

**EPSRC**

Engineering and Physical Sciences  
Research Council



UNIVERSITY OF  
BIRMINGHAM

# Charge Density Waves in High Temperature Superconductors

Elizabeth Blackburn

School of Physics and Astronomy

University of Birmingham

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# Acknowledgements



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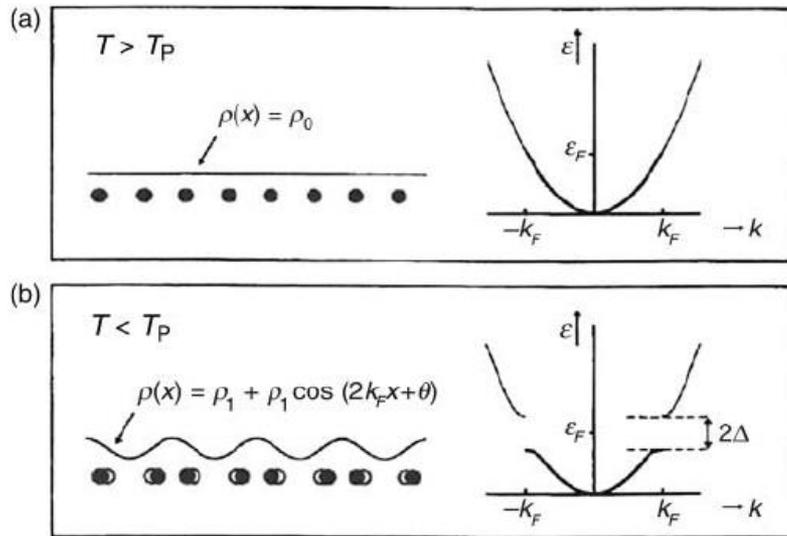


Ruixing Liang

Doug Bonn

Walter Hardy

# CDWs



Monceau, Advances in Physics **61**, 325 (2012).

# Superconductors

each electron in a pair does its own thing ...

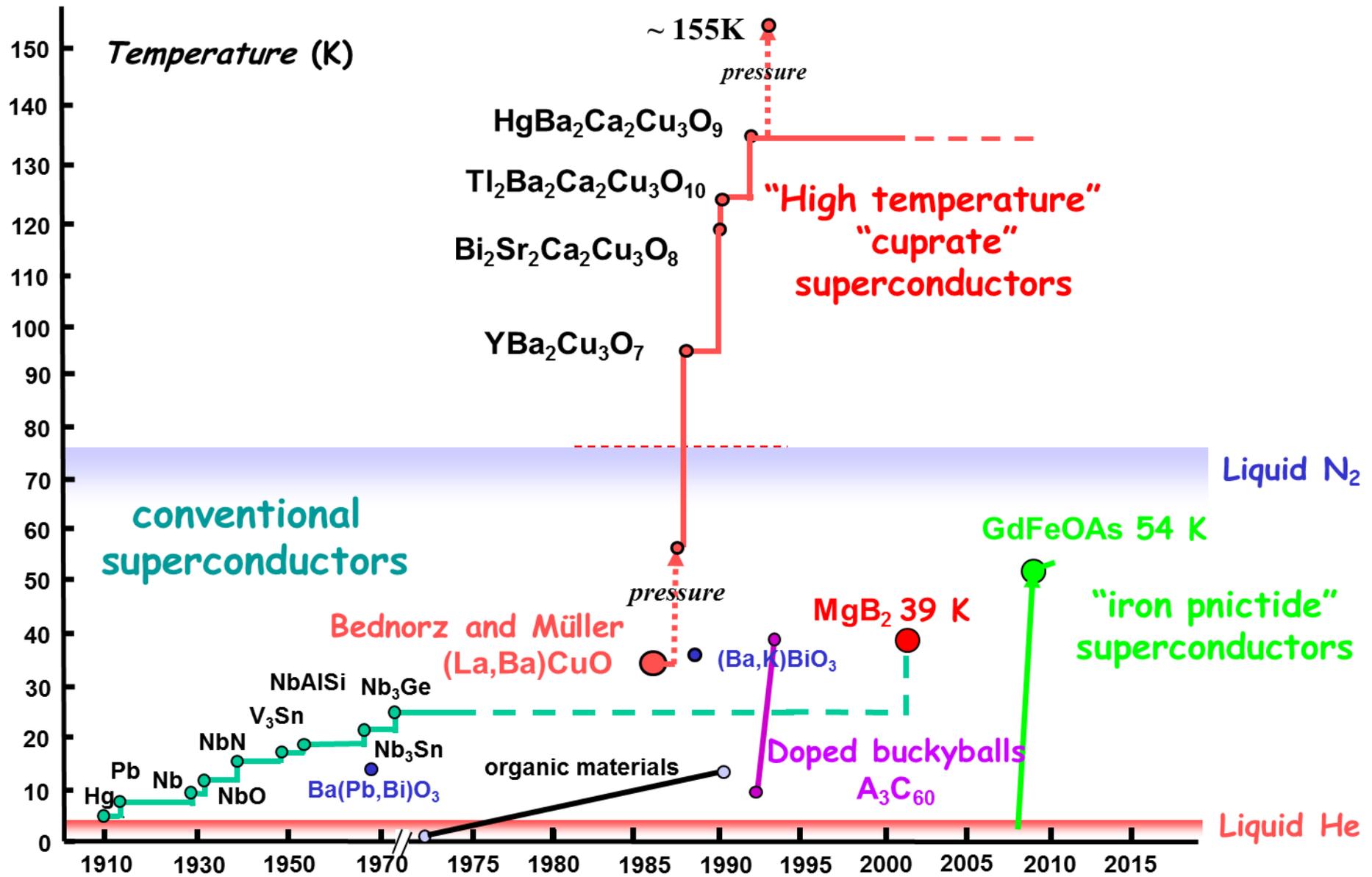
(as the Pauli Exclusion Principle says it must)

Principle says it must)

... but the CENTRES OF MASS of ALL the pairs do exactly the SAME thing – like in a laser or a BEC

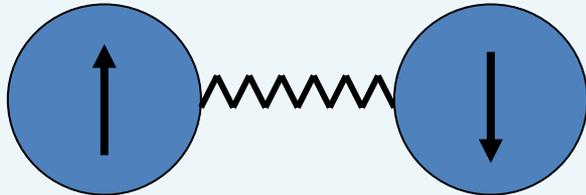
... but what force holds the electrons together?

( ~ a “coherence length”  $\xi$  apart)



# Cooper pairs in superconductors

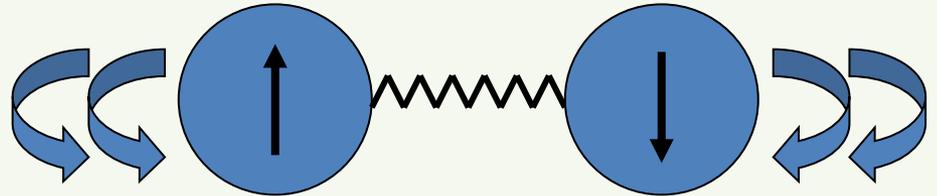
Conventional 's-wave'  
electron pairs



not circulating ...

