

Why study the normal state ?

Superconductivity competes with normal state

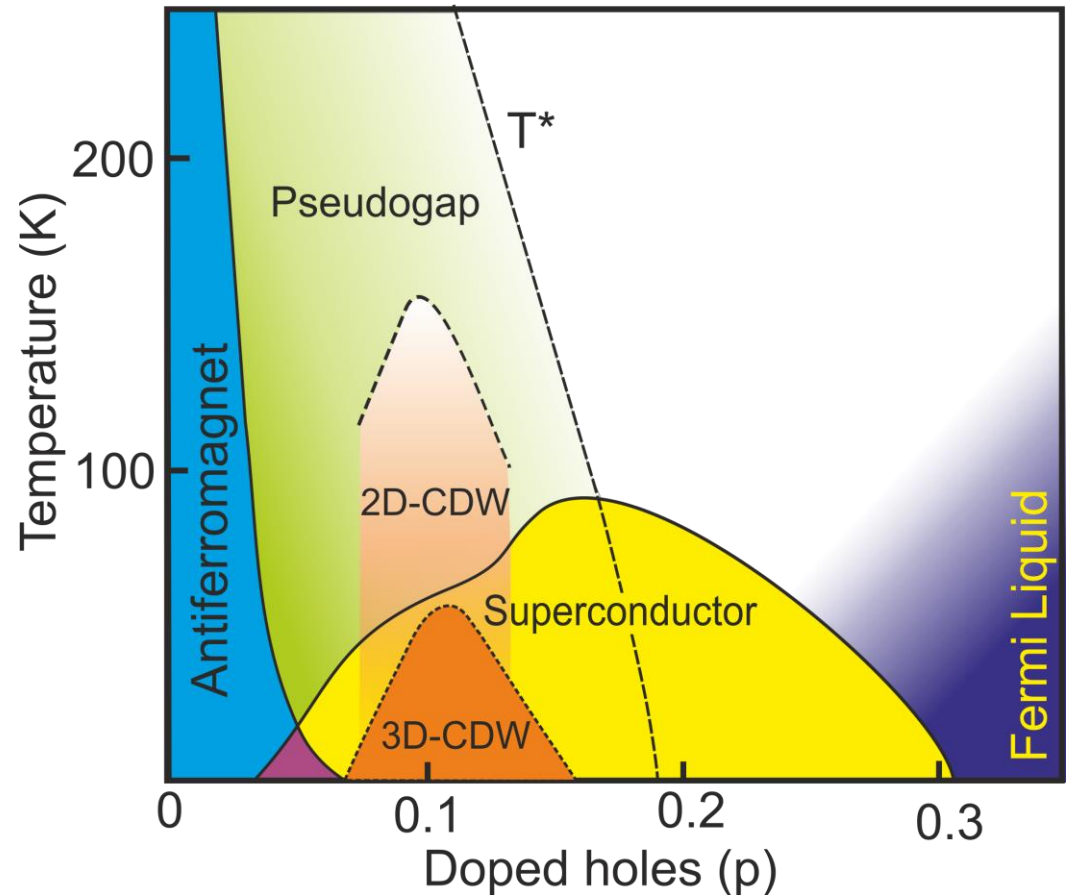
Need superconducting state to have lower energy for $T < T_c$

So need to understand details of normal state

- Competing phases
- Anomalous scattering
- Quasiparticle / coherence / collective excitations

Bulk transport and thermodynamic properties

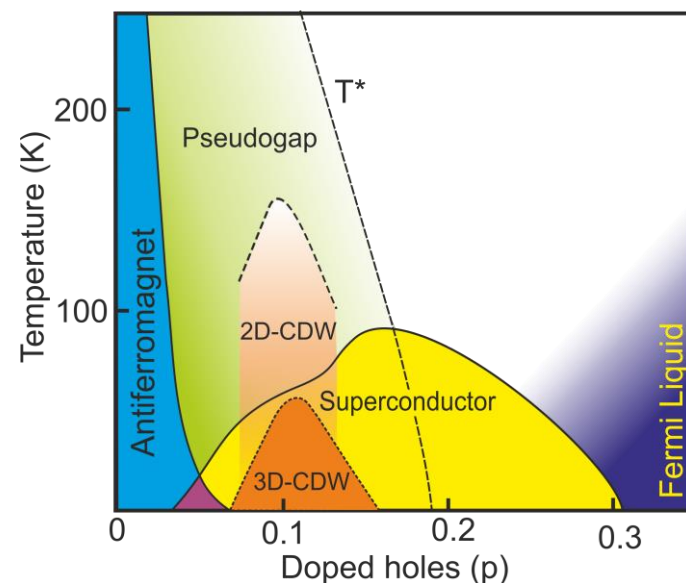
1. Phase diagram
2. Electronic structure
3. Resistivity
4. Hall Effect
5. Boltzmann theory
6. Quantum Oscillations



Cuprates: Materials

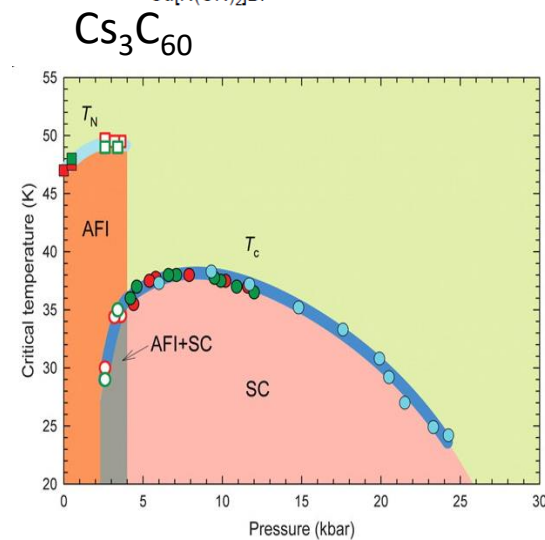
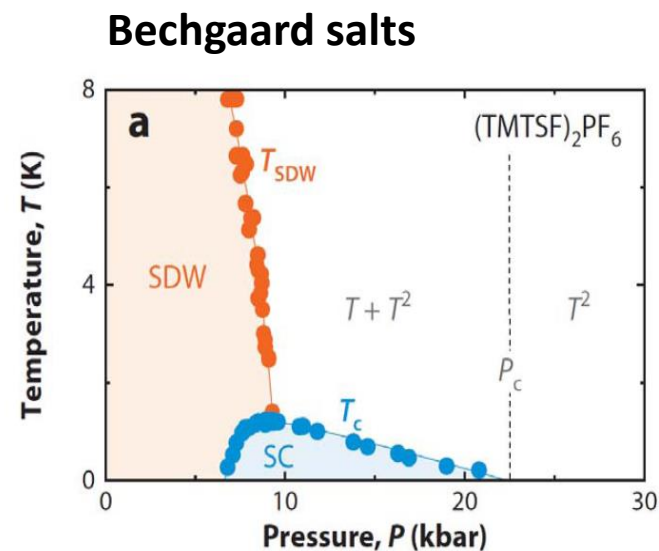
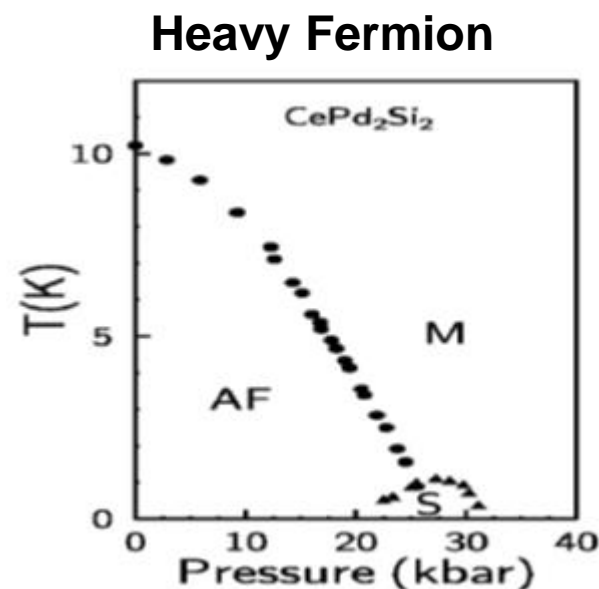
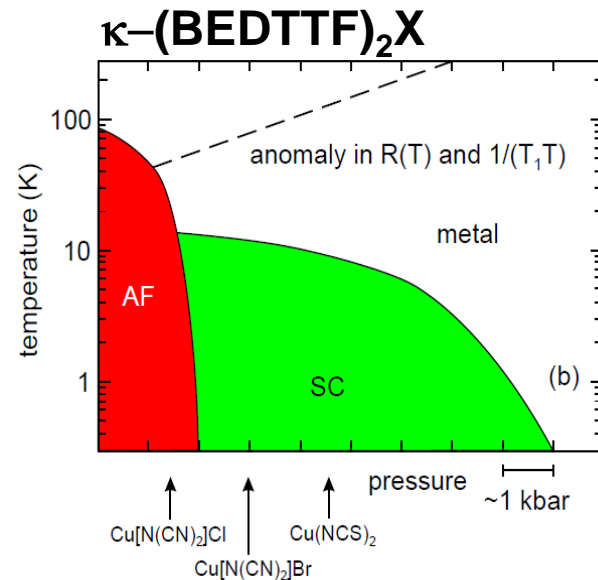
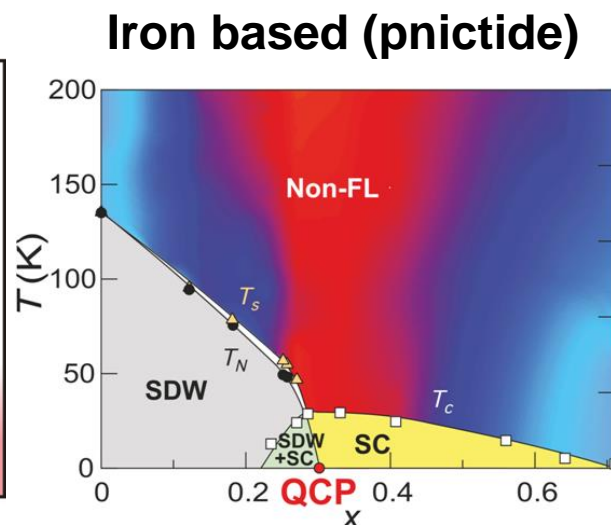
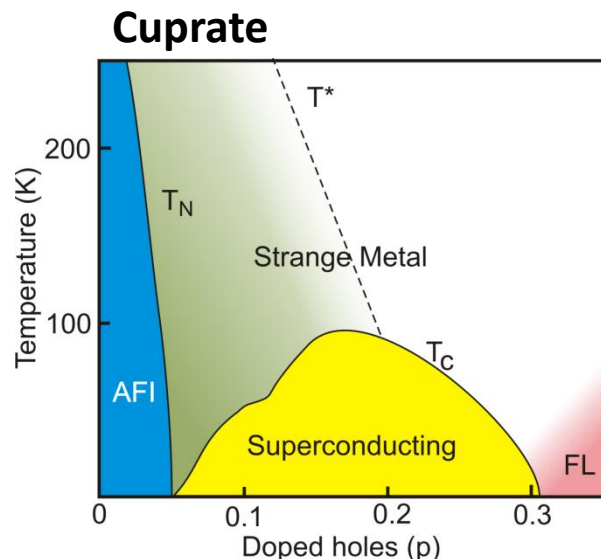
Hg-Family	Abbrev.	T_c
HgBa ₂ Ca ₃ Cu ₄ O _{10+δ}	Hg-1234	125 K
HgBa ₂ Ca ₂ Cu ₃ O _{8+δ}	Hg-1223	134 K (164 K @ 30GPa) – highest T_c
HgBa ₂ CuO _{4+δ}	Hg-1201	95 K
Tl-Family		
Tl ₂ Ba ₂ Ca ₂ Cu ₃ O _{10+δ}	Tl-2223	128 K
Tl ₂ Ba ₂ CaCu ₂ O _{6+δ}	Tl-2212	118 K
Tl ₂ Ba ₂ CuO _{6+δ}	Tl-2201	95 K (can be highly overdoped)
Bi-Family		
Bi ₂ Sr ₂ Ca ₂ Cu ₃ O _{10+δ}	Bi-2223	110 K
Bi ₂ Sr ₂ CaCu ₂ O _{8+δ}	Bi-2212	91 K (photoemission/tunneling –cleaves)
Bi ₂ Sr ₂ CaCu ₂ O _{8+δ}	Bi-2201	35 K
Y-Family		
YBa ₂ Cu ₃ O _{7+δ}	Y-123	94 K (clean – most highly studied)
Y ₂ BaCu ₄ O _{7+δ}	Y-124	82 K
La-Family		
La _{2-x} Sr _x CuO _{4+δ}	LaSr-214	40 K (full doping range)
La _{2-x} Ba _x CuO _{4+δ}	LaBa-214	30 K (1 st cuprate superconductor)
Others		
Ca _{1-x} Sr _x CuO ₂		110 K
Nd _{2-x} Ce _x CuO _{4+δ}		30K

Hole doped

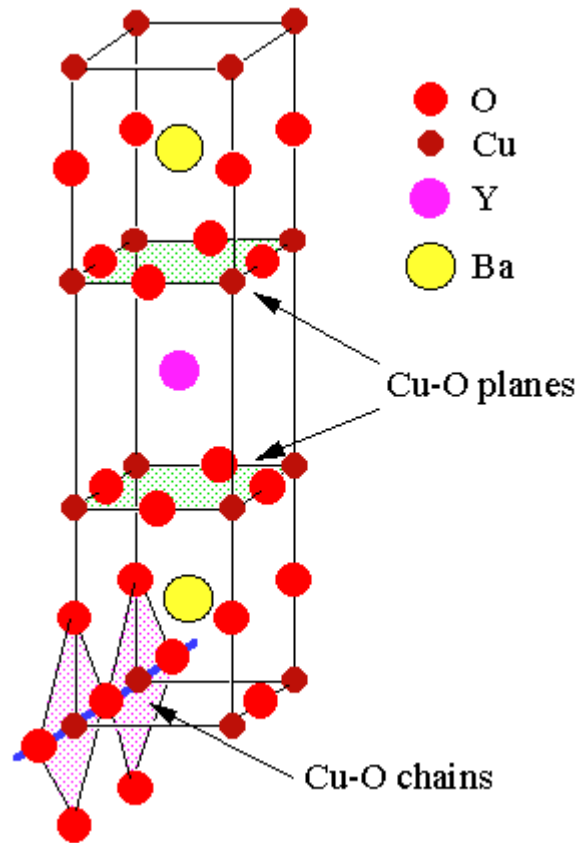


Electron doped

Superconductors mediated by magnetic interactions ?



