heat is $C = C_{\text{amplitude}} + C_{\text{phase}}$



$\text{YBa}_2\text{Cu}_3\text{O}_{6.73}$ specific heat. (exp.: Loram *et al*, PRL 71, 1740 (1993))

variational method: specific heat

The specific heat is $C = C_{\text{amplitude}} + C_{\text{phase}}$



T_ϕ is the temperature above which phase correlations are negligible.

$\text{YBa}_2\text{Cu}_3\text{O}_{6.73}$ specific heat. (exp.: Loram *et al*, PRL 71, 1740 (1993))

average value approach

- Expand the energy around the average amplitude:

$$U = \langle S \rangle_S \approx S_0(\langle |\psi| \rangle) + \langle S_\phi \rangle_S + \mathcal{O}(\langle \delta |\psi| \rangle^2)$$

average value approach

- Expand the energy around the average amplitude:

$$U = \langle S \rangle_S \approx S_0(\langle |\psi| \rangle) + \langle S_\phi \rangle_S + \mathcal{O}(\langle \delta |\psi| \rangle^2)$$

- Replace averages over S by averages over the Ginzburg-Landau action $S_{GL} = U_{GL}(|\psi|) + S_\phi$:

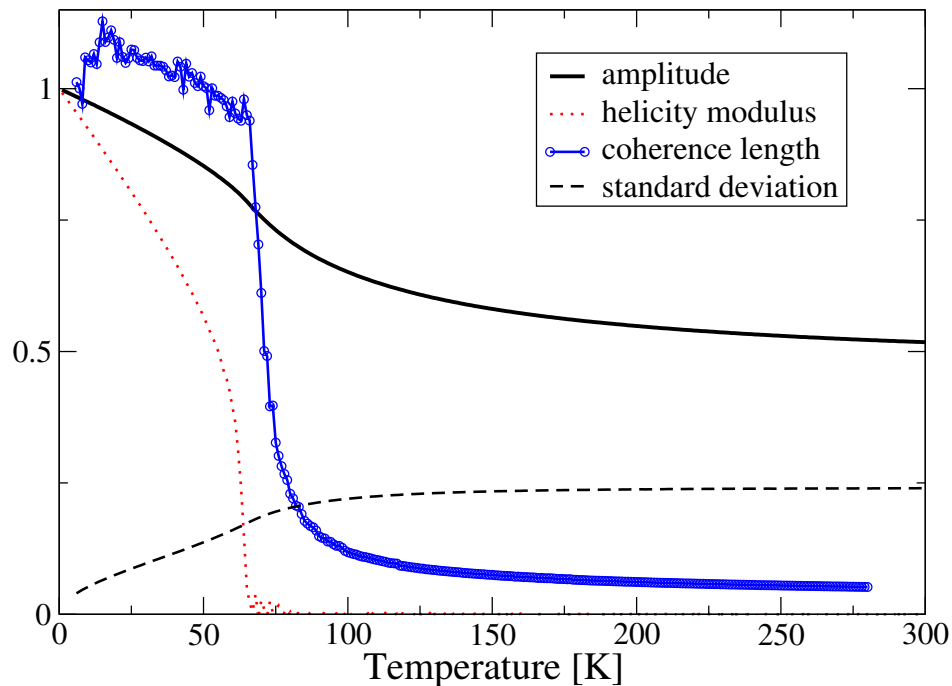
$$\langle \cdots \rangle_S \longrightarrow \langle \cdots \rangle_{S_{GL}}$$