Unconventional 'd-wave'

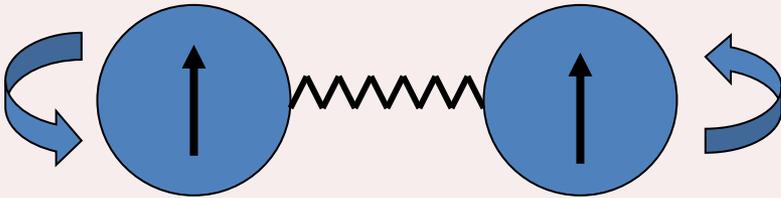
e.g. High-Tc, CeCoIn<sub>5</sub>



circulating *both* ways -  $l = 2$

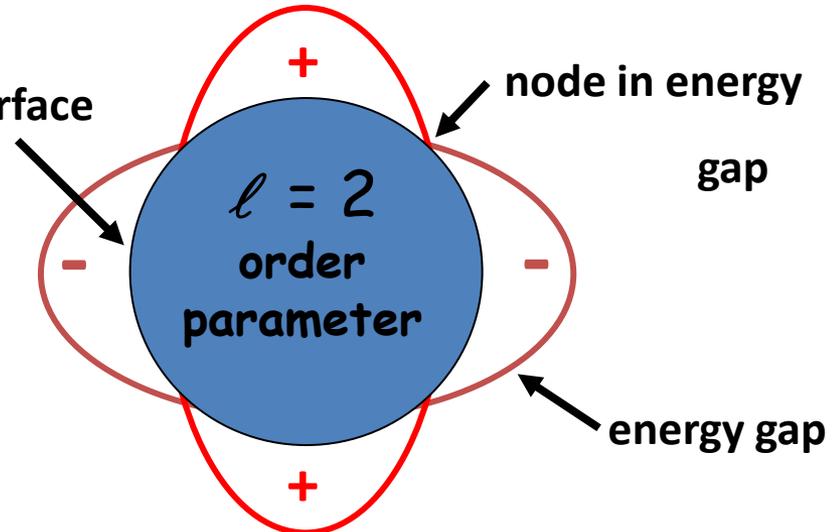
Unconventional: 'p-wave'

e.g. Sr<sub>2</sub>RuO<sub>4</sub>



circulating:  $l = 1$

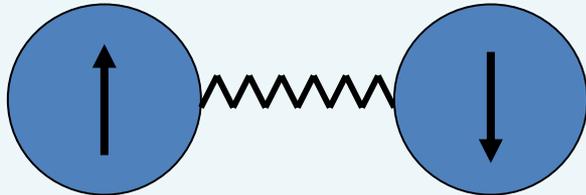
Fermi surface



# Cooper pairs in superconductors

Conventional 's-wave'

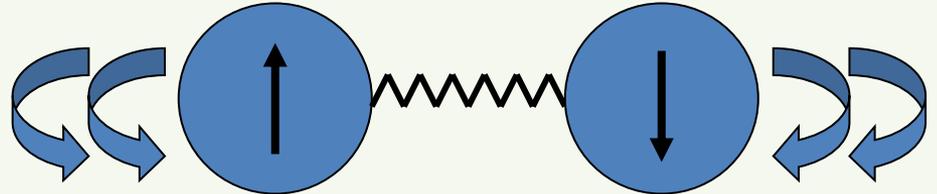
electron pairs



not circulating ...

Unconventional 'd-wave'

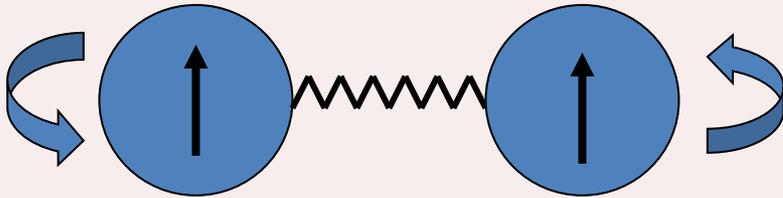
e.g. High-T<sub>c</sub> , CeCoIn<sub>5</sub>



circulating *both* ways -  $\ell = 2$

Unconventional: 'p-wave'

e.g. Sr<sub>2</sub>RuO<sub>4</sub>

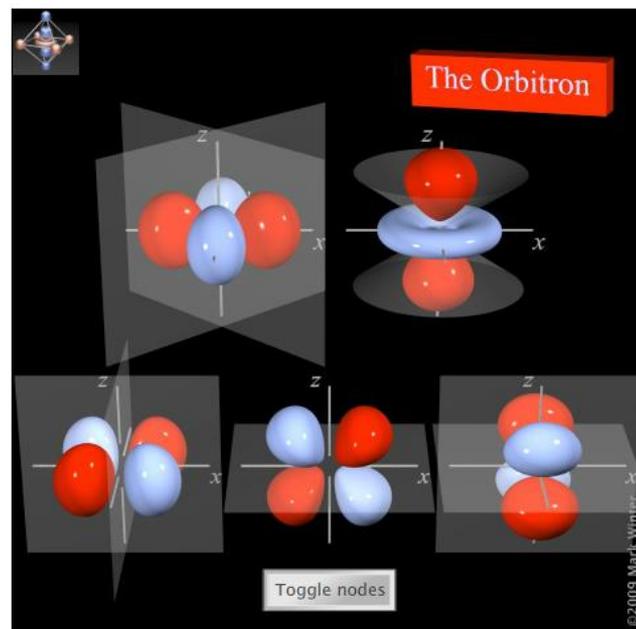
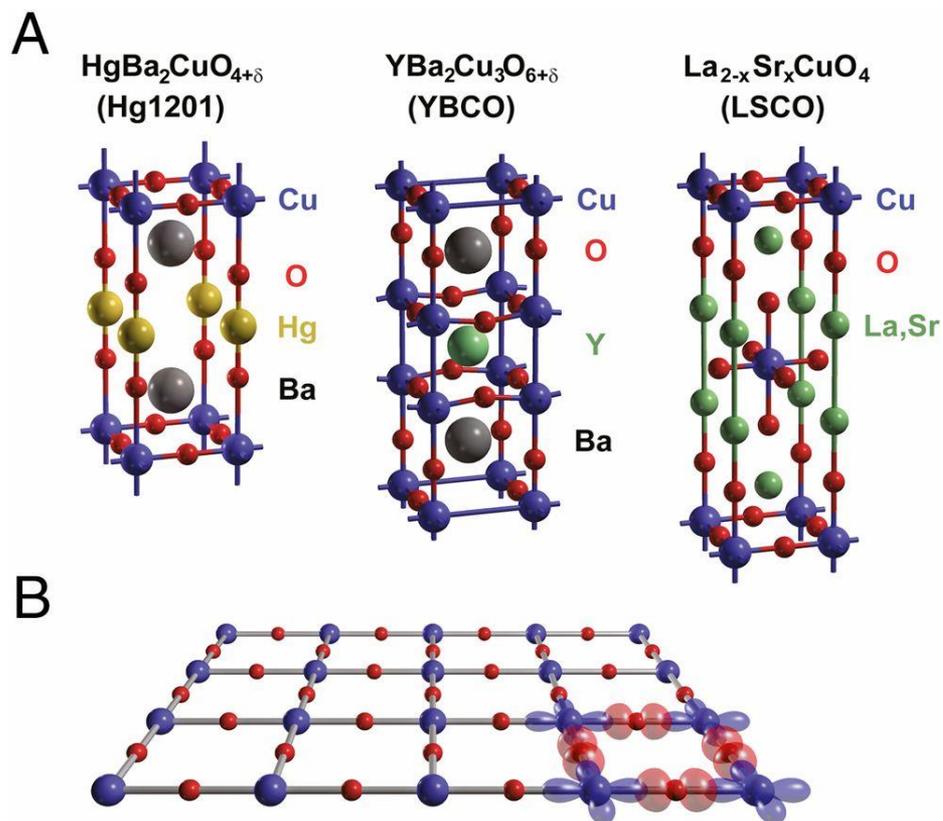


circulating:  $\ell = 1$

The type of pairing controls the symmetry of the superconducting gap function, which, amongst other things, affects flux line and Josephson tunnelling properties