Cuprates : Basic structure



Two dimensional copper-oxides

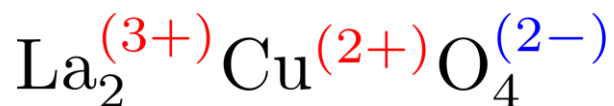
draws electrons away from
 CuO_2 layer (hole dopes)



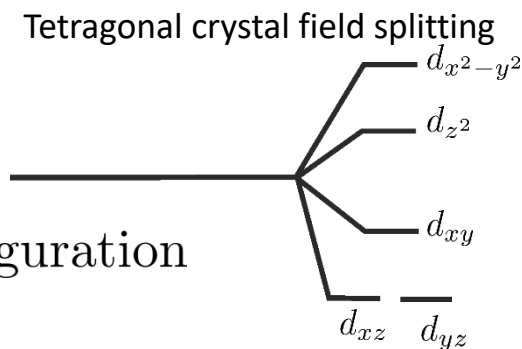
Electronic structure : Parent compound La_2CuO_4



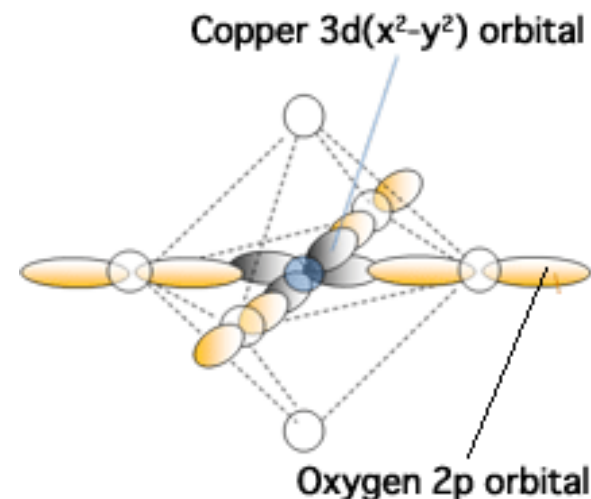
Formal valence counting



Cu^{2+} is in $3d^9$ configuration

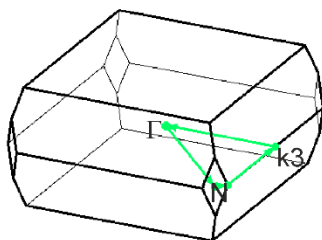
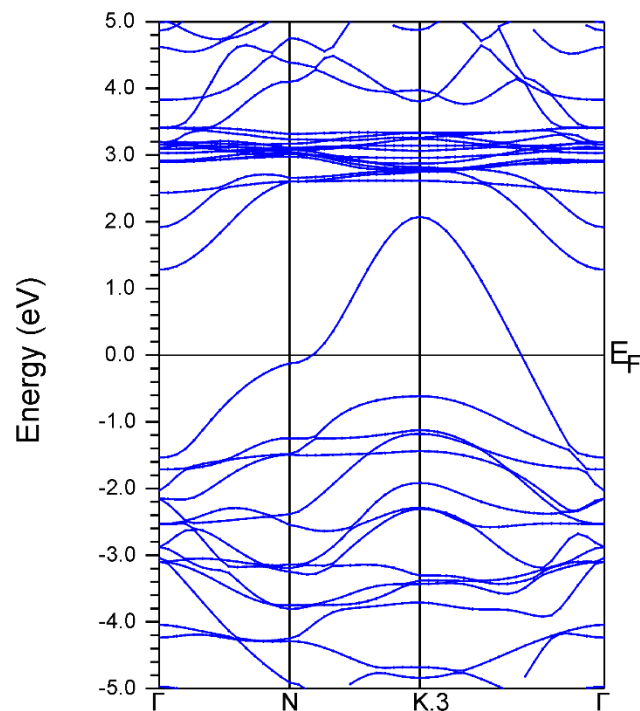


- Single unpaired electron on $3d$ orbitals.
- Cu is in tetragonal structure: leads to Crystal field splitting of d orbitals
- Highest energy orbital which contains a hole is $d_{x^2-y^2}$ orbital
- Cu $3d_{x^2-y^2}$ level strongly hybridises with O $2p$

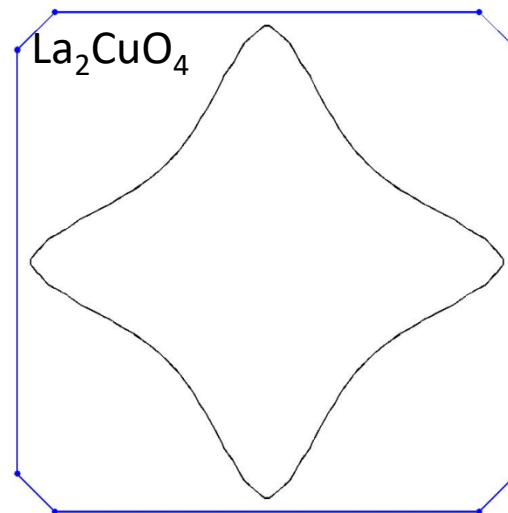


Density functional theory band-structure : DFT-LDA : La_2CuO_4

Single hole band
from Cu and O orbitals

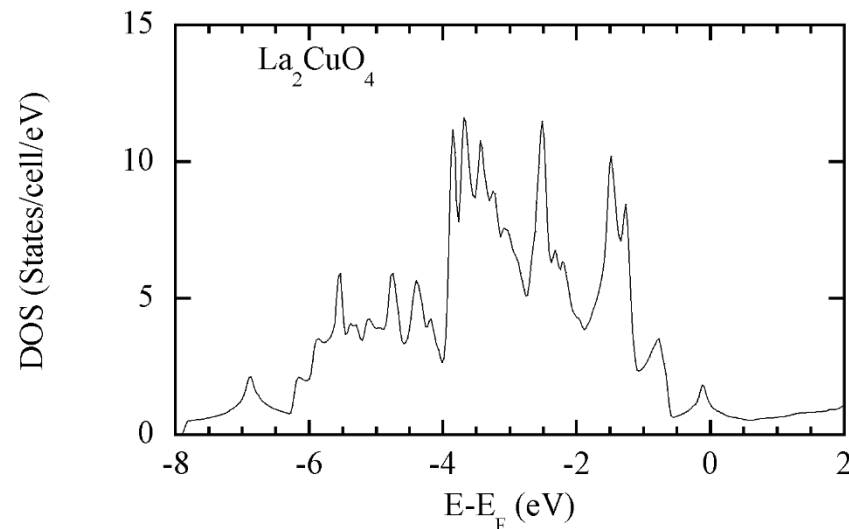


Fermi surface



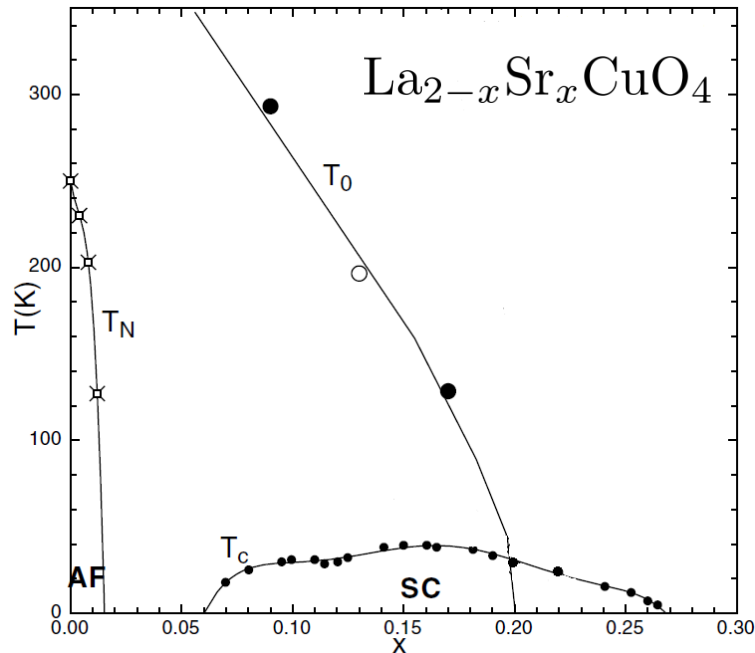
DFT-LDA predicts that
 La_2CuO_4 is half filled
i.e., 1 electron per unit cell

Fermi surface almost 2D
Weak c-axis dispersion



La₂CuO₄ Mott Physics

DFT-LDA is wrong !



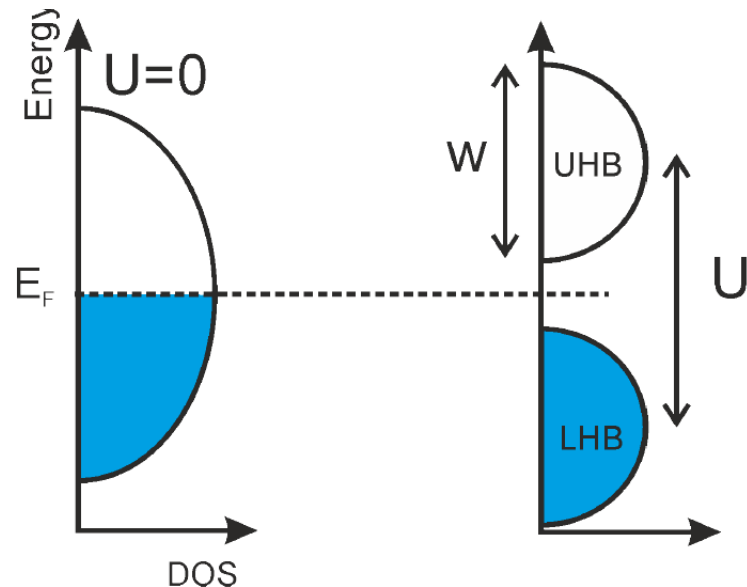
How does gap close ?
How much 'Mottness' remains in metallic state?

Undoped La_2CuO_4 is an antiferromagnetic insulator

Gap formed at the Fermi level because of electronic correlations (fluctuating U) not included in LDA band-structure

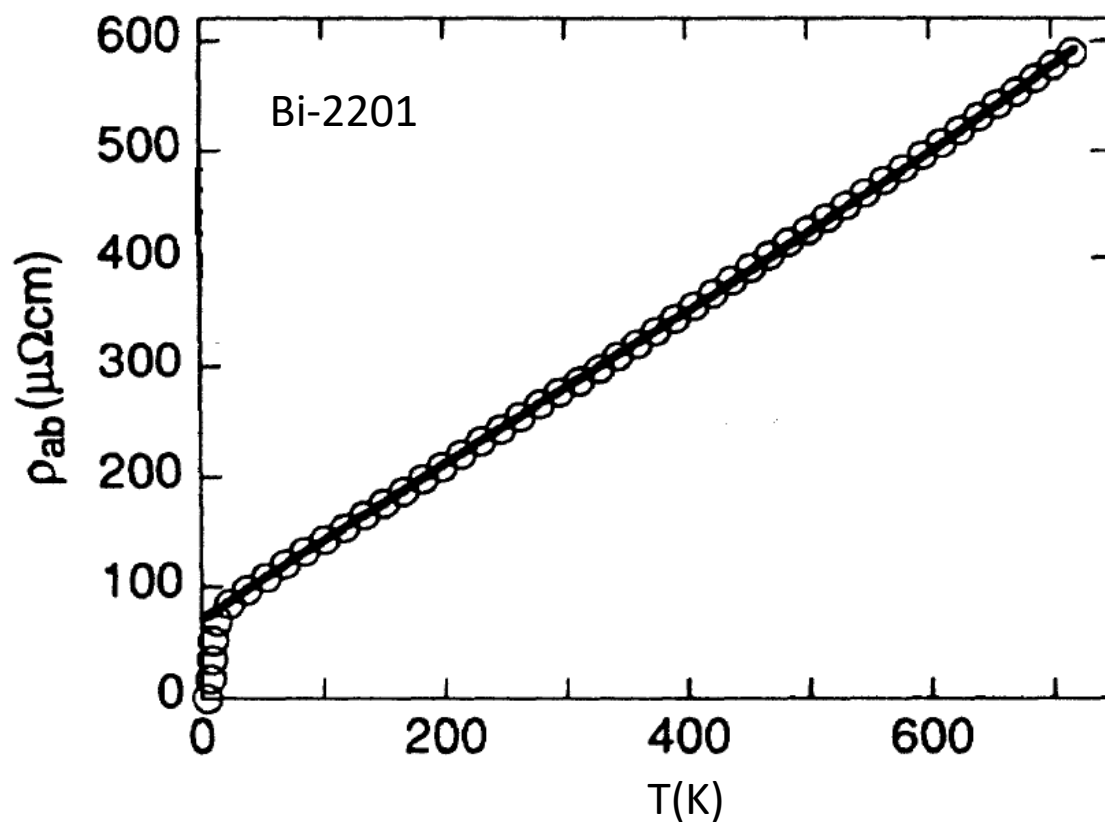
Hubbard Model

$$\mathcal{H} = - \sum_{i,j,\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Transport properties in the metallic state

Normal state properties: Linear resistivity



Resistivity linear with T
over an anomalously large
range of temperature

C.f. Simple metals where

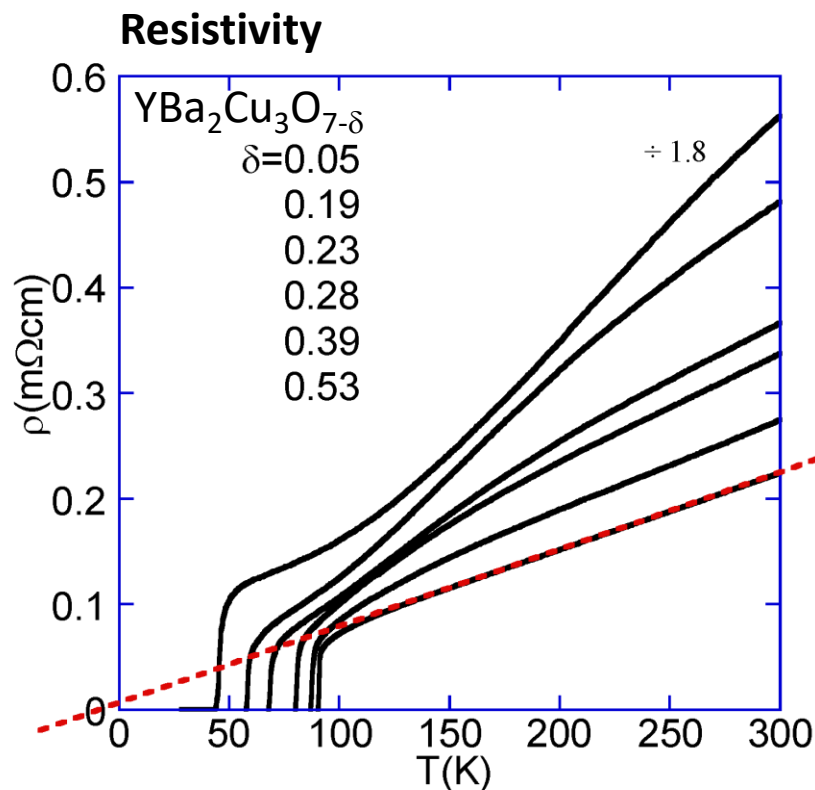
$$\rho \propto T \text{ for } T \gtrsim \theta_D/3$$