Computation

$$Z = \int D\psi e^{-\frac{V_0}{T} \sum_i (\sigma(t|\psi_i|^2 + \frac{1}{2}|\psi_i|^4) + \frac{1}{2}|\nabla\psi_i|^2)} \text{ where } t = T/T_0 - 1, \text{ and}$$

$$S_\phi = \sum_i \frac{1}{2} |\nabla\psi_i|^2$$

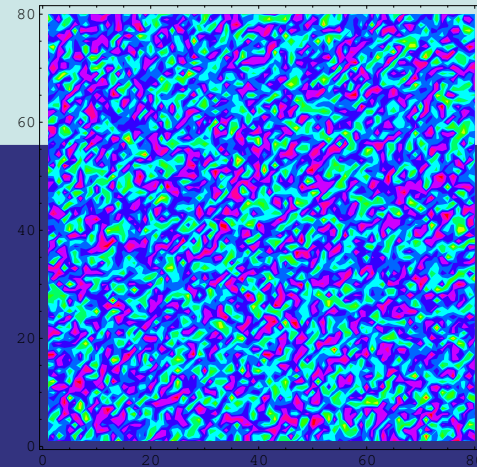
Monte Carlo cluster simulations



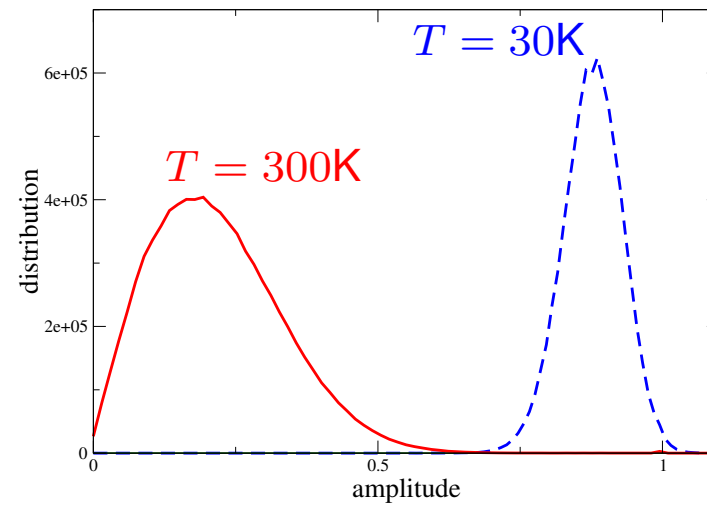
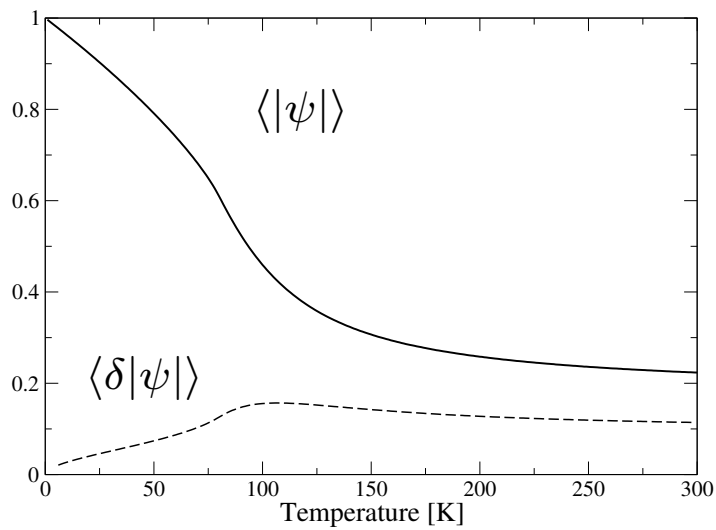
output needed:
 $\langle |\psi| \rangle$
 $U_\phi = \langle S_\phi \rangle$
for all parameters.

Fluctuations

$$\langle \delta|\psi| \rangle = \sqrt{\langle |\psi|^2 \rangle - \langle |\psi| \rangle^2}$$