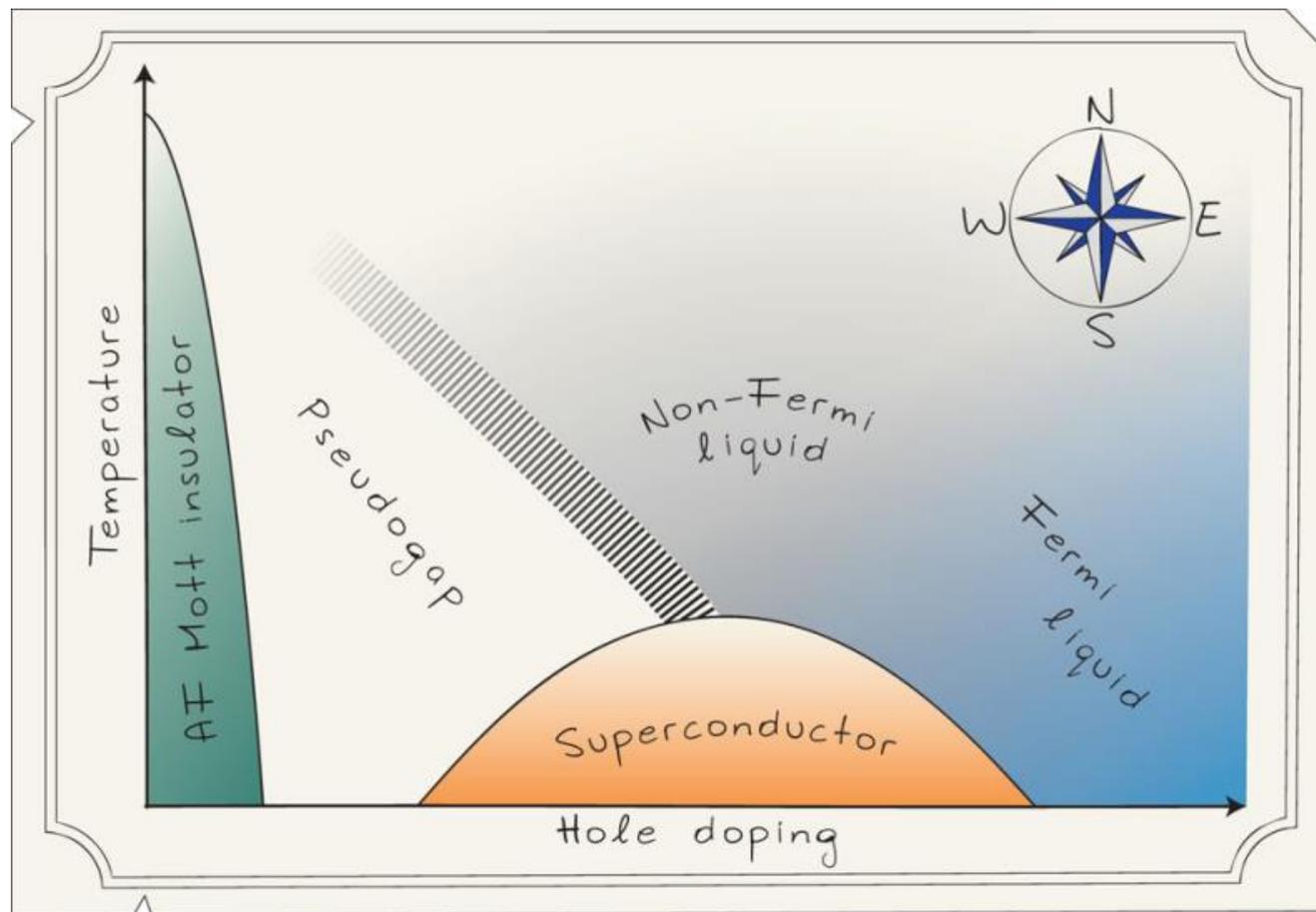
How does the pairing arise??

# The Copper-Oxygen Planes



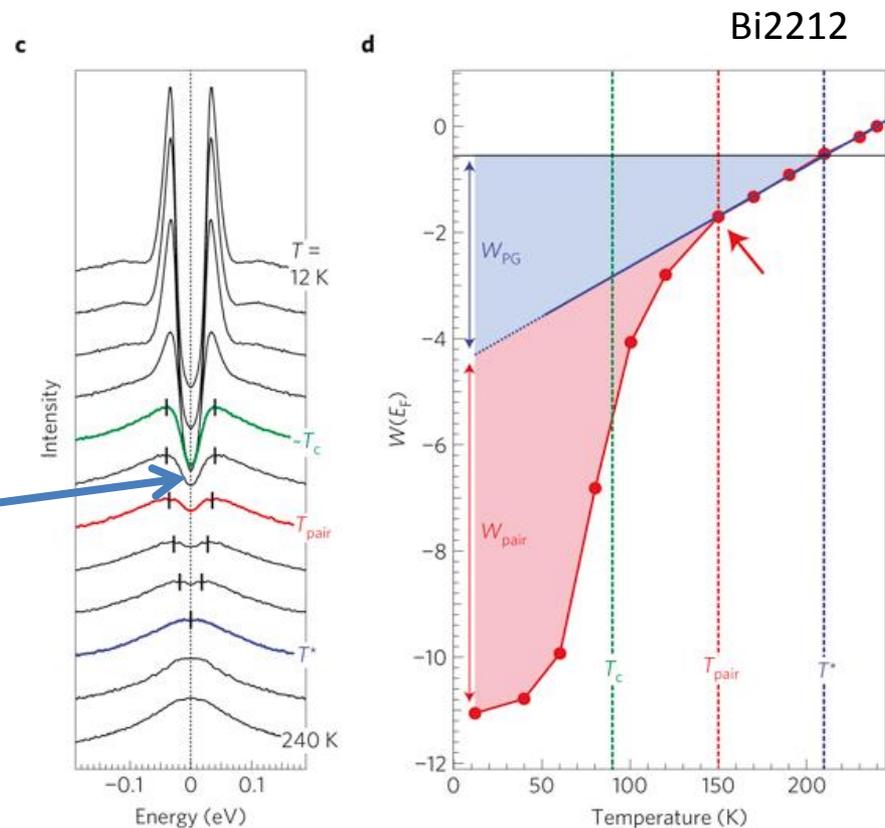
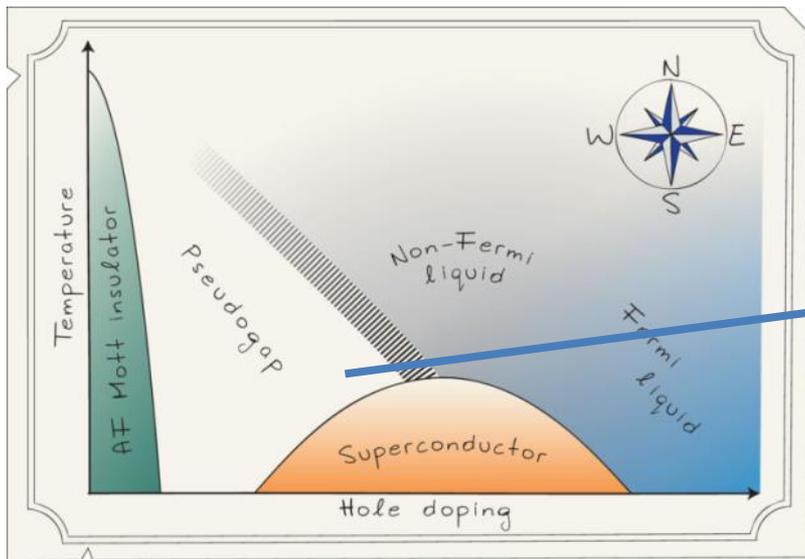
*The shape of the five 3d orbitals. From left to right: (top row)  $3d_{x^2-y^2}$  and  $3d_{z^2}$  (bottom row)  $3d_{xy}$ ,  $3d_{xz}$ , and  $3d_{yz}$ . For each, the yellow zones are where the wave functions have negative values and the blue zones denote positive values.*