Suggests that mechanism of
scattering in cuprates has no
energy scale

S. Martin et al, Phys. Rev. B 41, 846 (1990).

Anomalous normal state : optimal and underdoped

A. Carrington et al. PRB 1993



Optimal doped

$$\rho \propto T$$

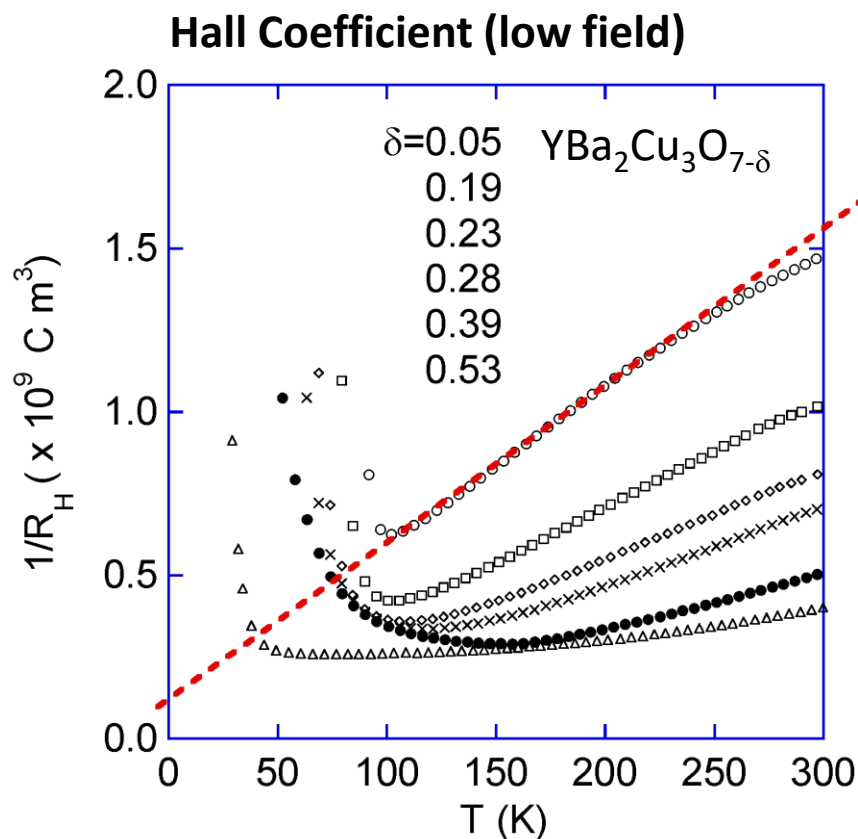
$$1/R_H \propto T$$

Underdoped

Downward curvature in $\rho(T)$

$\rho(T) \rightarrow T^2$ at low T

R_H less T dependent



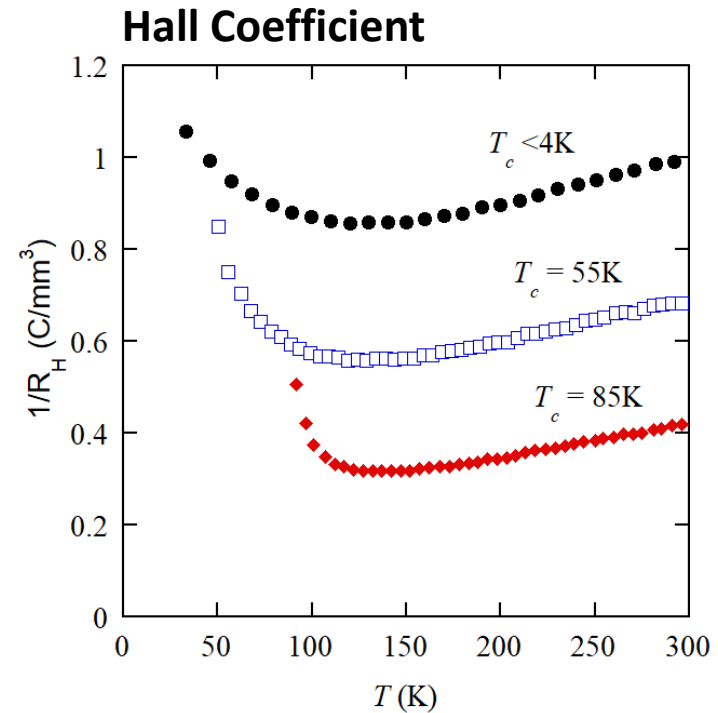
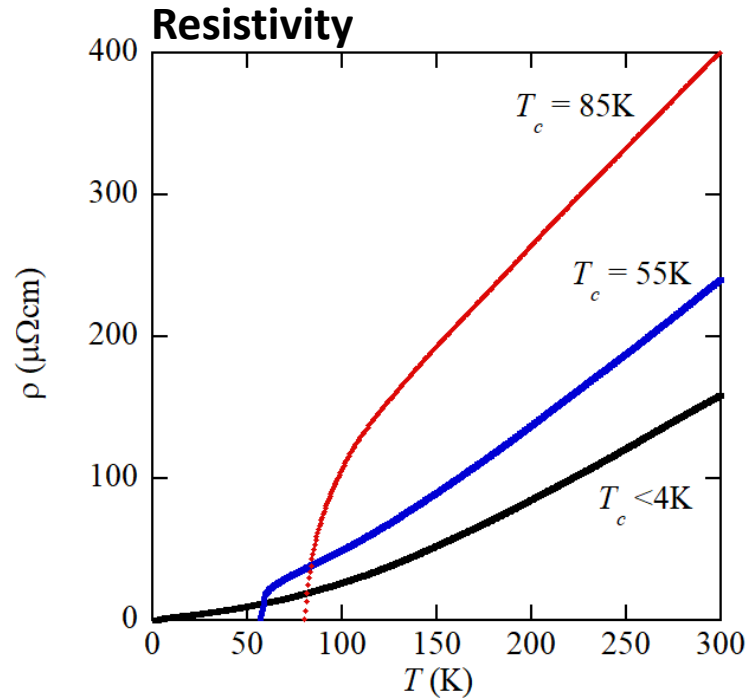
Simple metals

$$\rho \propto T \text{ for } T \gtrsim \theta_D/3$$

$$1/R_H = -ne$$

Anomalous normal state : Overdoped

A. Tyler, PhD Thesis, Univ. Cambridge 1997

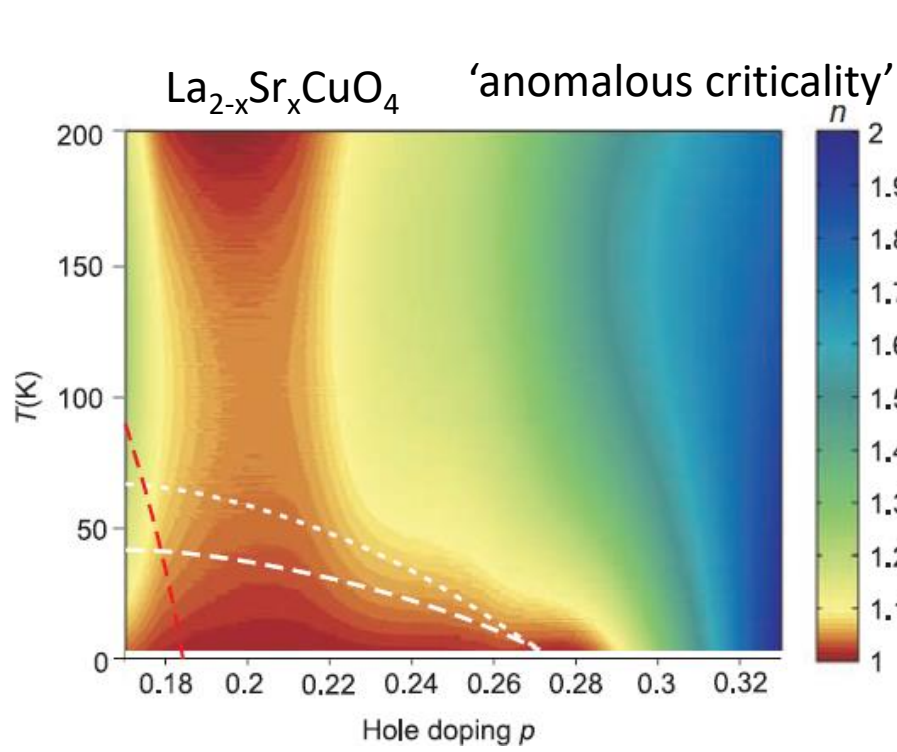


Overdoped

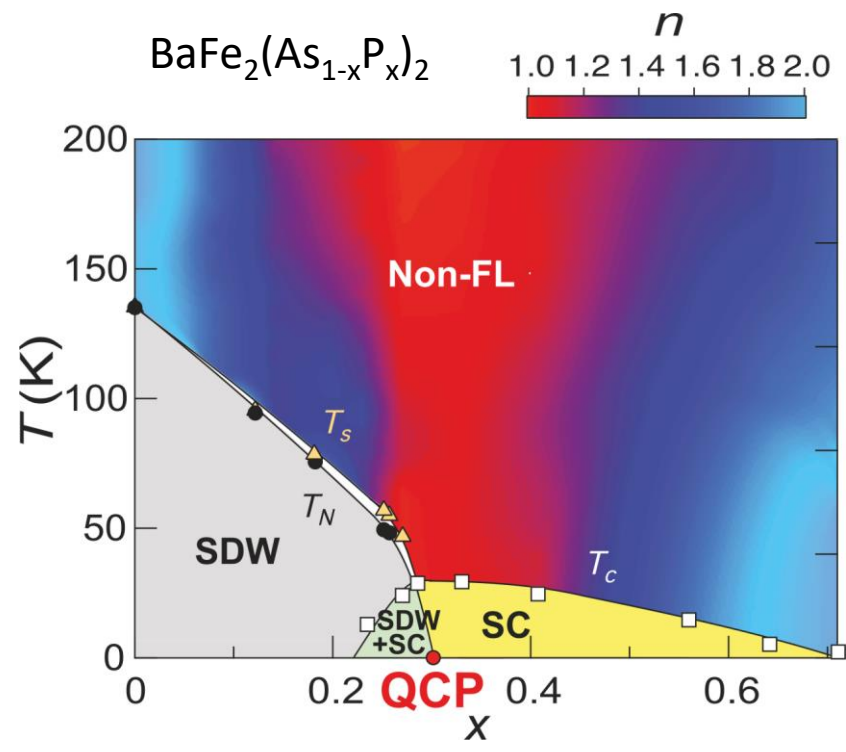
$$\rho(T) \rightarrow T^2$$

R_H less T dependent

Resistivity exponent



R. Cooper et al Science 2009



S. Kasahara et al., PRB (2010)

$$\rho(T) \sim T^\alpha$$

Linear Component in resistivity

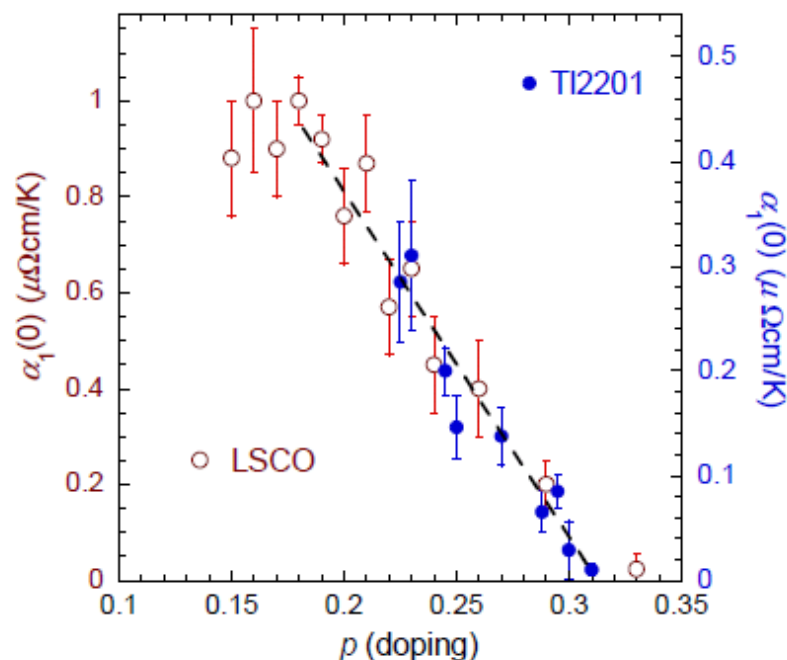
Two ways of viewing the same data

$$\rho(T) = \alpha T + \beta T^2 \quad \text{or} \quad \rho(T) \sim T^\alpha$$

Two different current carriers

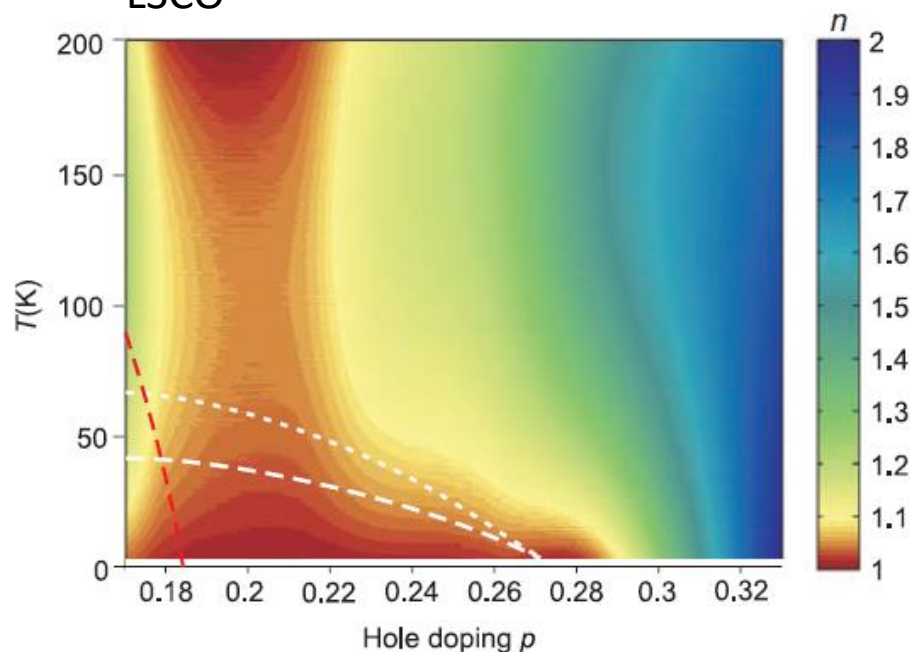
Anisotropic scattering

T linear component



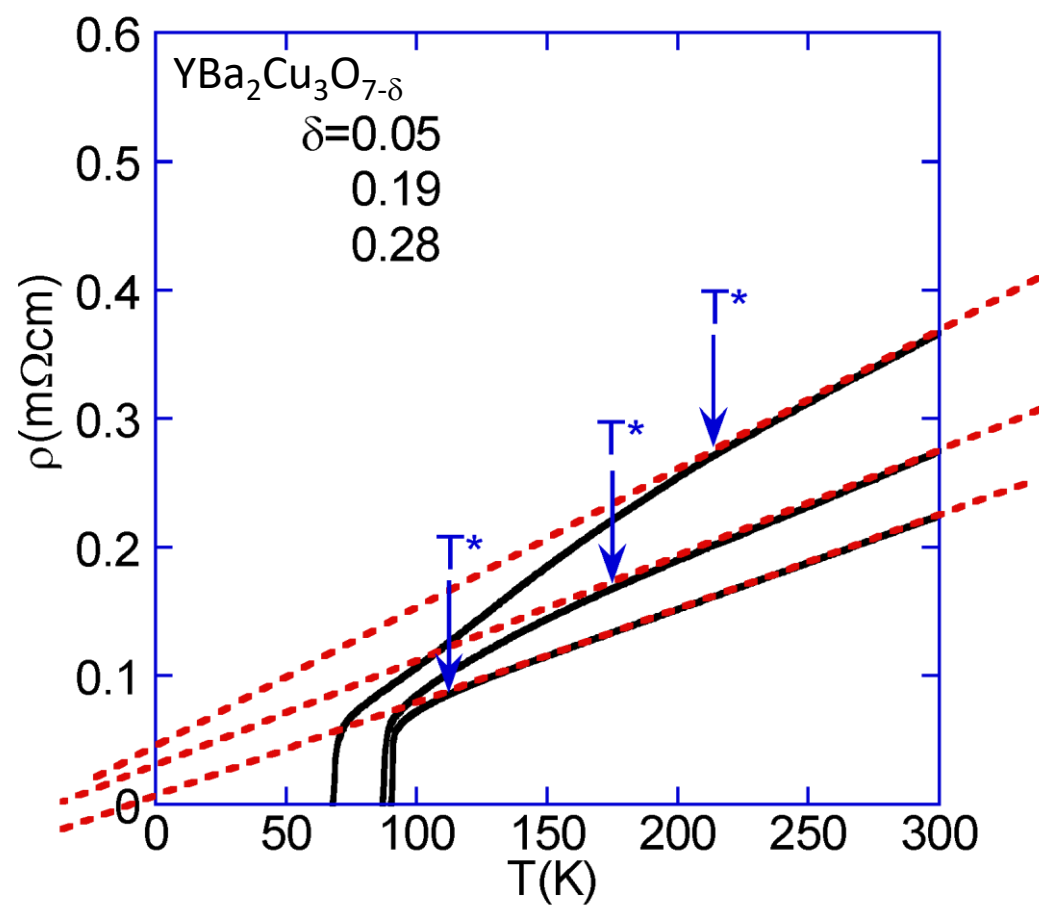
N. Hussey et al Journal of Physics:
Conference Series **449** (2013)