Amplitude Distribution

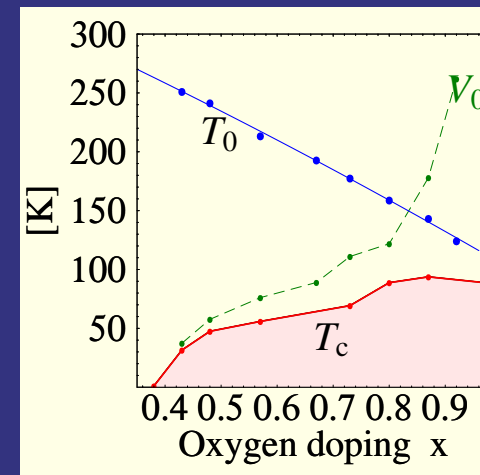
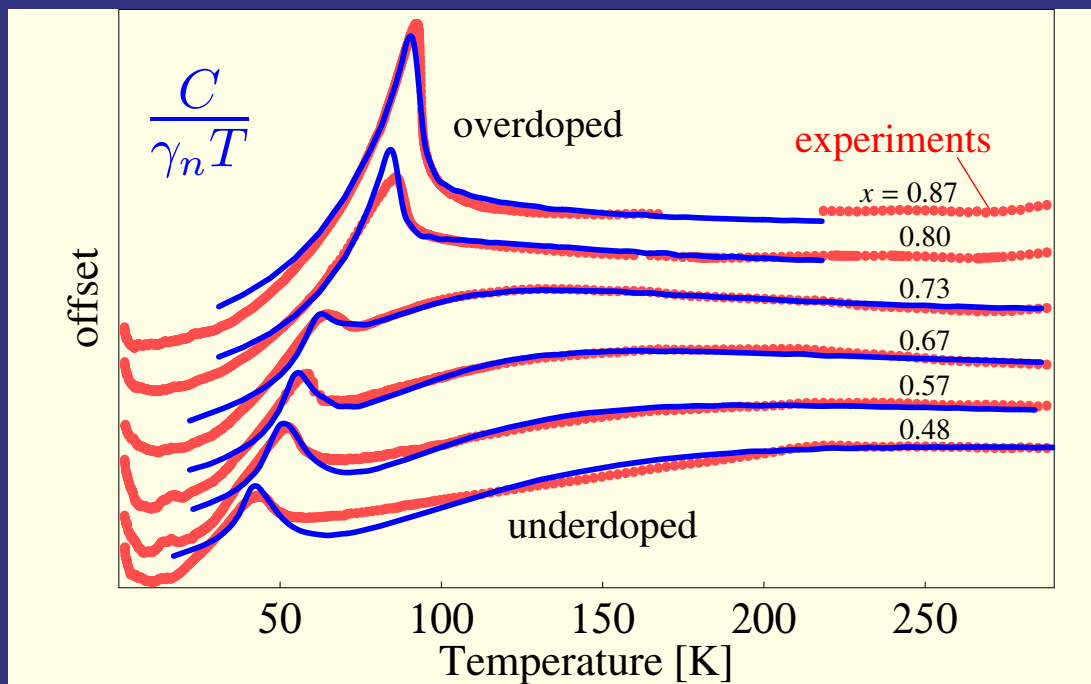


average value: YBCO specific heat

The specific heat is $C = C_0 (\langle |\psi| \rangle) + C_{phase}$

where $\langle |\psi| \rangle = Z^{-1} \int D^2\psi |\psi| e^{-\beta S_{GL}[\psi]}$

V_0 (phase stiffness) and T_0 (MF temperature) are extracted from the best plots: underdoped, overdoped

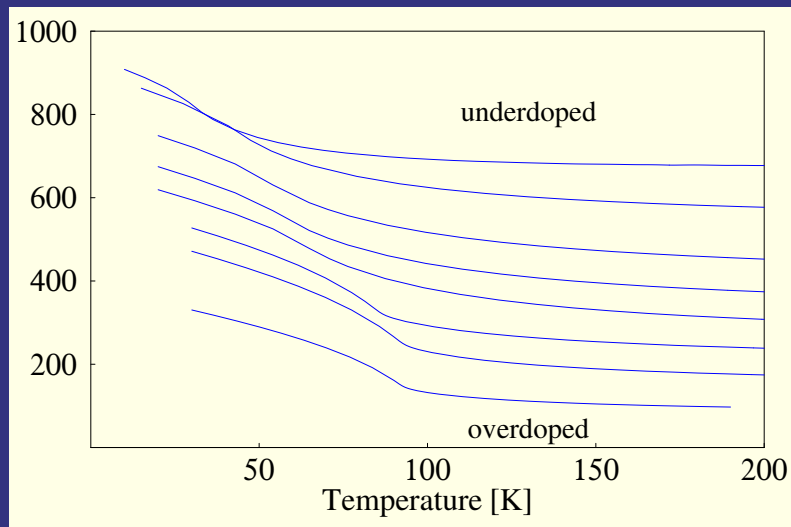


$\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$: underdoped: 2D d -wave, overdoped: 3D d -wave (s -wave)