# The cuprate superconductor phase diagram



# The pseudogap – loss of DOS at Fermi Level, well above $T_c$

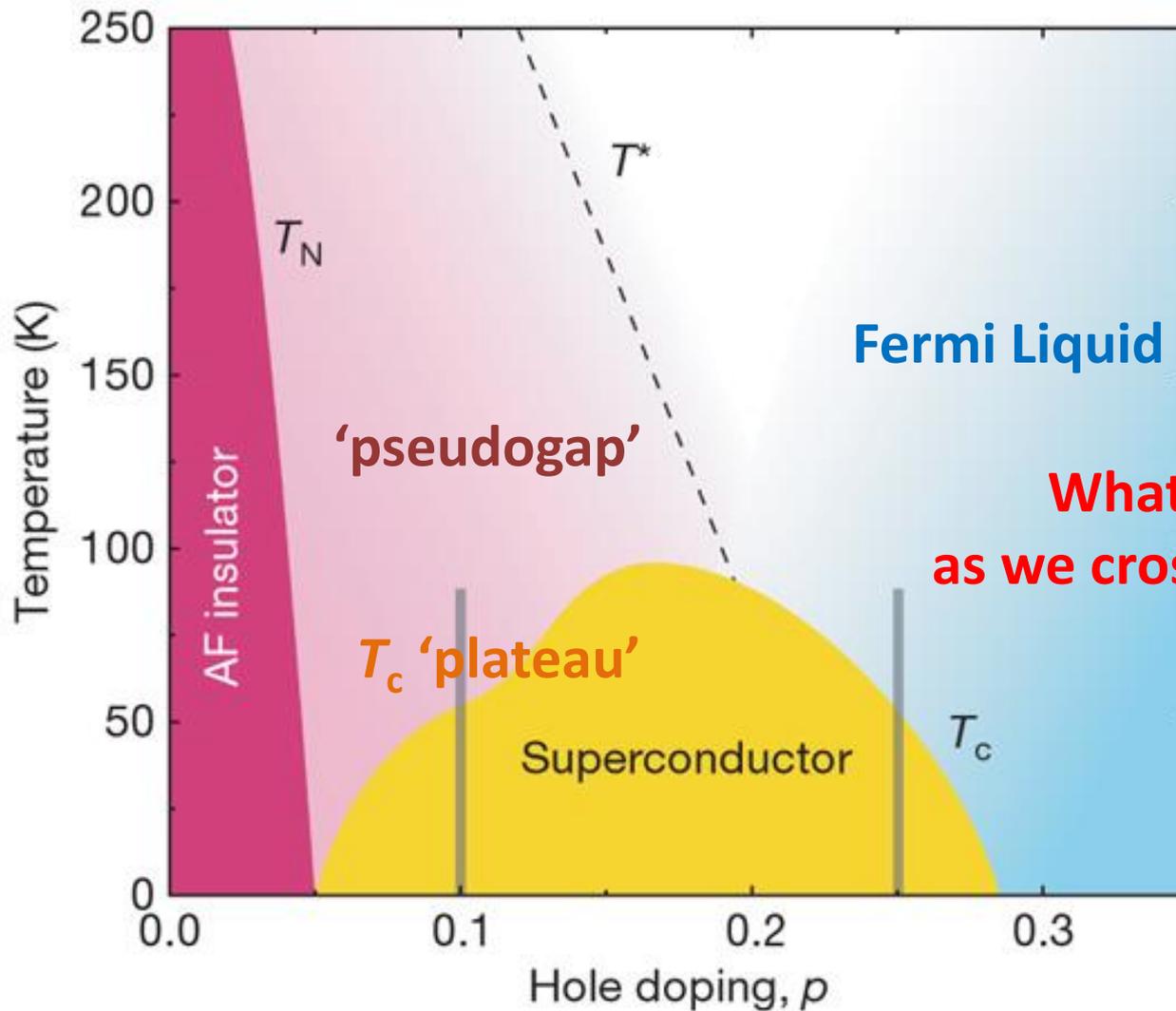
- Pre-formed pairs?
- Competing order?



Wahl, Nature Physics (2012)

Kondo *et al.*, Nature Physics (2011)

# Phase diagram of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ versus doping

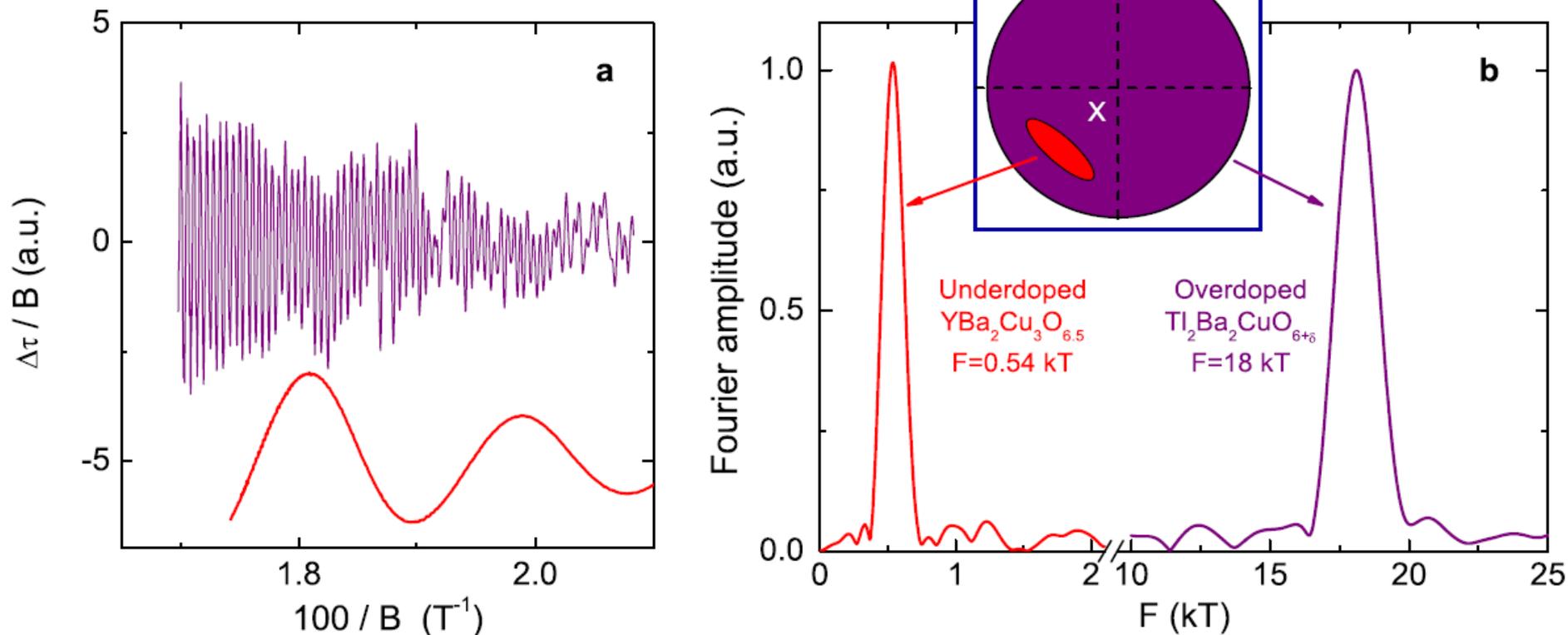


What changes  
as we cross the 'dome'?