LSCO



R. Cooper et al Science 2009

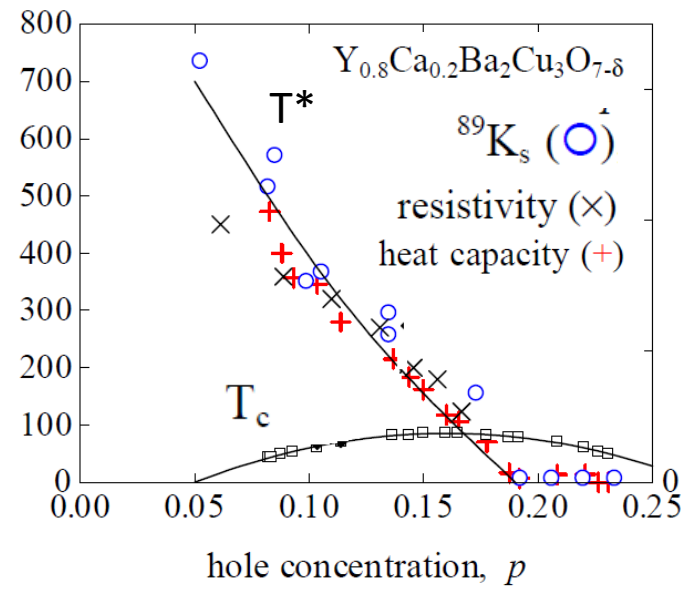
Pseudo-gap in resistivity data



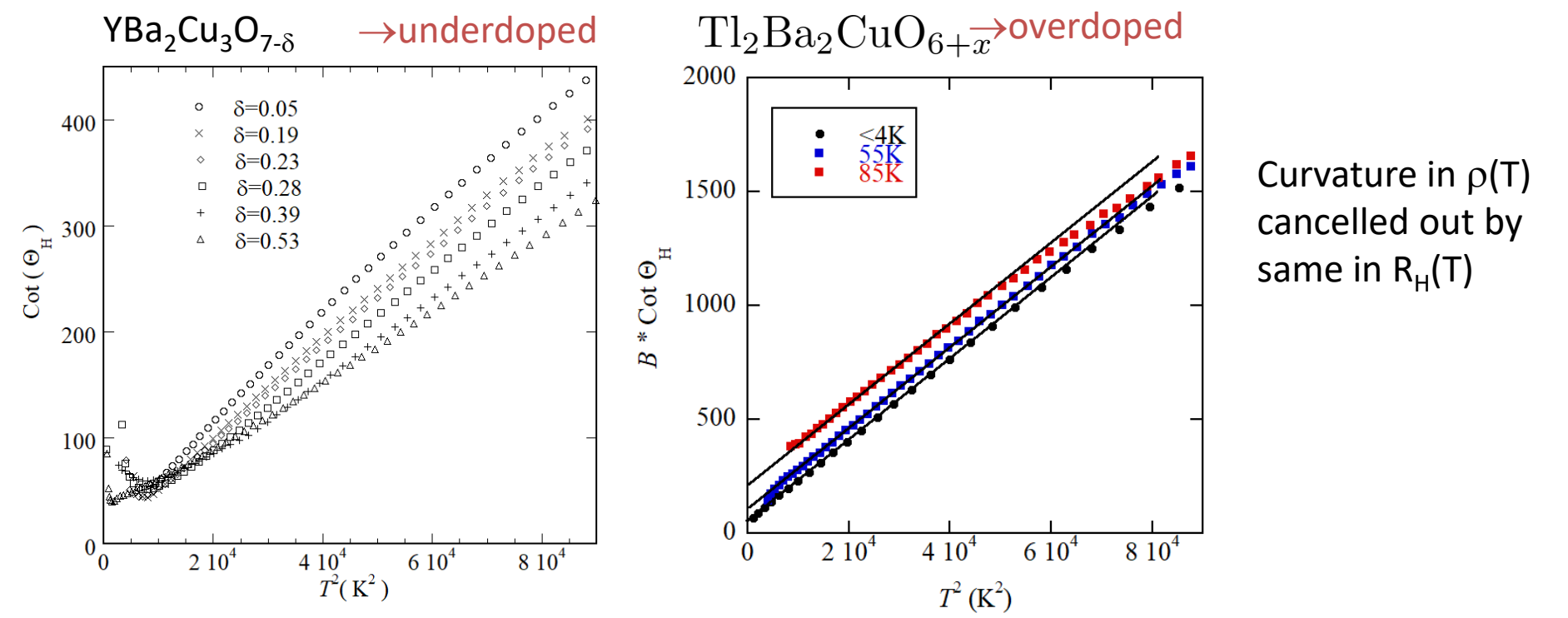
In some other cuprates ρ(T) increases at T*

Is the pseudogap T* a phase transition or energy scale ?
No specific heat anomaly..but abrupt change in torque anisotropy*
(*Sato et al. Nat.Phys 2017)

J. Loram and J Tallon
Physica C 349, 53 (2001)



Anomalous normal state : Hall Angle



$$\cot \theta_H = \frac{\rho_{xx}}{\rho_{xy}} = \frac{\rho_{xx}}{R_H B}$$

in Drude Theory ...

$$= \frac{n}{eB} \frac{m}{ne^2 \tau} = \frac{1}{\omega_c \tau}$$

$$\cot \theta_H \sim T^2$$
over most of phase diagram

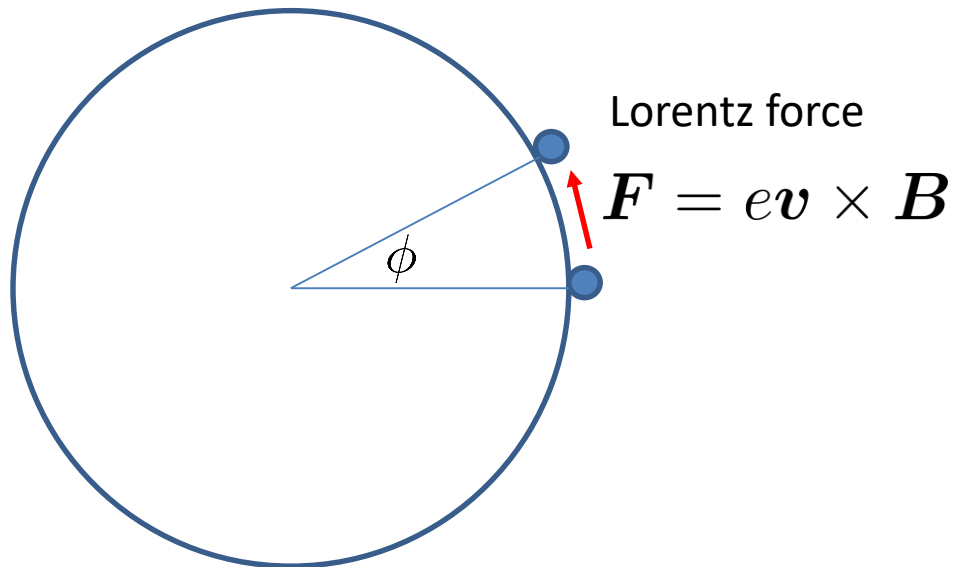
Implies a ‘Hall’ scattering rate τ_H^{-1} , which is distinct from that for longitudinal scattering from $\rho(T)$

Chien, Wang, Ong et al PRL 1991

Boltzmann Transport theory : Hall coefficient

Shockley-Chambers tube integral formula (in 2D)

$$\sigma_{xy} = \frac{e^3 B}{2\pi^2 \hbar^2 c \omega_c^2} \int_0^{2\pi} \int_0^\infty v_x(\phi) v_y(\phi - \phi') e^{-\frac{\phi'}{\omega_c \tau}} d\phi' d\phi$$



Boltzmann Transport theory : Hall coefficient (in 2D)

Hall conductivity

$$\sigma_{xy} = \frac{e^3 B}{2\pi^2 \hbar^2 c \omega_c^2} \int_0^{2\pi} \int_0^\infty v_x(\phi) v_y(\phi - \phi') e^{-\frac{\phi'}{\omega_c \tau}} d\phi' d\phi$$

Longitudinal Conductivity

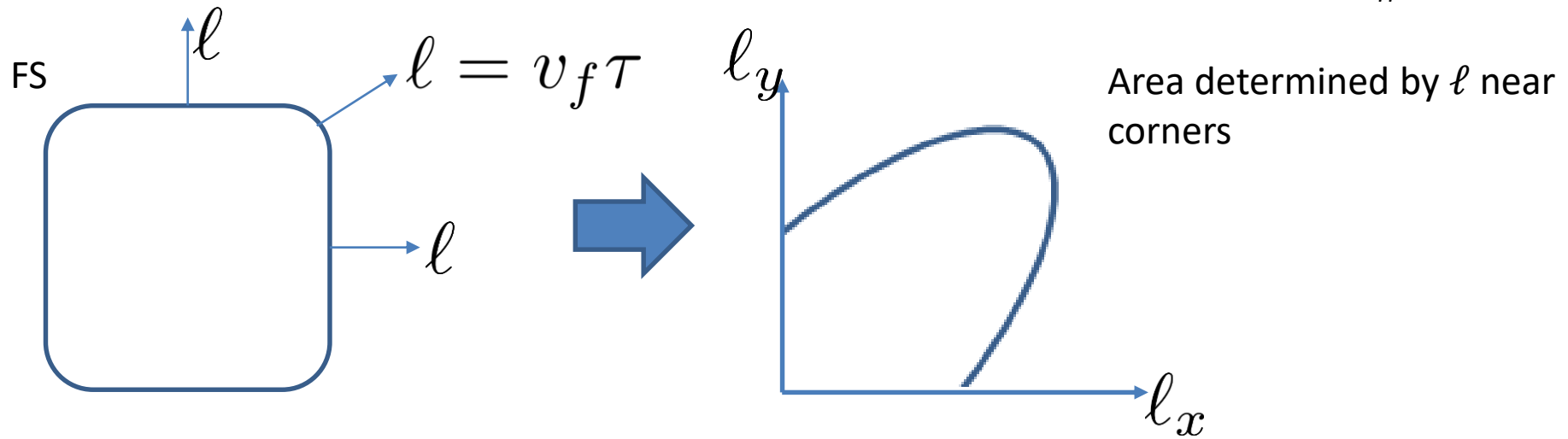
$$\sigma_{xx} = \frac{e^3 B}{2\pi^2 \hbar^2 c \omega_c^2} \int_0^{2\pi} \int_0^\infty v_x(\phi) v_x(\phi - \phi') e^{-\frac{\phi'}{\omega_c \tau}} d\phi' d\phi$$

$$R_H B = \rho_{xy} = \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

$$\rho_{xx} = \frac{\sigma_{xx}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

Hall coefficient: weak field

Geometrical construction (*N.P Ong PRB 1991*) Weak field = first order terms only (R_H linear in B)



Area enclosed by mean-free-path ℓ vector as move around FS determines Hall cond.

$$\sigma_{xy} = 2 \frac{e^2}{h} \frac{B A_\ell}{\phi_0}$$

$$\sigma_{xx} = \frac{e^2}{2\pi h} S \ell_{av}$$

$$R_H B = \rho_{xy} = \frac{\sigma_{xy}}{\sigma_{xx}^2 + \sigma_{xy}^2}$$

Spherical Fermi surface, isotropic scattering:

$$R_H = \frac{1}{ne}$$

Models of separation of transport lifetimes

$$\tau_{\rho}^{-1} \sim T \qquad \tau_H^{-1} \sim T^2$$

Spin-charge separation (Holons and spinons) P.W. Anderson 1991

Quantum-critical metal:

Holographic metal (dissipative and charge-conjugation symmetric currents)
(Blake & Donos, PRL 2015)

Anisotropic scattering (conventional Fermi surface, but unconventional scattering):

Curve parts of FS dominate Hall response

(J.R. Cooper PRL 1992, Stojkovic and Pines PRB 1997)

Weak field : Two bands

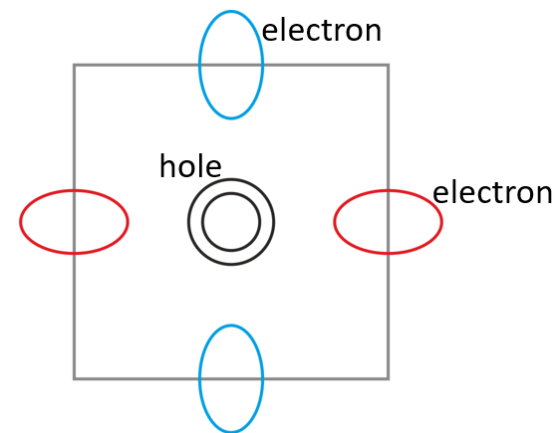
Add the conductivities for each band, assume very weak field (ρ and R_H indep. of H)

$$\begin{aligned}\sigma_{xy} &= \sigma_{xy}^1 + \sigma_{xy}^2 \\ \sigma_{xx} &= \sigma_{xx}^1 + \sigma_{xx}^2\end{aligned}\quad \underline{\sigma} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{pmatrix}^{-1}$$

e.g., iron-based supercond.

$$R_H = \frac{R_1 \rho_2^2 + R_2 \rho_1^2 + R_1 R_2 (R_1 + R_2) B^2}{(\rho_1 + \rho_2)^2 + (R_1 + R_2)^2 B^2}$$

$$\rho = \frac{\rho_1 \rho_2 (\rho_1 + \rho_2) + (\rho_1 R_2^2 + \rho_2 R_1^2) B^2}{(\rho_1 + \rho_2)^2 + (R_1 + R_2)^2 B^2}$$

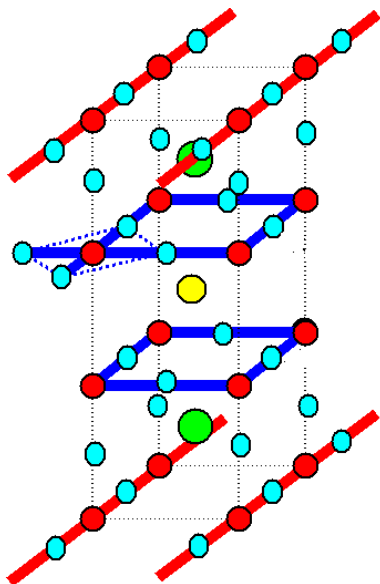


Now ρ and R_H have a field dependence even if ρ and R_H in each band do not

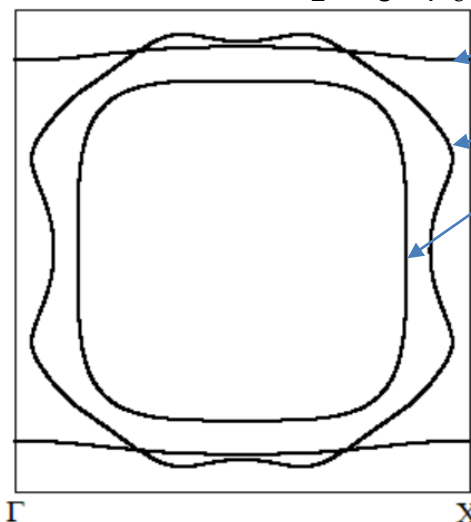
Now a new 'weak field' regime is where B^2 term in R_H is small

Note this is a different 'weak-field' regime from that where $\omega_c \tau \gg 0$

Two bands in Cuprates: Chains and planes in YBCO

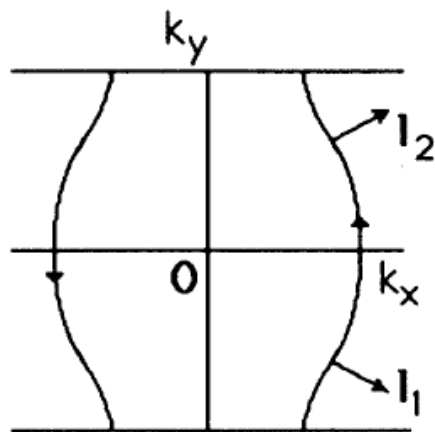


Fermi surface $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$

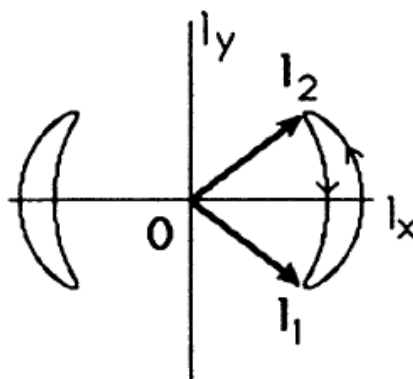


$\sim 1\text{D}$ CuO chain

2D CuO planes



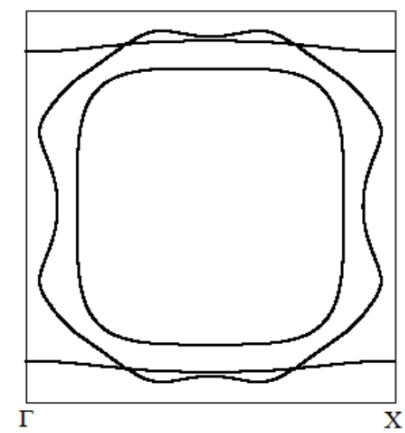
Fermi Surface



l curve

Quasi 1D Fermi surface
For isotropic ℓ , $\sigma_{xy} = 0$

Chains and planes : add conductivities

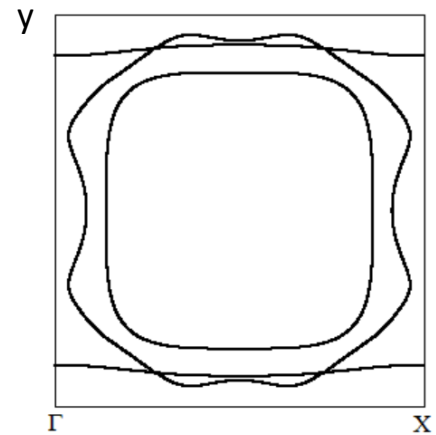


$$\sigma_{xy} = \sigma_{xy}^c + \sigma_{xy}^p$$

$$\sigma_{xx} = \sigma_{xx}^p + \sigma_{xx}^c$$

$$\sigma_{yy} = \sigma_{yy}^p + \sigma_{yy}^c$$

Chains and planes



$$\sigma_{xy} = \cancel{\sigma_{xy}^c} + \sigma_{xy}^p$$

$$\sigma_{xx} = \sigma_{xx}^p + \cancel{\sigma_{xx}^c}$$

$$\sigma_{yy} = \sigma_{yy}^p + \sigma_{yy}^c$$

$$R_H B = \rho_{xy} = \frac{\sigma_{xy}}{\sigma_{xx}\sigma_{yy} + \sigma_{xy}^2}$$