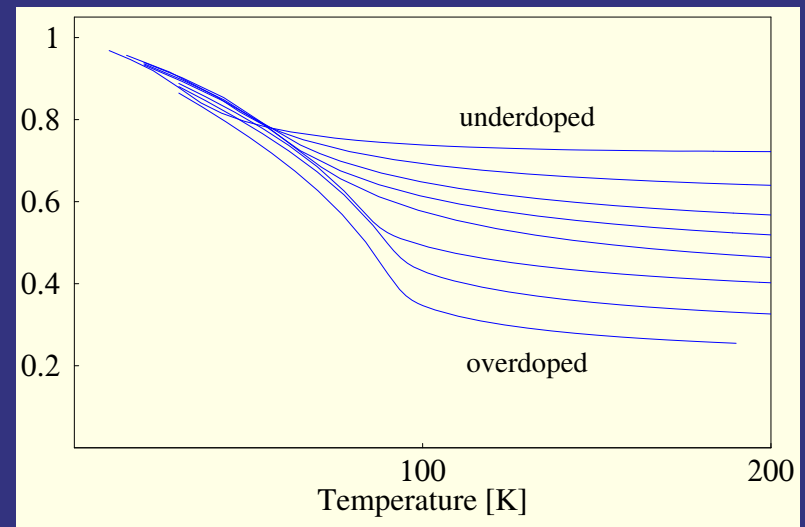
average value: amplitude for YBCO

The average amplitude is $\langle |\psi| \rangle = Z^{-1} \int D^2\psi |\psi| e^{-\beta S_{GL}[\psi]}$