# The Fermi surface – quantum oscillation data

Overdoped – all holes visible - obeys Luttinger theorem

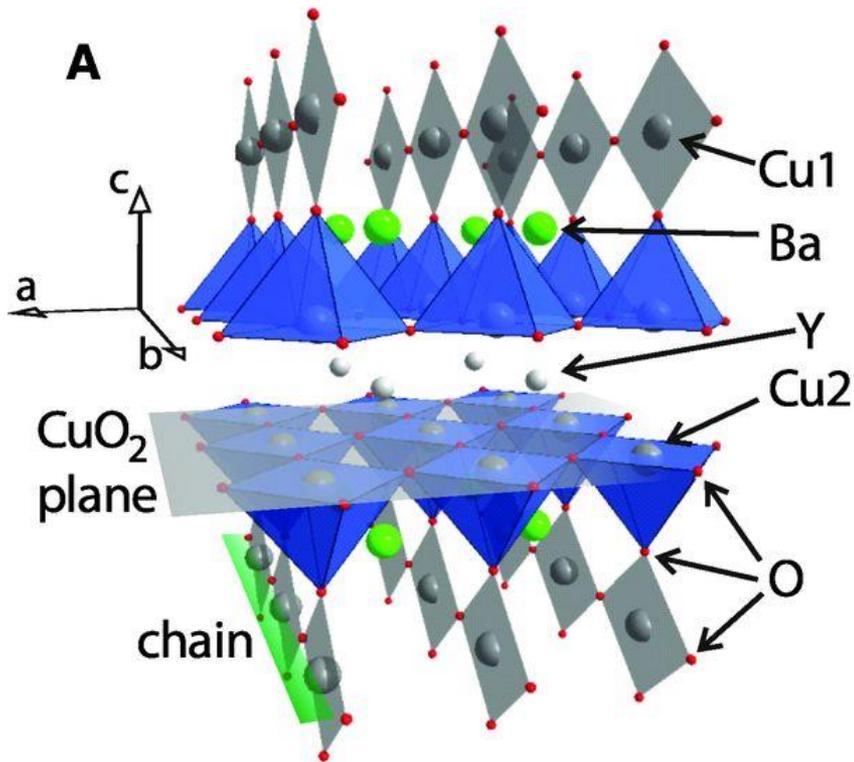
B. Vignolle *et al.* Comptes Rendus Physique (2011)



Underdoped – tiny number of *electrons* not holes

N.B. QOs give the *area* of the electron pocket

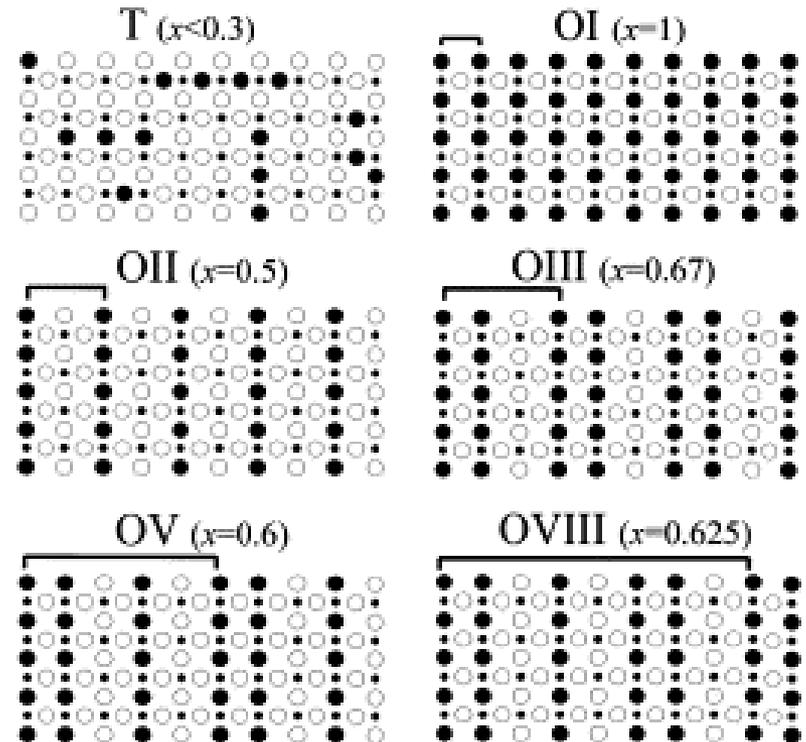
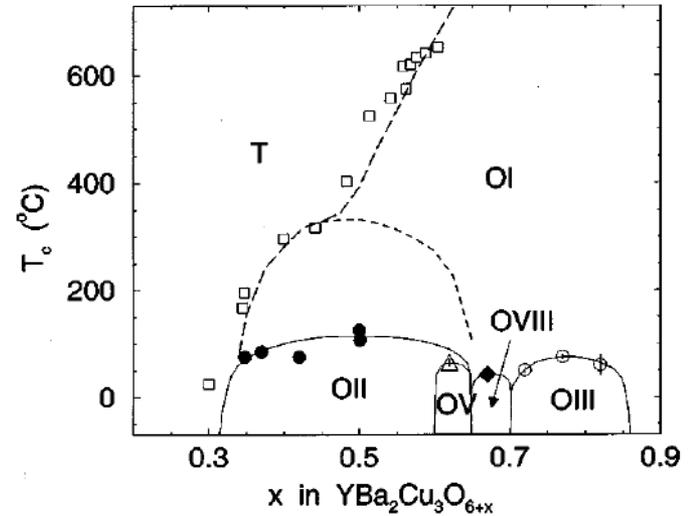
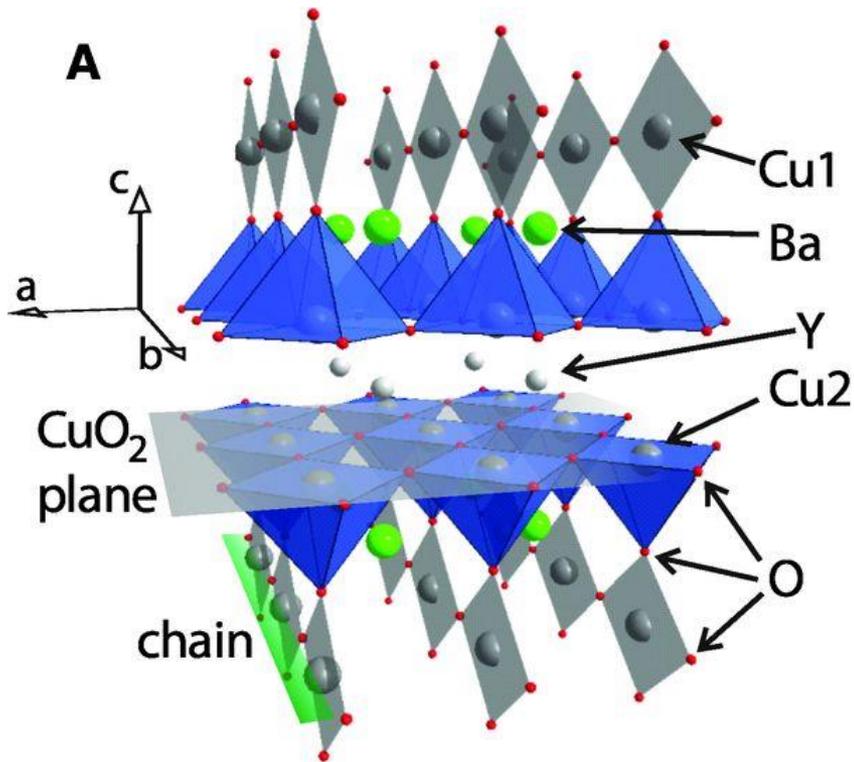
# Superconductivity in $\text{YBCO}_{6+x}$