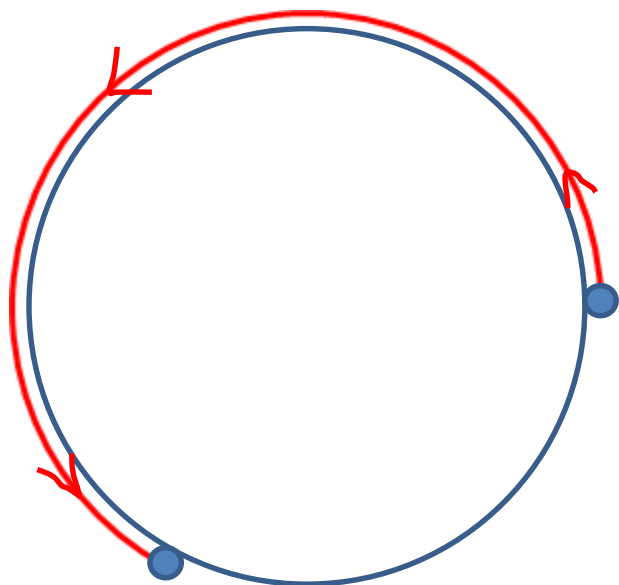
For overdoped YBCO

$$R_H = R_H^p \frac{\rho_b}{\rho_a} \simeq 1.5 R_H^p$$

Hall coefficient : high field

Shockley-Chambers tube integral formula (in 2D)

$$\sigma_{xy} = \frac{e^3 B}{2\pi^2 \hbar^2 c \omega_c^2} \int_0^{2\pi} \int_0^\infty v_x(\phi) v_y(\phi - \phi') e^{-\frac{\phi'}{\omega_c \tau}} d\phi' d\phi$$



High field limit

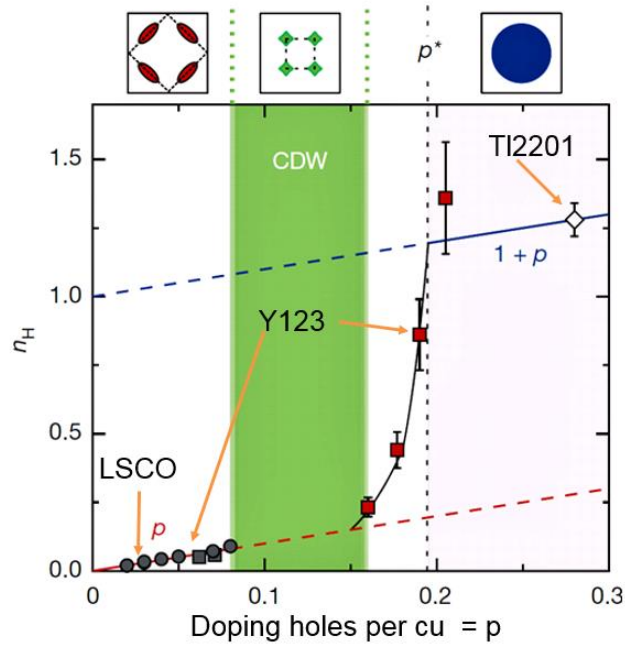
$$\omega_c \tau \gg 1$$

$$R_H \rightarrow \frac{1}{ne}$$

Recover simple connection between Hall coefficient and Fermi volume in high field limit (single band) for systems with anisotropic scattering or Fermi velocity

High field Hall effect in YBCO: Is pseudogap a Fermi surface shape effect?

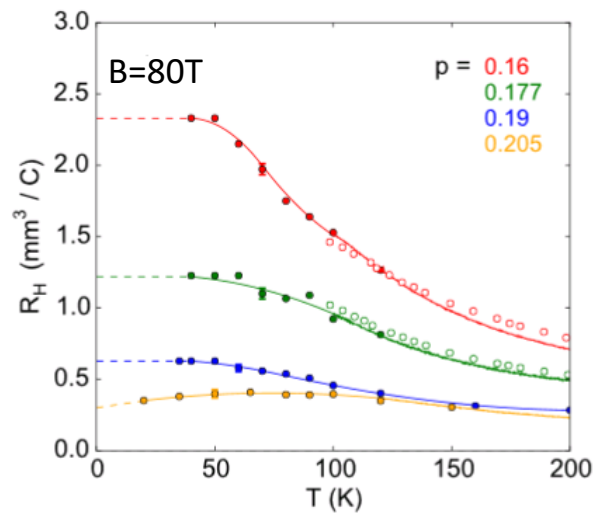
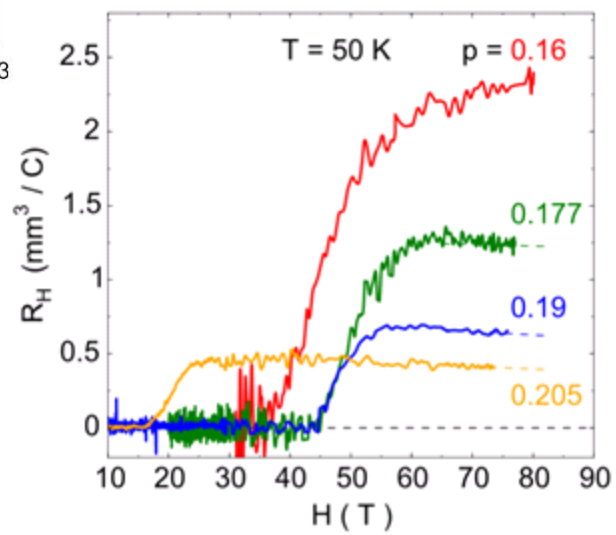
‘Abrupt’ change in high field, low T, n_H at point where pseudogap starts



S. Badoux *et al* Nature 2016

Questions

- 1) How do chains influence n_H
- 2) Is high field, low T limit reached ?
- 3) **What happens in far overdoped regime?**

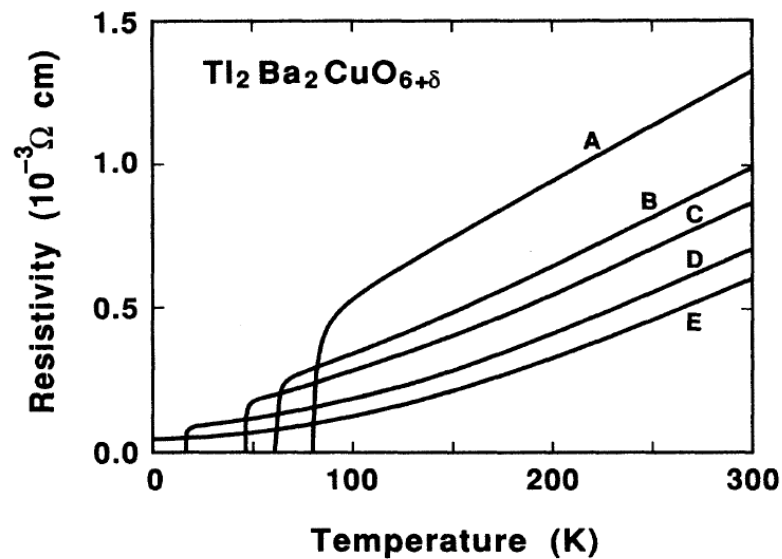


Transport properties in the overdoped regime



$\text{Ti}_2\text{Ba}_2\text{CuO}_{6+x}$: access overdoped regime

Single Cu layer (no chains)
Electronically clean (cf: LSCO, Nd-LSCO)
Single band, no Lifshitz transitions

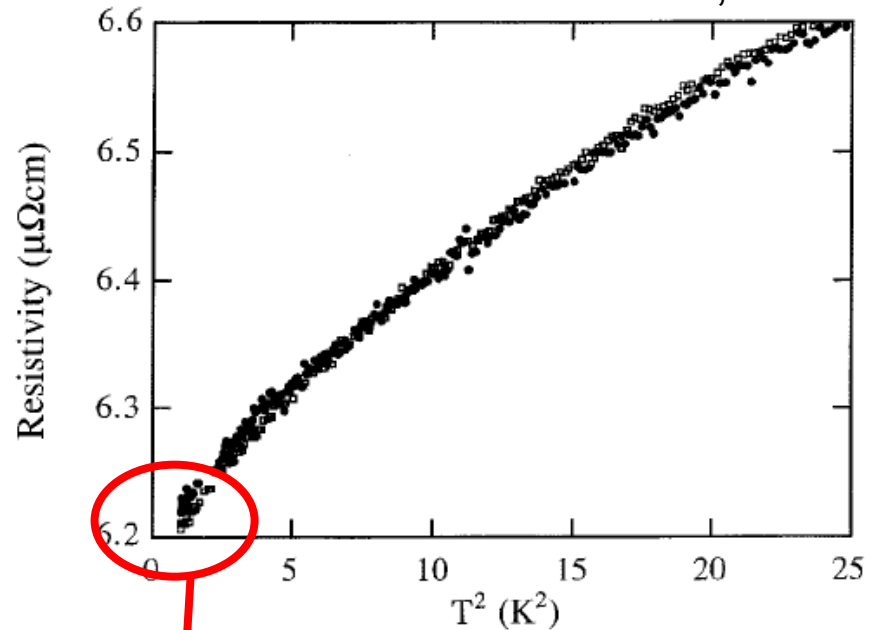


Kubo et al., PRB 1991

Superficially evolution from $\rho \sim T$ to $\rho \sim T^2$?

Ti-2201 , $T_c = 11\text{K}$

A.P.Mackenzie et al, PRB 1996

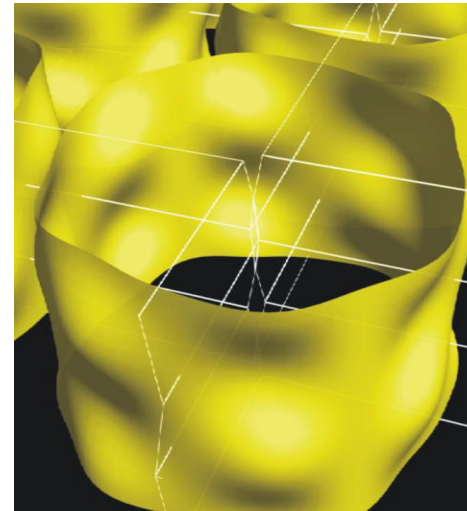
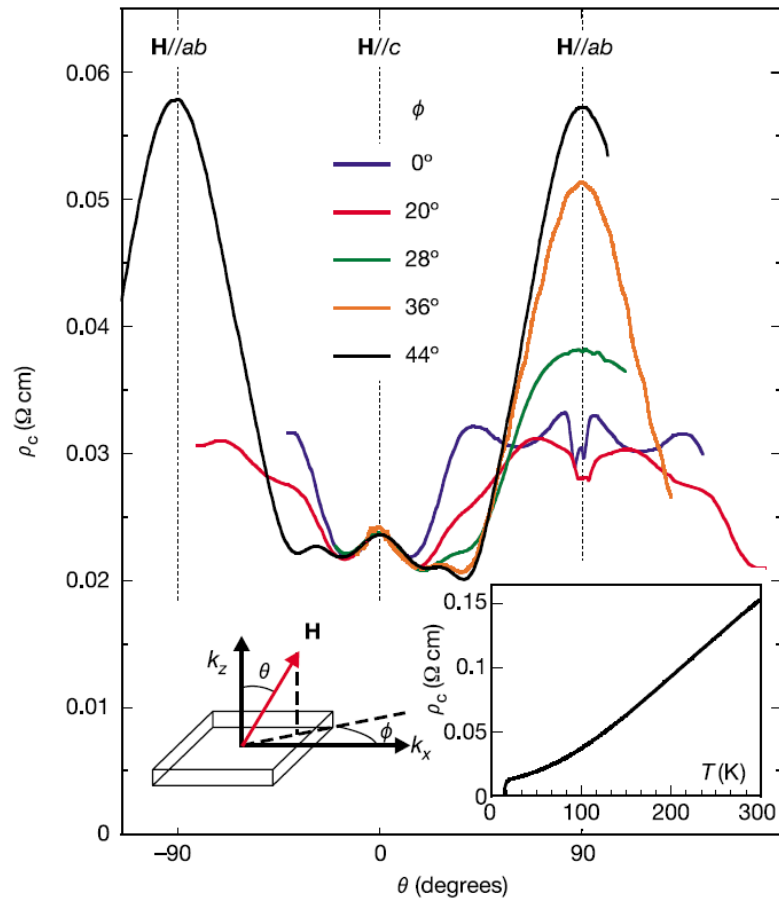


Very low residual resistance, mfp $\sim 1000 \text{ \AA}$

Far overdoped $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+x}$: what we know

Angular Dependence Magnetoresistance *N.Hussey et al, Nature 2003*

$T_c = 20\text{K}$



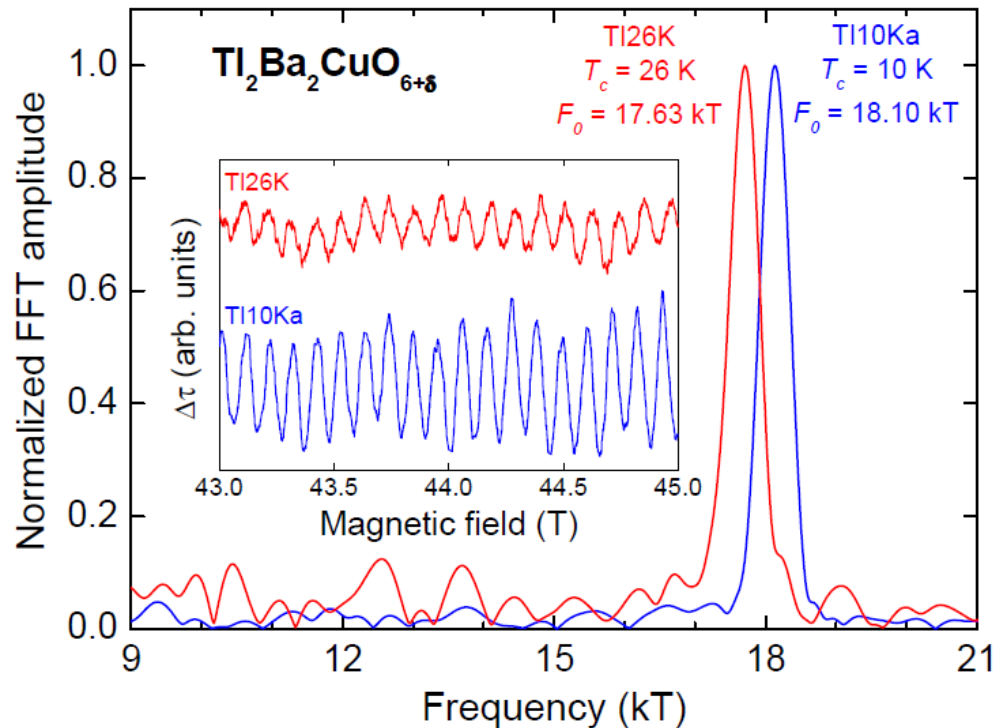
Semiclassically coherent Fermi surface

Highly 2D

Fermi surface shape close to DFT calculations

Far overdoped $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+x}$: what we know