$$\langle |\psi| \rangle$$

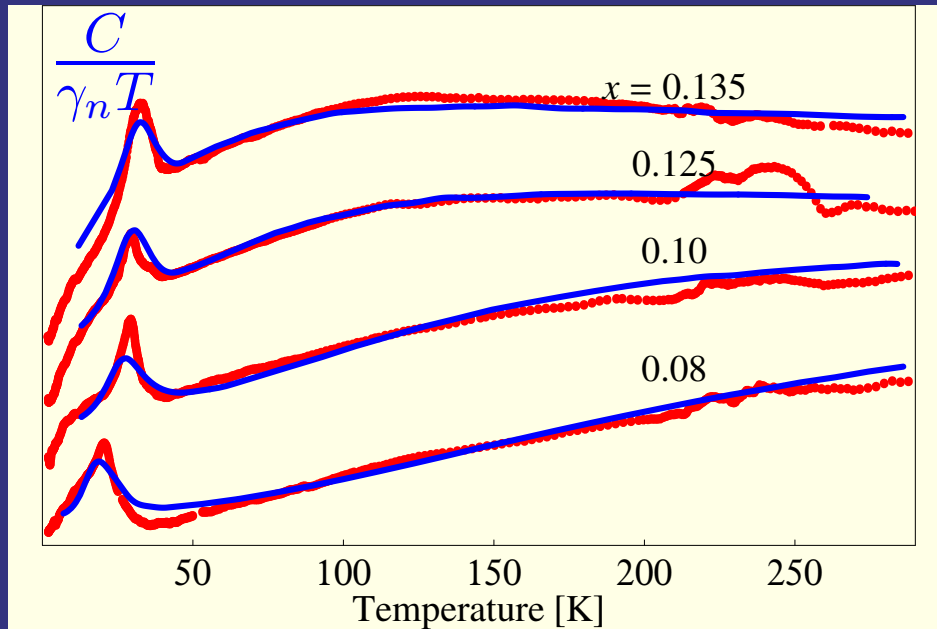


$$\langle |\psi| \rangle / \psi_0$$



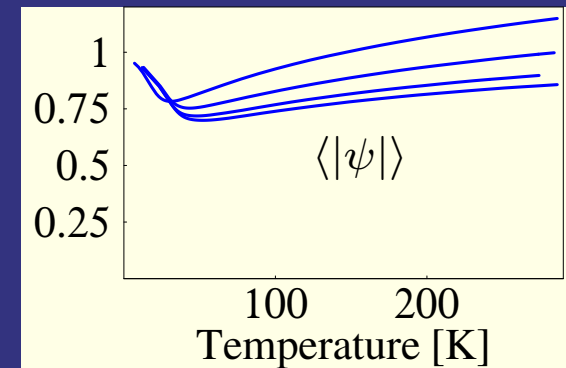
average value: LSCO specific heat

$$C = C_0 (\langle |\psi| \rangle) + C_\phi$$



La_{2-x}Sr_xCuO₄ specific heat for different dopings.
2D d-wave (exp.: Loram *et al*)

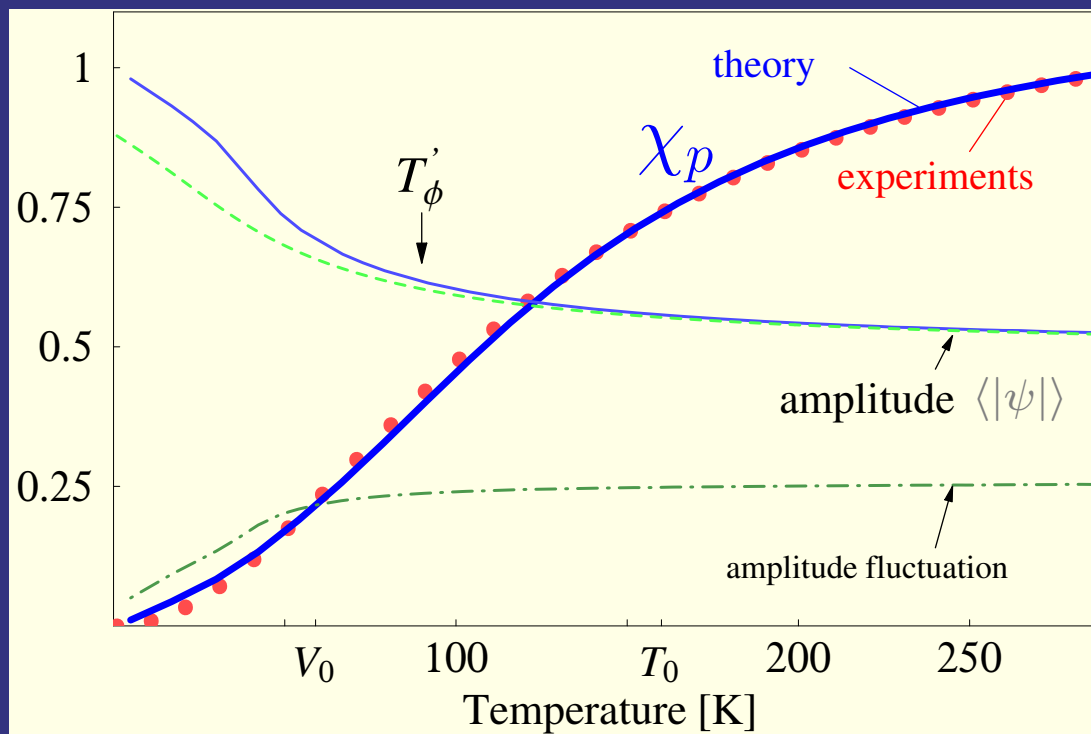
x	0.08	0.1	0.125	0.135
V_0	30	45	50	54
T_0	490	359	224	192



average amplitude.