Superconductivity mainly resides in the  $\text{CuO}_2$  bi-layered planes

Oxygen content is varied from  $\text{O}_7$  to  $\text{O}_6$  by removing  $\text{O}$  from the chains running along  $b$

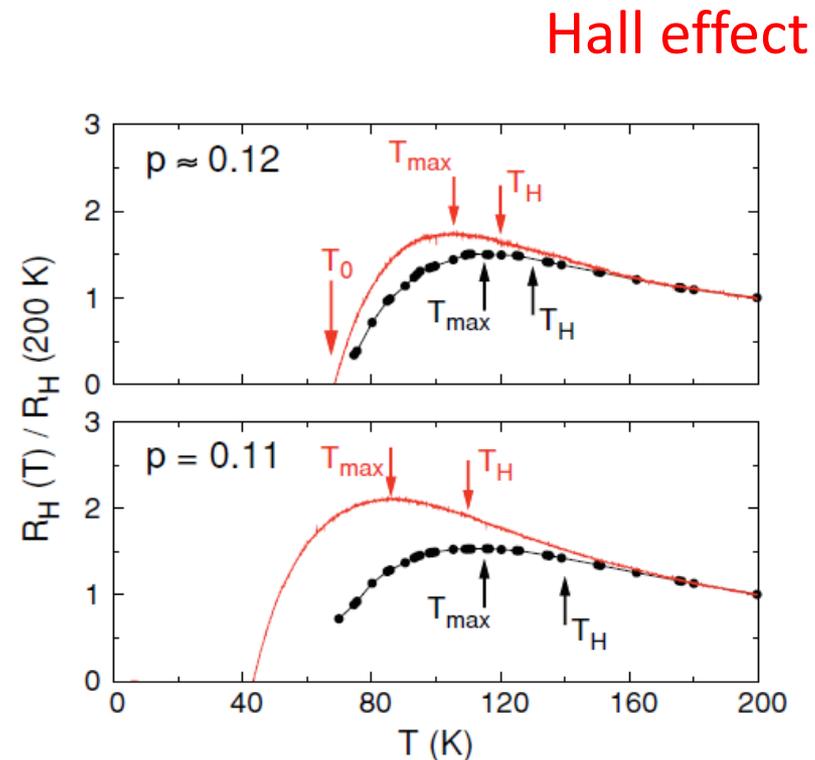
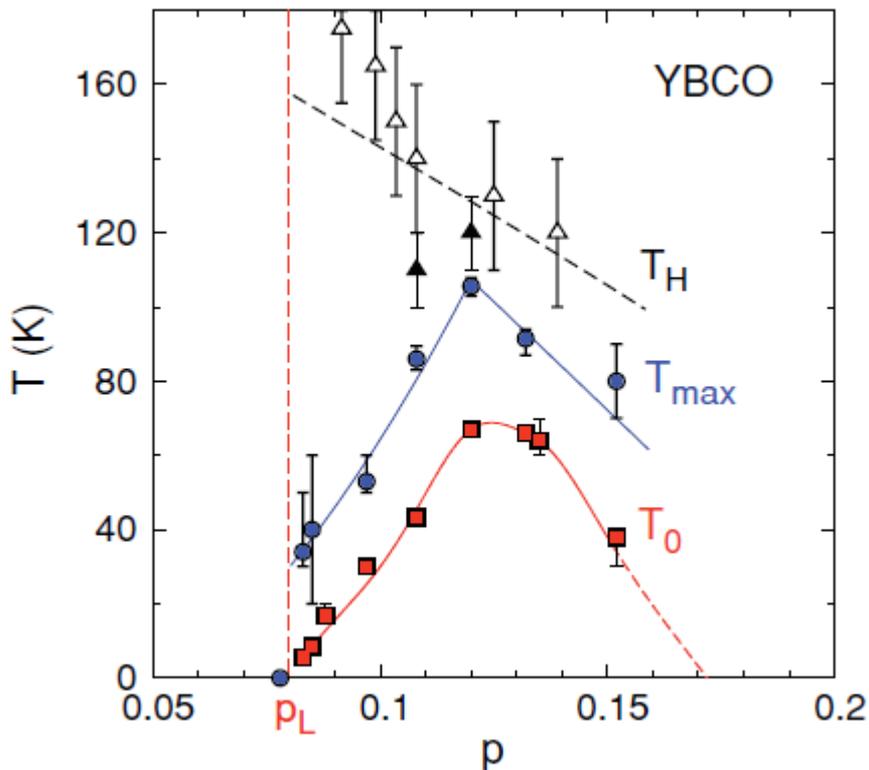
# Oxygen ordering in $\text{YBCO}_{6+x}$



Ghiringhelli *et al.*, Science (2012)  
 Andersen *et al.*, Physica C (1999)  
 v. Zimmerman *et al.*, Phys.Rev.B (2003)