Quantum Oscillations



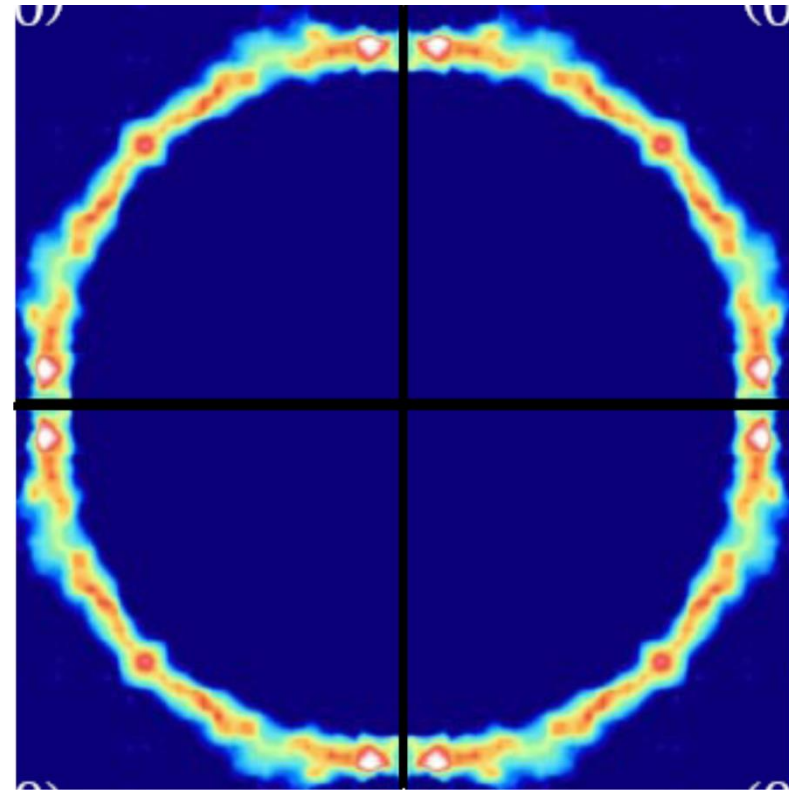
B. Vignolle, N Hussey, AC et al, Nature (2008)

A. Bangura, N Hussey, AC et al, PRB (2010)

P. Rourke, N Hussey, AC et al, NJP (2010)

ARPES

$T_c = 30 \text{ K}$, $p = 0.26 \pm 0.04$

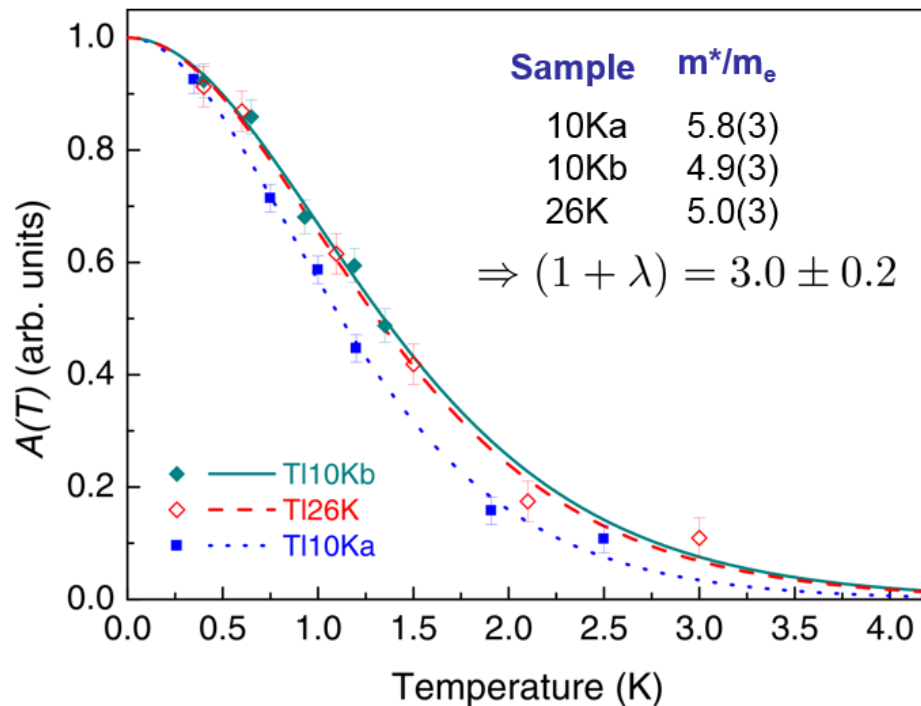


M. Platé et al, PRL (2005)

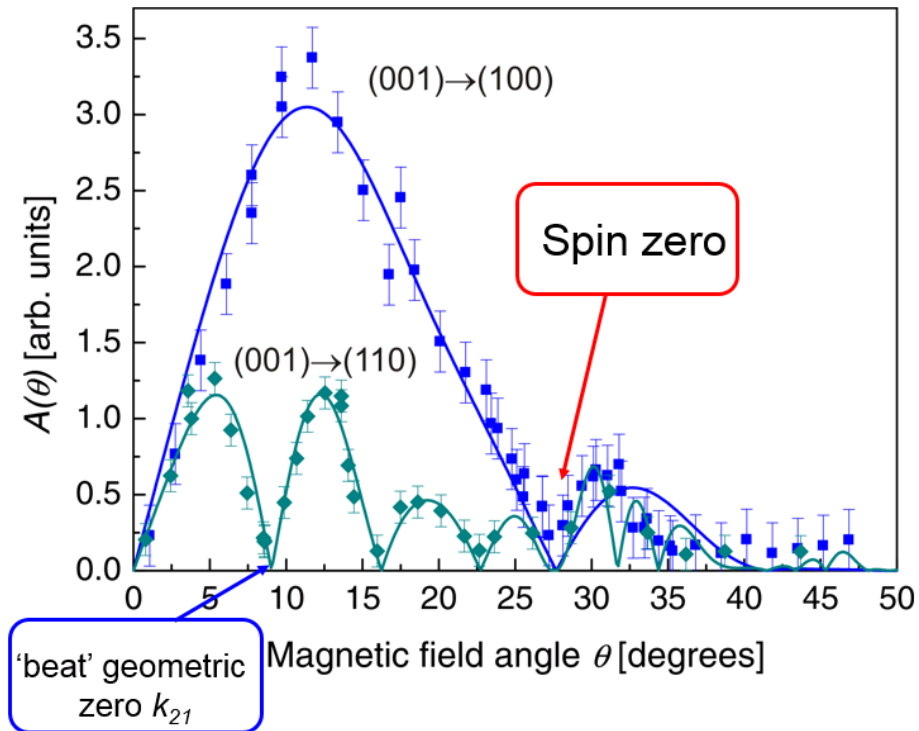
No observation of QO for $T_c > 26 \text{ K}$ (even after trying very hard!)

$\text{Ti}_2\text{Ba}_2\text{CuO}_{6+x}$: Fermi surface details

Tl2201: Effective mass determination



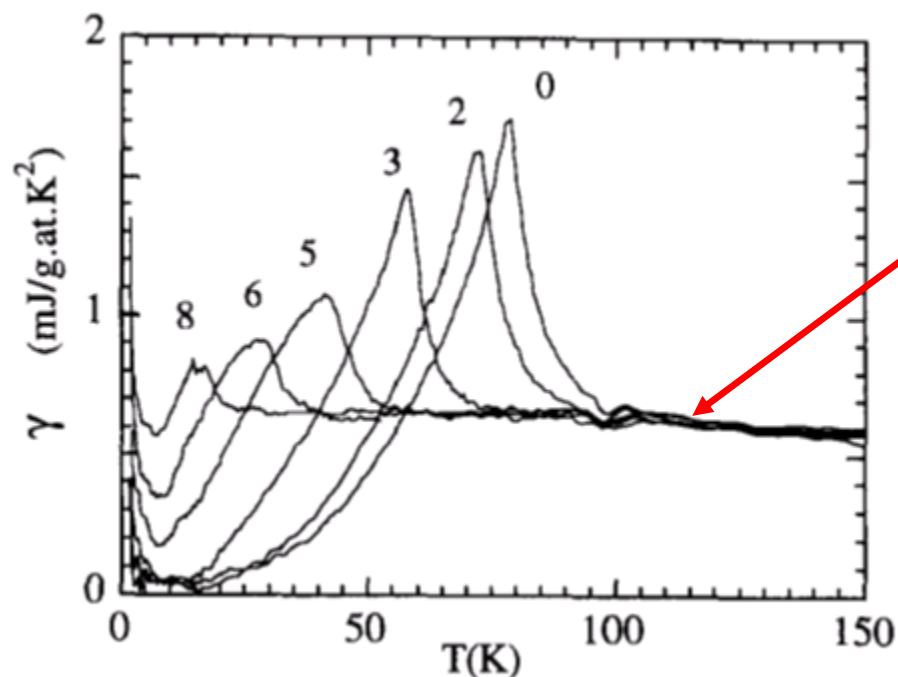
Tl-2201: dHvA Amplitude vs Field angle



Quite strong mass renormalisation, factor 3

Shape of FS determined from field angle dependence of quantum oscillation amplitude, not frequency, because of extreme 2D Fermi surface

Tl2201: Electronic Heat Capacity



John Loram et al., Physica C 1994

γ constant with doping

Specific heat anomalies conserve entropy
So NO pseduogap

Reduction of superconducting anomaly
height from pair breaking (disorder) when T_c
is low

$$\gamma(T_c^+) = 7 \pm 1 \text{ mJ/molK}^2$$

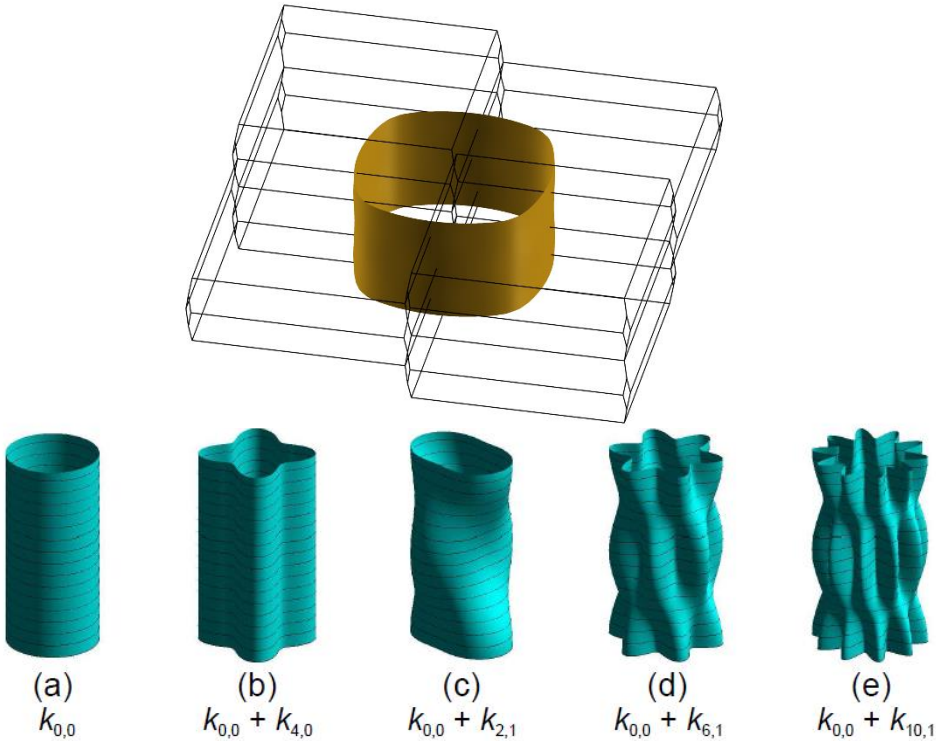
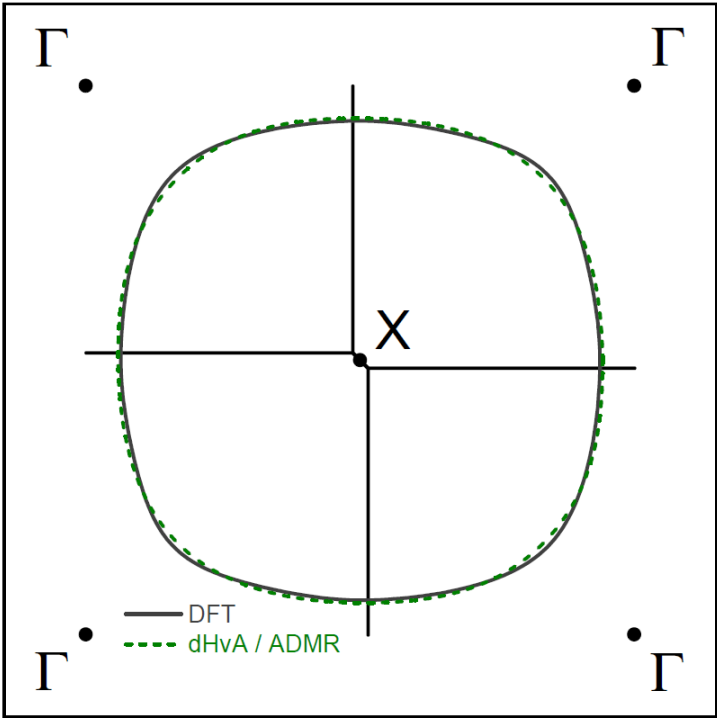
Cf: dHvA mass $m^* = 5.2 \pm 0.4 m_e$

$$\gamma_{\text{dHvA}} = 7.6 \pm 0.6 \text{ mJ/mol/K}^2$$

Measure electronic
specific heat in good
agreement with QO mass
So....

No missing FS sheets
Mass field independent

Compare measured Fermi surface to DFT



	$k_{0,0} \text{ (\AA}^{-1}\text{)}$	$\frac{k_{4,0}}{k_{0,0}}$	$\frac{k_{8,0}}{k_{0,0}}$	$\frac{k_{12,0}}{k_{0,0}}$	$\frac{k_{16,0}}{k_{0,0}}$	$k_{2,1} \text{ (\AA}^{-1}\text{)}$	$\frac{k_{6,1}}{k_{2,1}}$	$\frac{k_{10,1}}{k_{2,1}}$
DFT	0.7390	-0.047	0.0088	-0.00135	0.000436	-0.00287	0.50	-0.34
Exp	0.7416	-0.032	—	—	—	-0.00170	0.71	-0.25

dHvA

ADMR

dHvA

ADMR

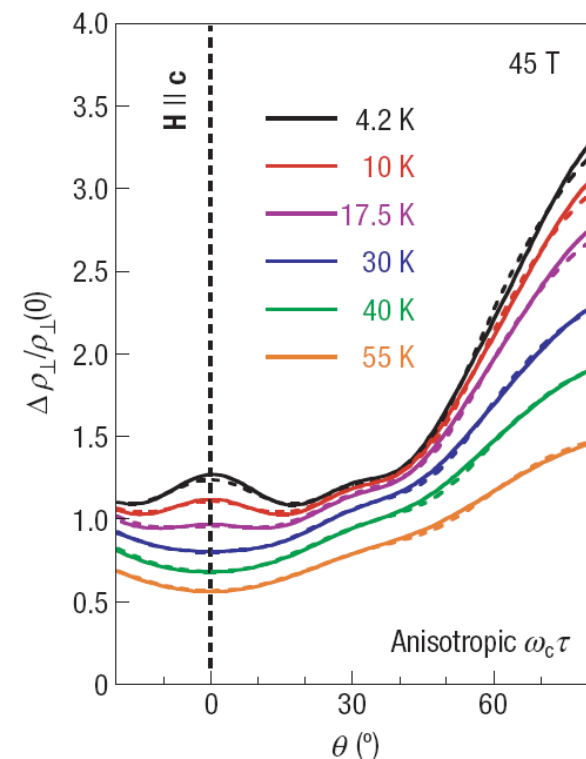
ADMR

$$\frac{k_{0,0}}{k_{2,1}} = 436$$

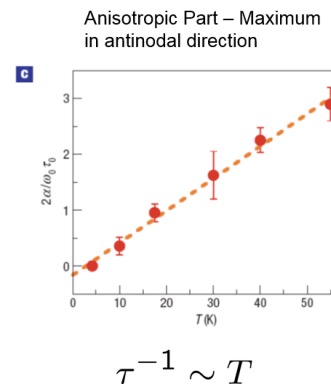
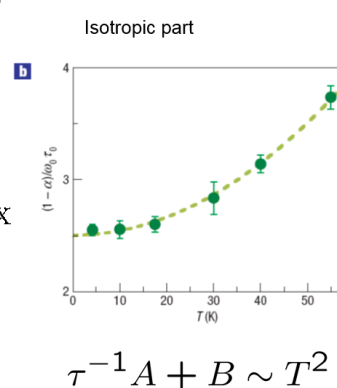
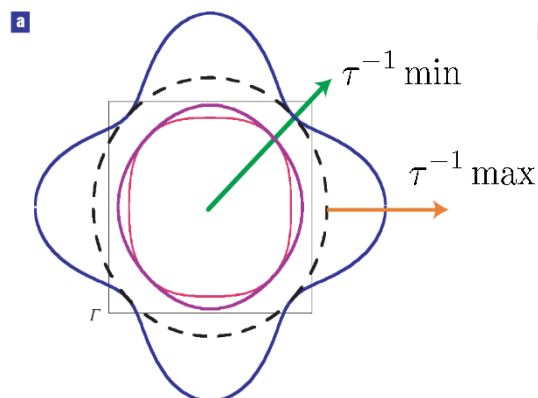
Details of Fermi surface warping agree well with DFT