magnetic spin susceptibility χ_p

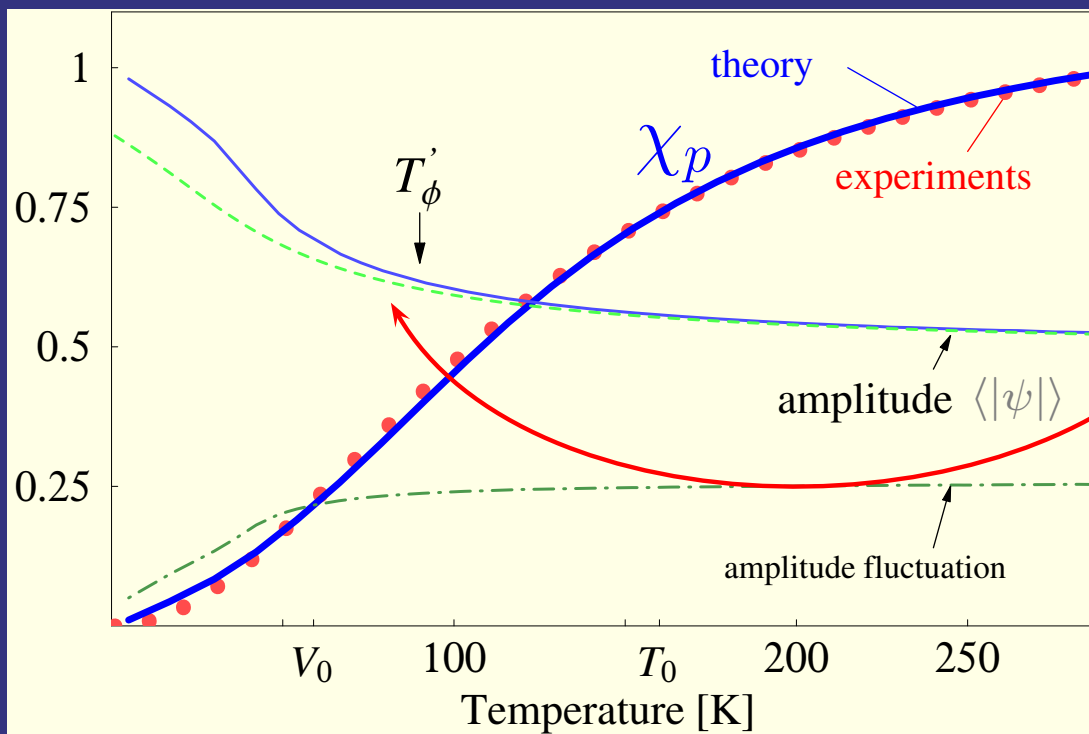
$$\chi_p = \chi_{BCS}(\langle |\psi| \rangle) \text{ where } \langle |\psi| \rangle = Z^{-1} \int D^2\psi |\psi| e^{-\beta S_{GL}[\psi]}$$



$\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ magnetic spin susceptibility: *d*-wave. (exp.: Takigawa *et al*)

magnetic spin susceptibility χ_p

$$\chi_p = \chi_{BCS}(\langle |\psi| \rangle) \text{ where } \langle |\psi| \rangle = Z^{-1} \int D^2\psi |\psi| e^{-\beta S_{GL}[\psi]}$$