# Signs of something changing inside the PG region

- Transport measurements

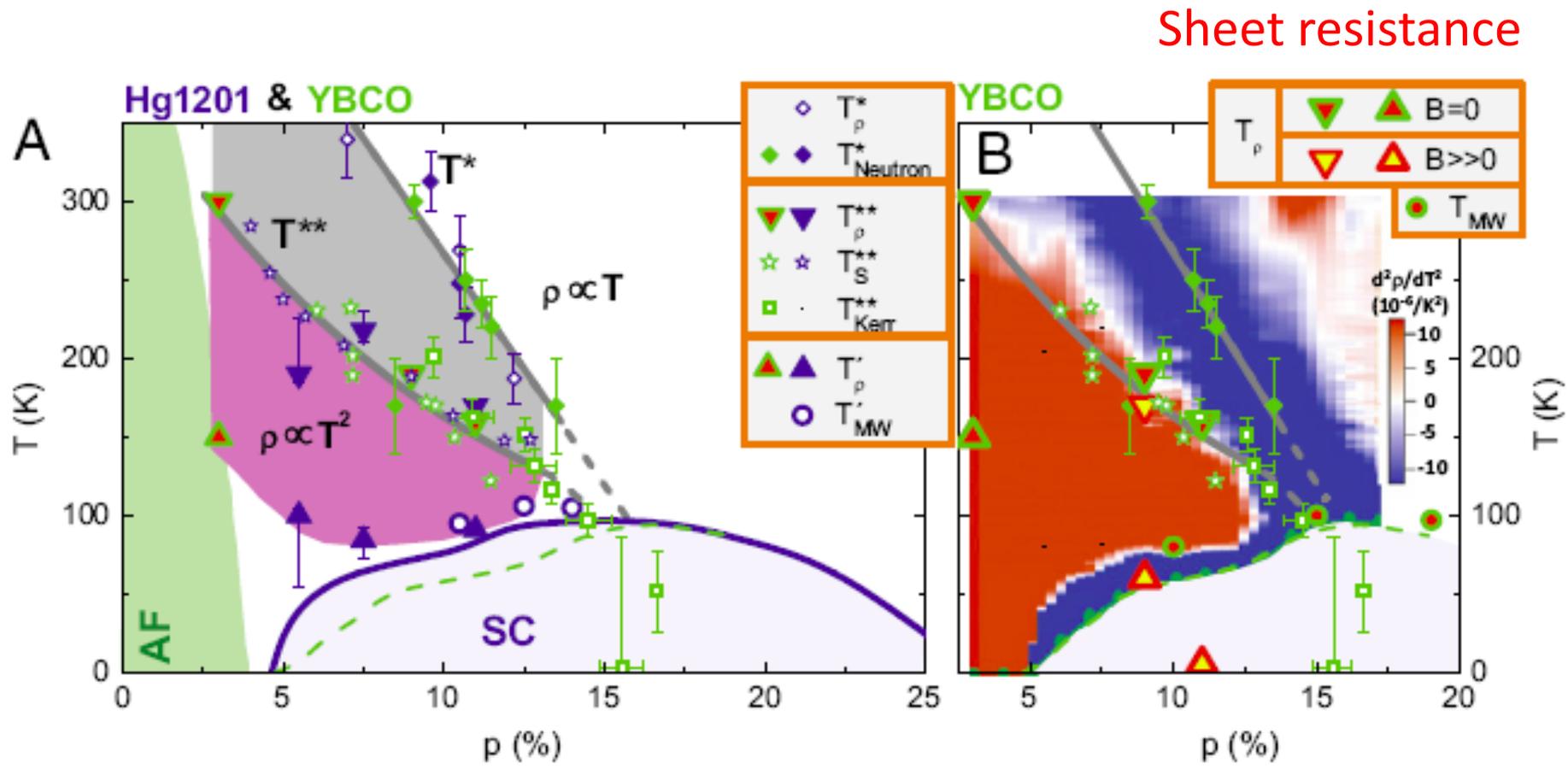


LeBoeuf *et al.*, Nature (2007),  
Phys. Rev. B (2011)

This suggests that the Fermi surface changes topology below  $T_{Hall}$

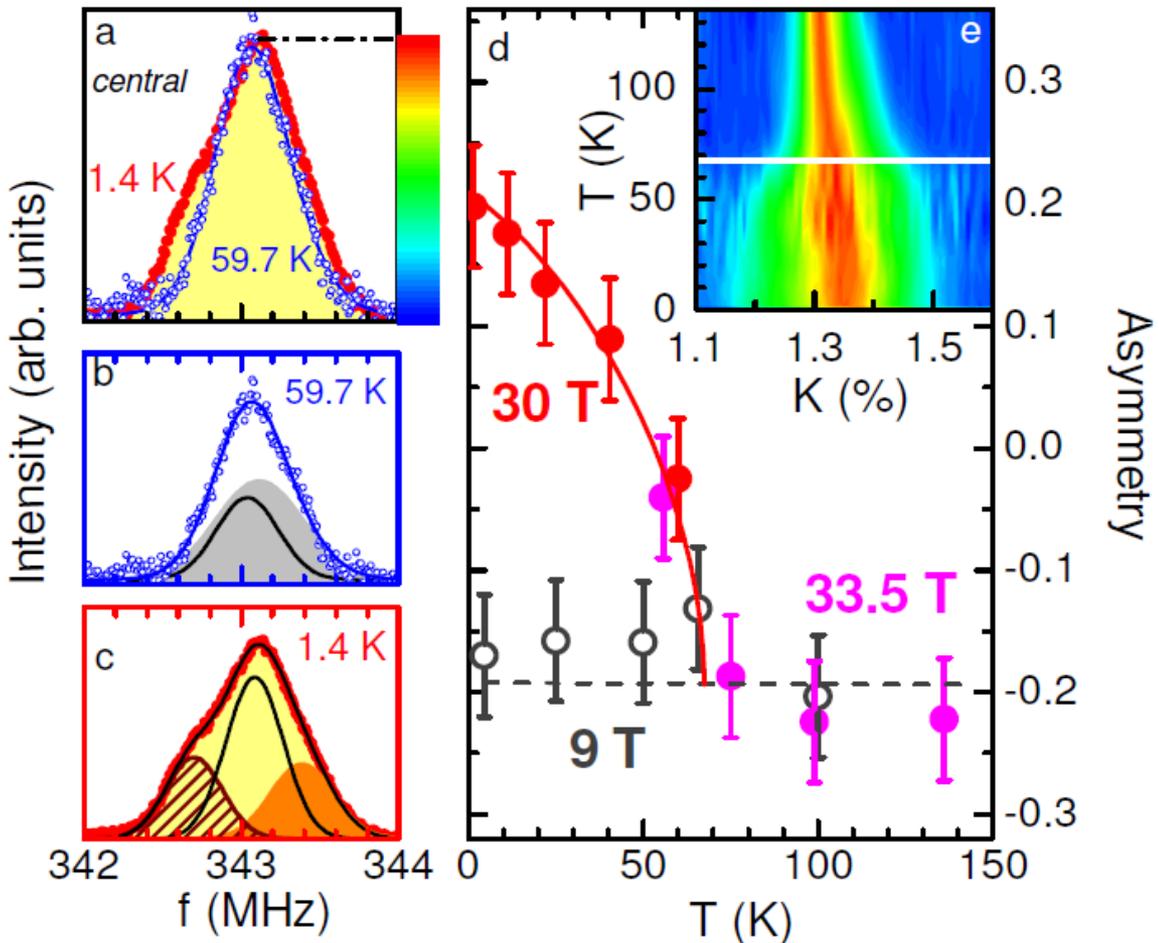
# Signs of something changing inside the PG region