TI2201: AMDR: Scattering rate

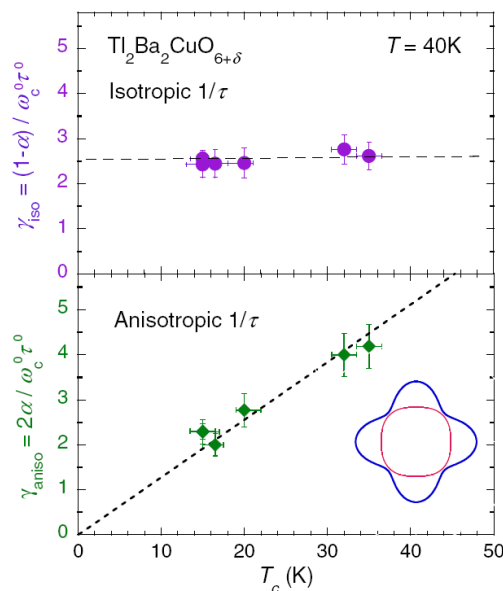
Temperature dependence of AMDR *M. Abdel-Jawad et al, Nature Physics 2006*



Scattering rate is anisotropic



M. Abdel-Jawad et al, PRL 2007



Isotropic T^2 term does not change with T_c

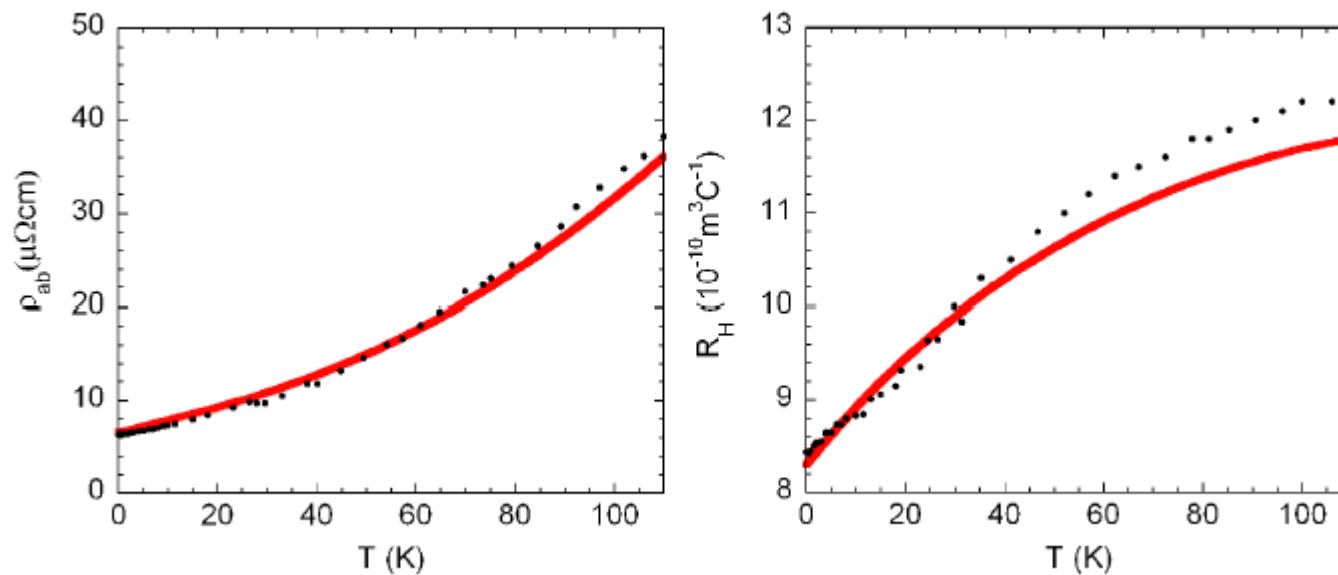
Anisotropic T term scales with T_c

But cannot fit data for $T_c > 45 K$ with same model

Low field Hall effect+ simulation: Tl2201

M. Abdel-Jawad et al, Nature Physics 2006

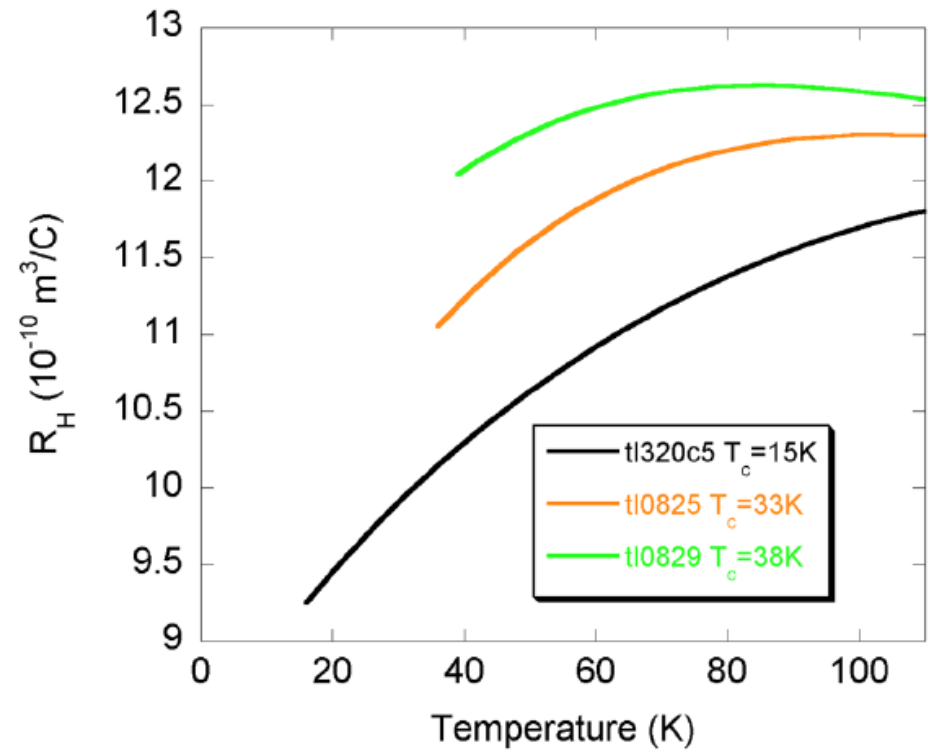
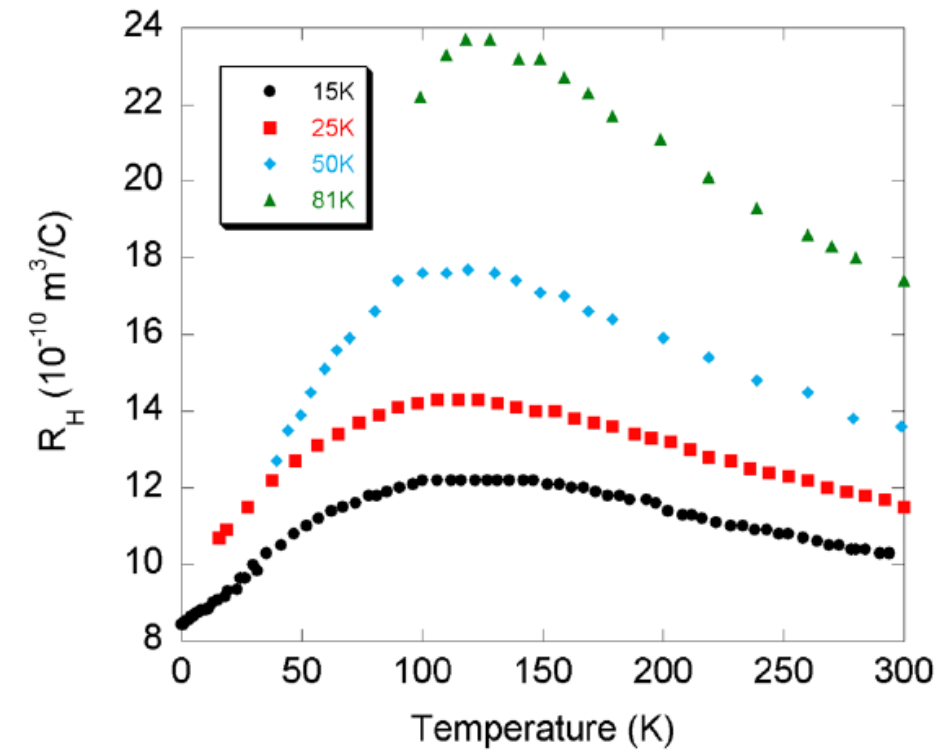
Low field limit, Tl-2201 parameter and data : $T_c=15$ K



Works well for most overdoped samples

Low field Hall effect+ simulation: Tl2201

M. French : PhD Thesis 2009



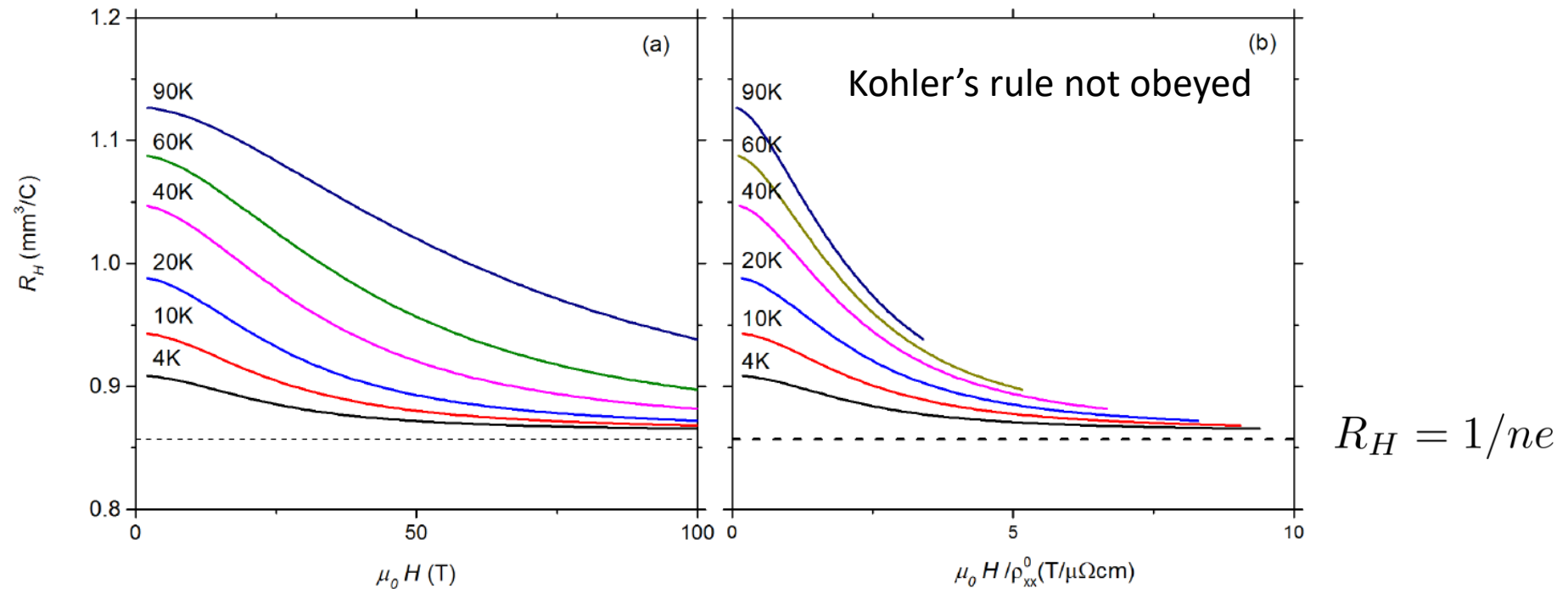
Experimental T dependence is far stronger than theory for higher T_c samples

High field R_H for Tl-2201 : Calculation

Shockley-Chambers formula to simulate within Boltzmann theory at arbitrary H

Parameters: measured anisotropy of scattering rate + Fermi surface geometry for Tl-2201

Parameters for Tl-2201 : $T_c=20\text{K}$

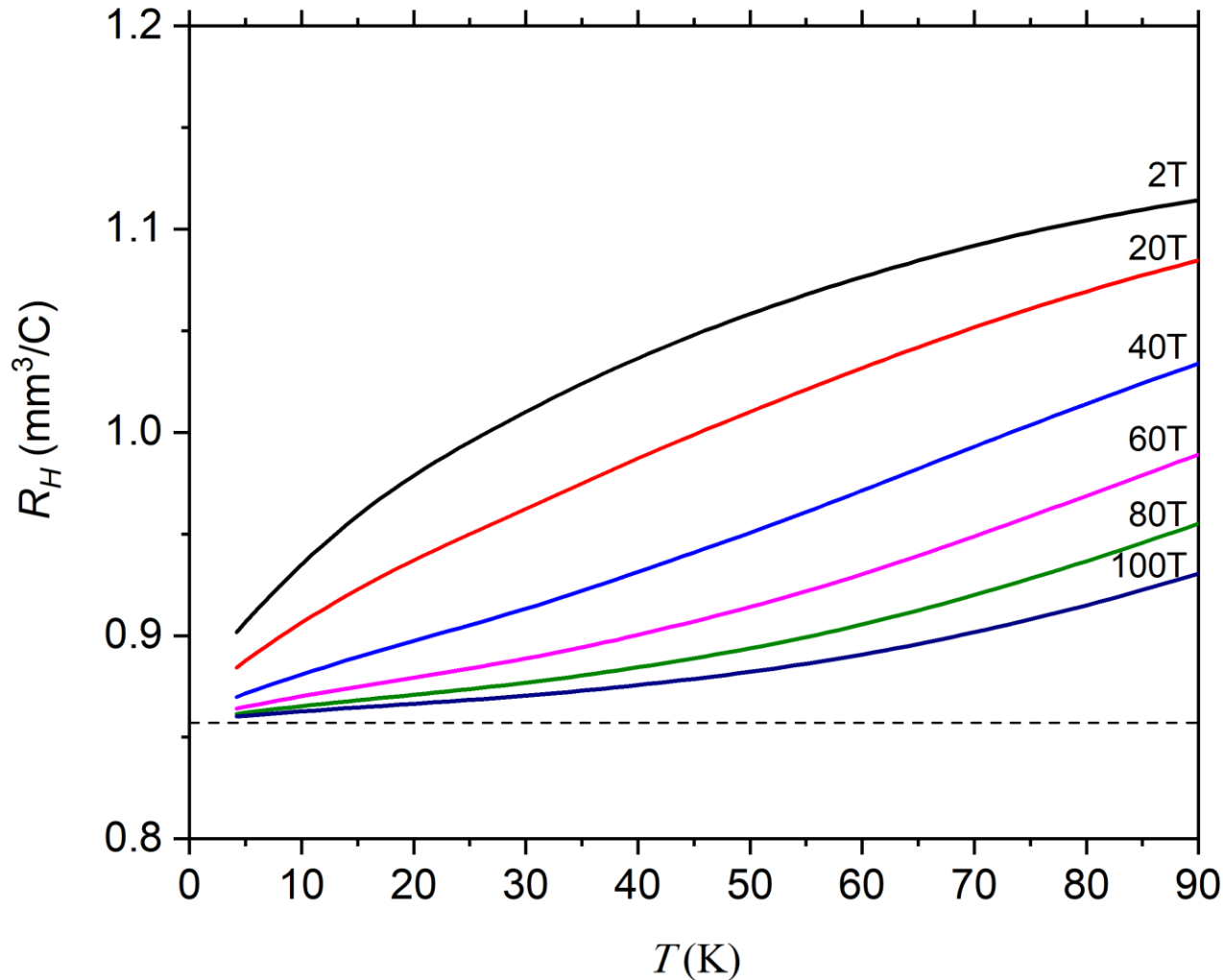


R_H tends to $1/ne$ at low T (isotropic scattering) or high B ($\omega_c \tau \gg 1$)