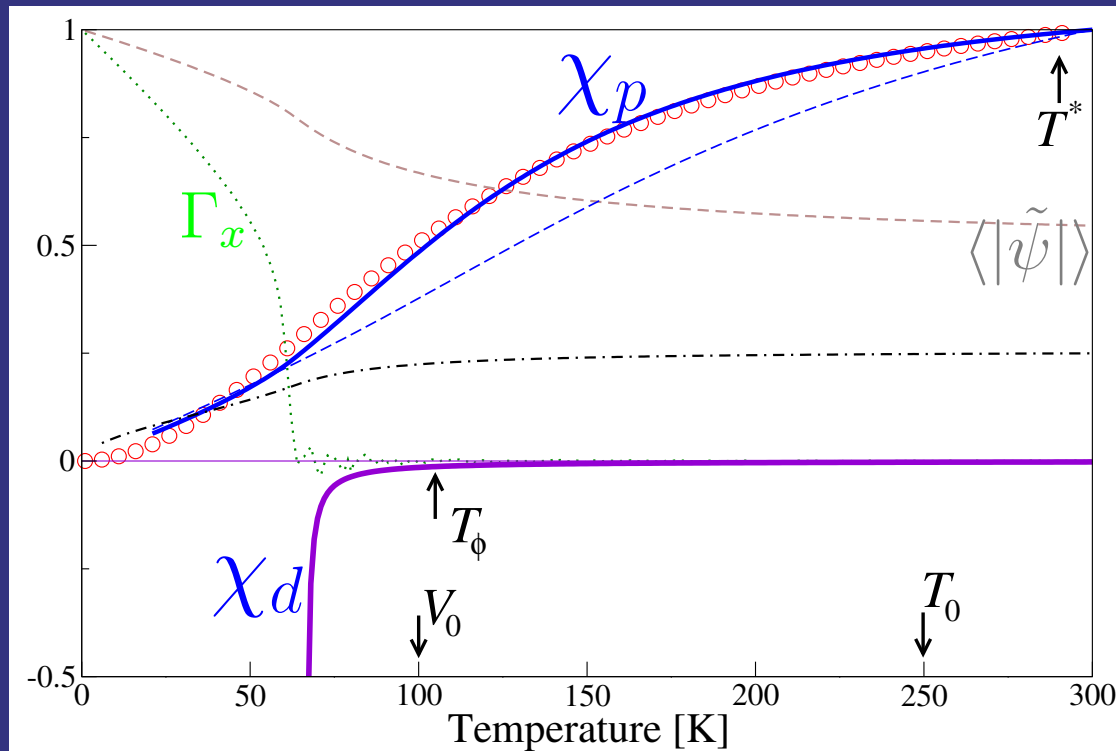


T'_ϕ is the temperature above which phase does not influence the amplitude (and χ_p)

$\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$ magnetic spin susceptibility: *d*-wave. (exp.: Takigawa *et al*)

magnetic susceptibility $\chi = \chi_p + \chi_d$

χ_p is the paramagnetic spin susceptibility and χ_d is the diamagnetic susceptibility.

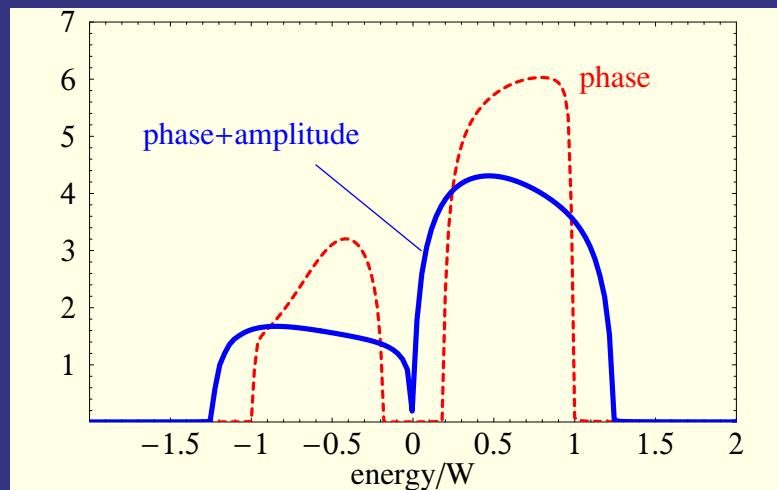


YBCO: magnetic spin susceptibility and diamagnetic susceptibility.