C. Putzke et al arXiv:1909.08102

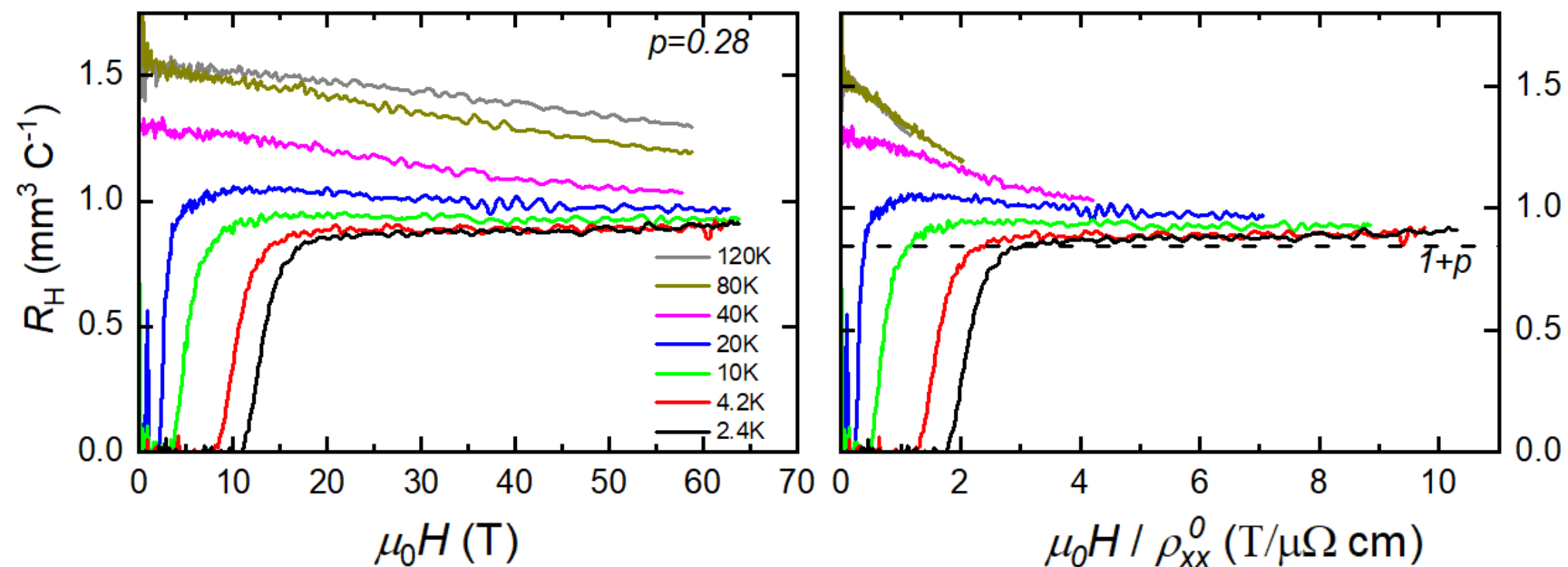
Simulate field dependence of R_H for Tl-2201

T dependence at fixed field



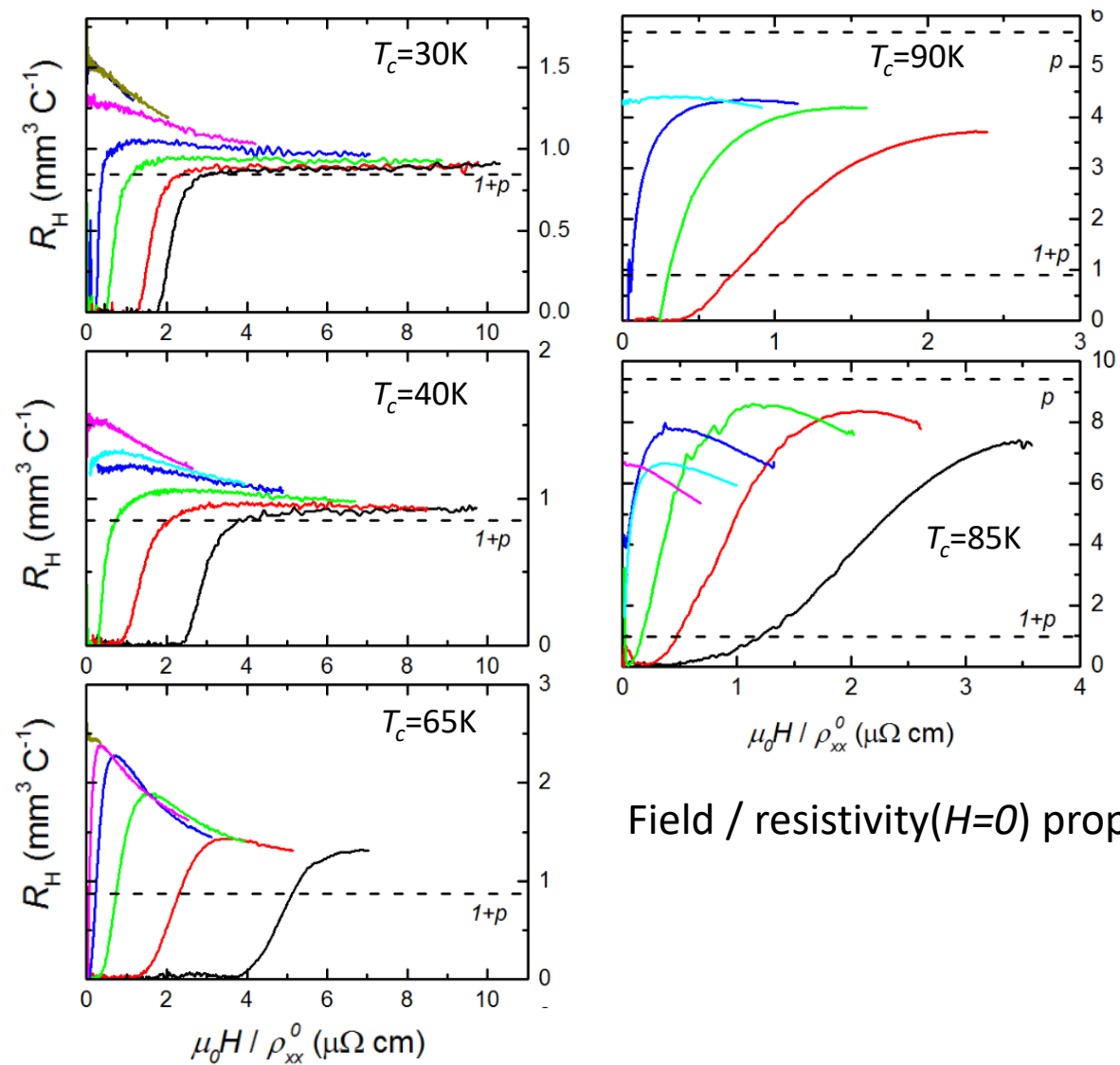
High field suppresses
T dependence

High field Hall coefficient in Tl2201



C. Putzke et al arXiv:1909.08102

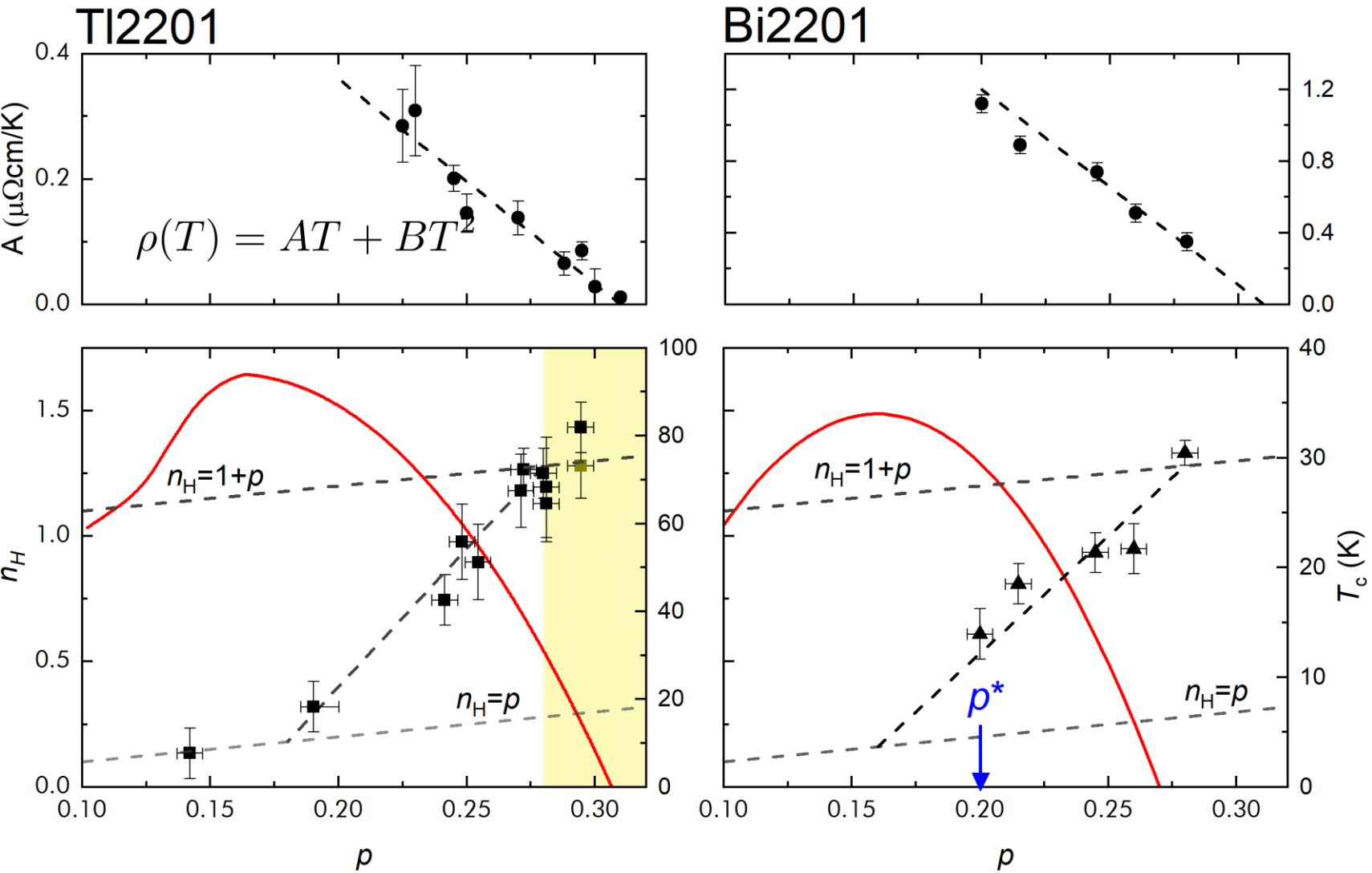
Hall data with scaled x-axis



Field / resistivity($H=0$) proportional to $\omega_c \tau$

C. Putzke et al arXiv:1909.08102

Evolution of n_H in overdoped regime



C. Putzke et al arXiv:1909.08102

Interpretation

Pseudogap hidden below T_c with critical point in far OD regime

✗ no rise of R_H below T_c ($H=0$)

Anisotropic scattering at $T=0$

✗ High field should quench this effect

Density wave, causing reconstruction of FS, for $T_c > 40\text{K}$ in overdoped regime

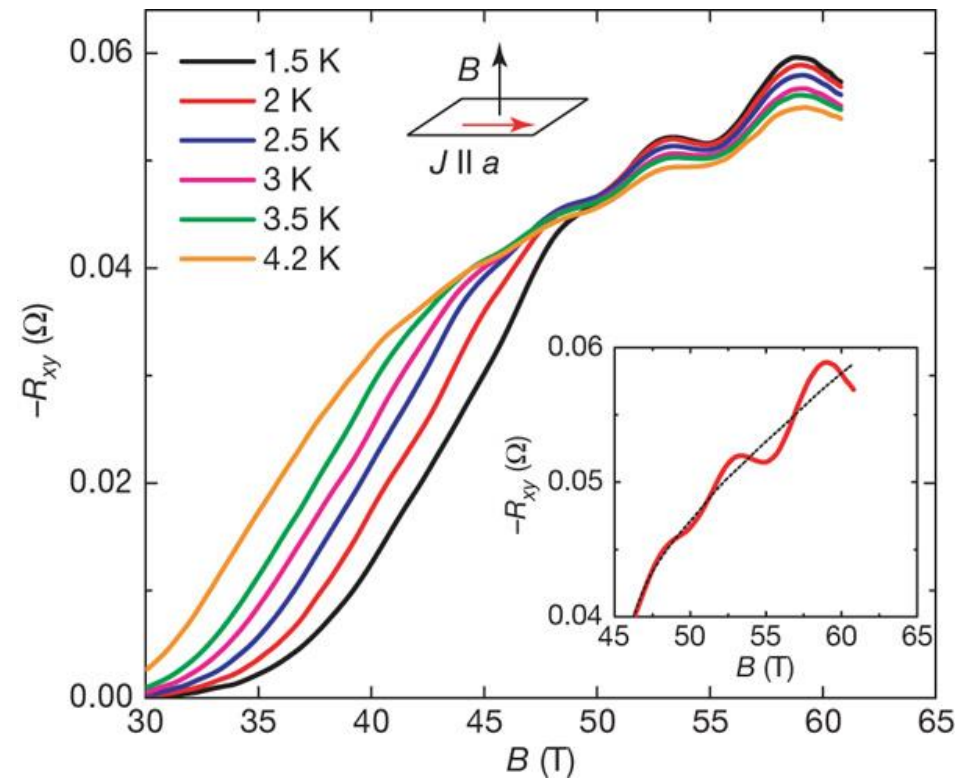
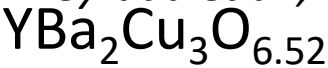
No evidence for this.

Non-conventional (Boltzmann) transport
incoherent or non-Fermi liquid transport

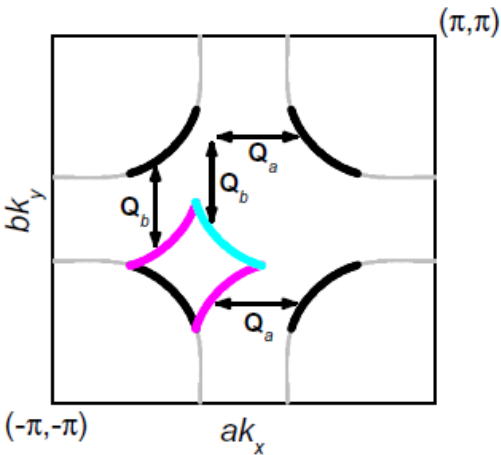
Potentially could also explain evolution of
linear-in- T term in $\rho(T)$ with doping.

Quantum oscillations in underdoped cuprates

N. Doiron-Leyraud et al., Nature 2007



CDW Fermi surface reconstruction



- Impossible from Fermi arcs.
- Inconsistent with band-structure (observed Fermi surface is only 2% of the Brillouin zone area)
- Must be some form of Fermi surface reconstruction due to change of Brillouin zone

Conductivity tensor

$$\mathbf{J} = \boldsymbol{\sigma} \cdot \mathbf{E} \quad \boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

$$\boldsymbol{\rho} = \begin{pmatrix} \rho_{xx} & \rho_{xy} & \rho_{xz} \\ \rho_{yx} & \rho_{yy} & \rho_{yz} \\ \rho_{zx} & \rho_{zy} & \rho_{zz} \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}^{-1}$$

$$\boldsymbol{\rho} = \boldsymbol{\sigma}^{-1} = \frac{1}{\det|\boldsymbol{\sigma}|} \begin{pmatrix} \sigma_{yy}\sigma_{zz} - \sigma_{yz}\sigma_{zy} & \sigma_{xz}\sigma_{zy} - \sigma_{xy}\sigma_{zz} & \sigma_{xy}\sigma_{yz} - \sigma_{xz}\sigma_{yy} \\ \sigma_{yz}\sigma_{zx} - \sigma_{yx}\sigma_{zz} & \sigma_{xx}\sigma_{zz} - \sigma_{xz}\sigma_{zx} & \sigma_{xz}\sigma_{yx} - \sigma_{xx}\sigma_{yz} \\ \sigma_{yx}\sigma_{zy} - \sigma_{yy}\sigma_{zx} & \sigma_{xy}\sigma_{zx} - \sigma_{xx}\sigma_{zy} & \sigma_{xx}\sigma_{yy} - \sigma_{xy}\sigma_{yx} \end{pmatrix}$$

It is in general complex to go between conductivity and resistivity!