density of states: CPA

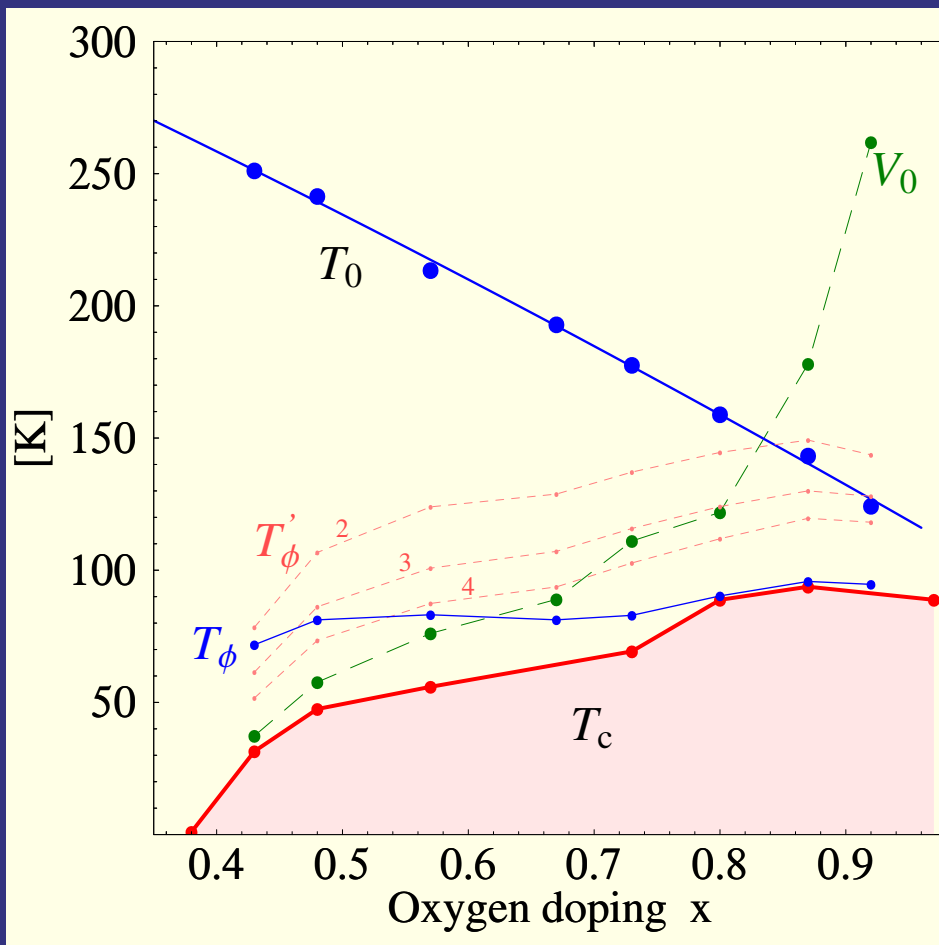
CPA (Coherent Phase Approximation):

$$\underbrace{\langle G(r, r) \rangle_{\psi_r}}_{\text{average local GF}} = \underbrace{\mathcal{G}(0, z)}_{\text{effective local GF}}$$

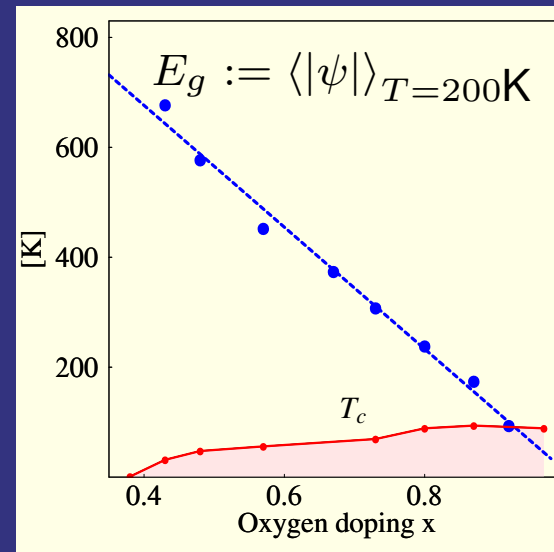


Average over amplitude and phase (thick line).

resulting phase diagram.



Phase diagram of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$.



pseudogap energy scale E_g

$$\Rightarrow T_0 \sim T^*$$

$$\Rightarrow T_\phi \sim T'_{Hall}, T'_{Nernst}$$

conclusion and perspective

- Superconductivity and pseudogap have the same origin.
- Two regimes in the pseudogap: correlated (phase) and uncorrelated (amplitude). (\neq phase scenario.)

To do: Nernst effect, transport, etc..