- Transport measurements



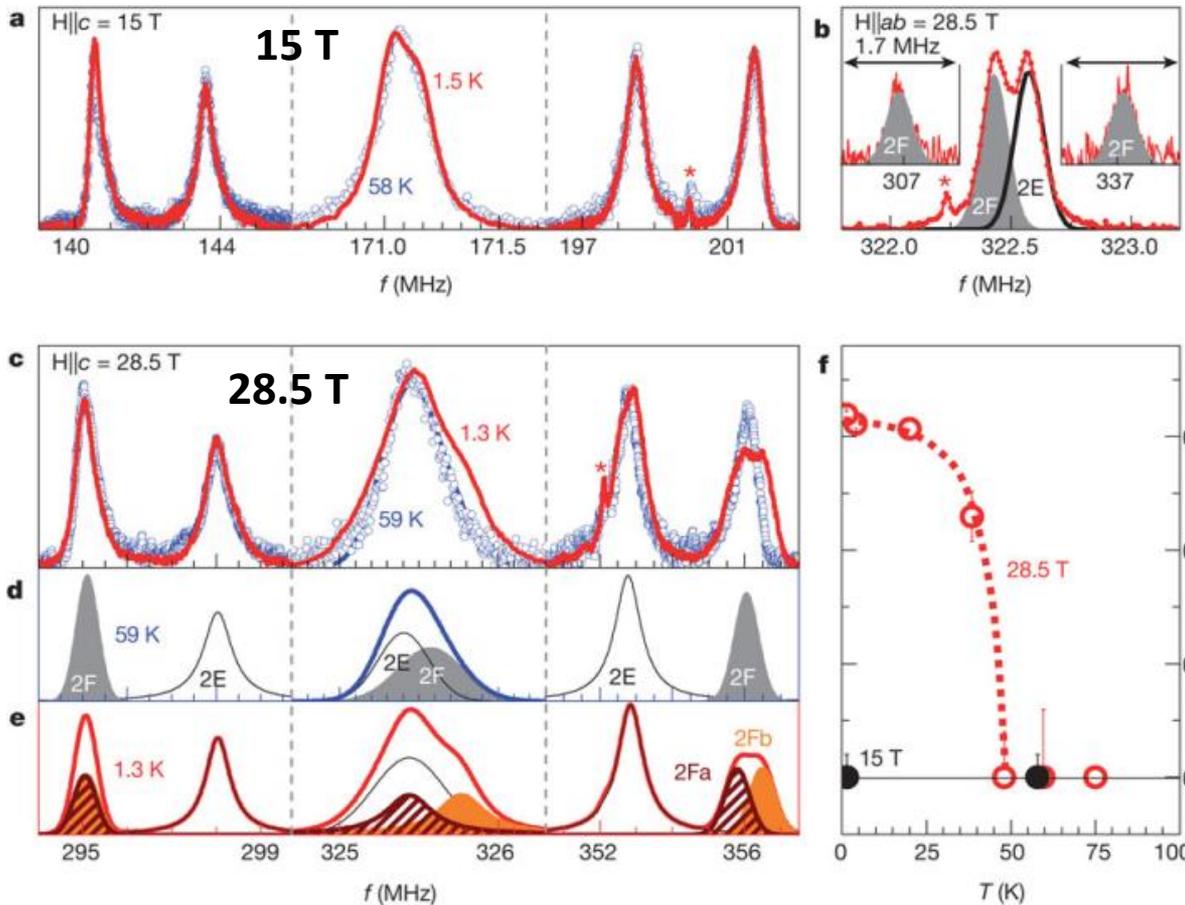
# Signs of something changing inside the PG region

- Transport measurements
- NMR/NQR



Wu *et al.*, Nature **477**, 7363 (2011) – picture is ortho-VIII.

# $^{63}\text{Cu}$ NQR shows signs of charge order in o-II YBCO



Wu *et al.*, Nature (2011)  
(& Nature Comms .2013)

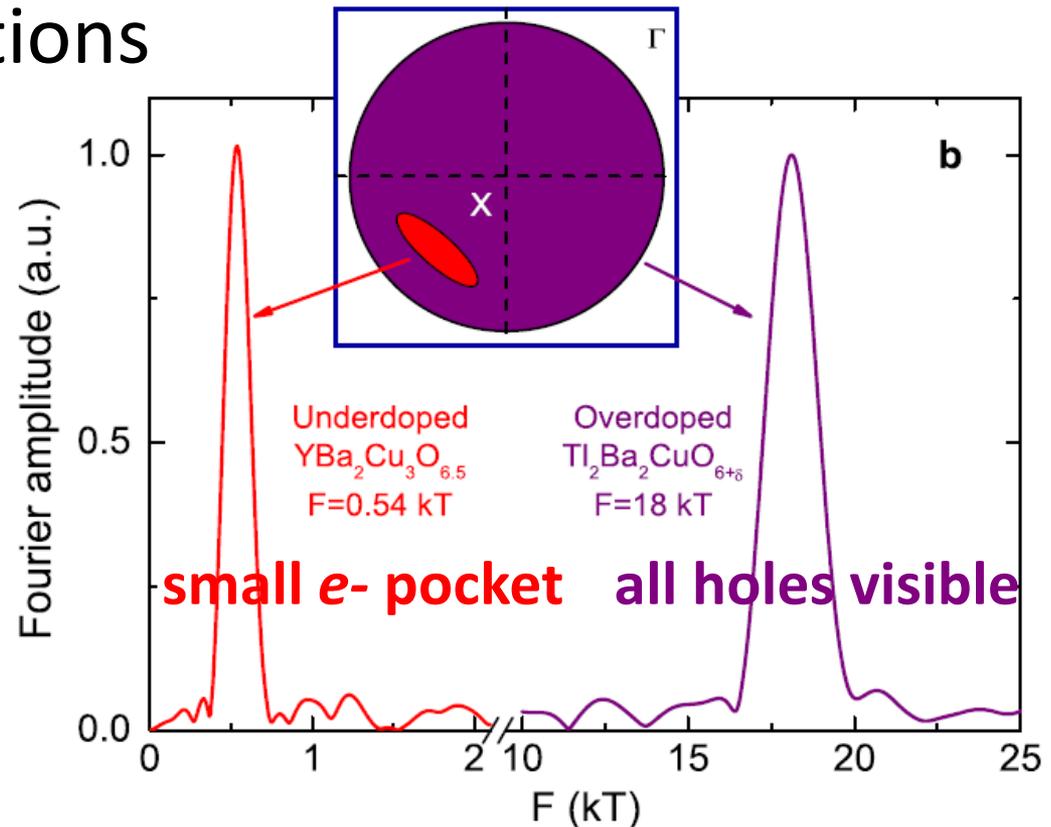
Splitting in a Cu line appears at high field and low temperature.

They suggested a charge modulation along  $a$  with period  $4a$ ...

... beware: NMR/NQR is a 'local' probe

# Signs of something changing inside the PG region

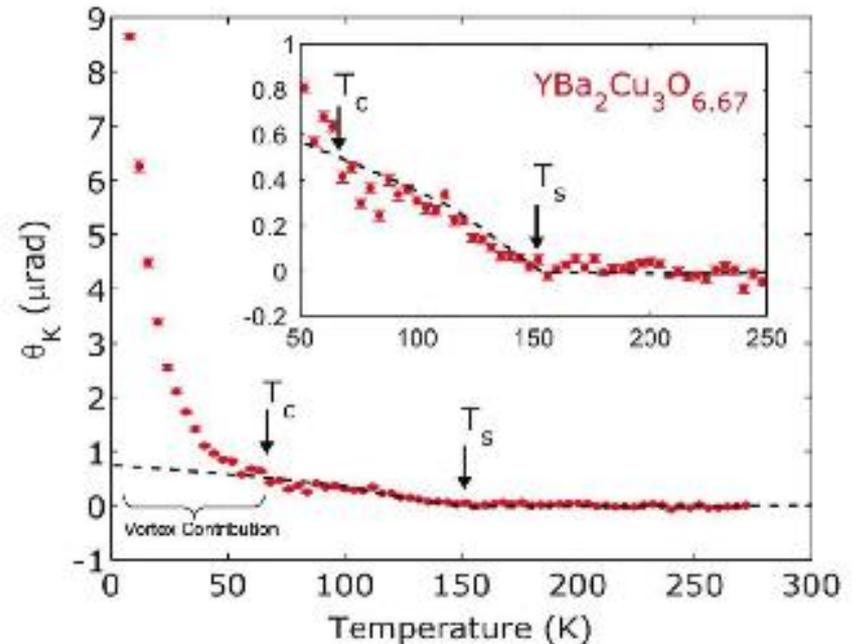
- Transport measurements
- NMR/NQR
- Quantum oscillations



# Signs of something changing inside the PG region

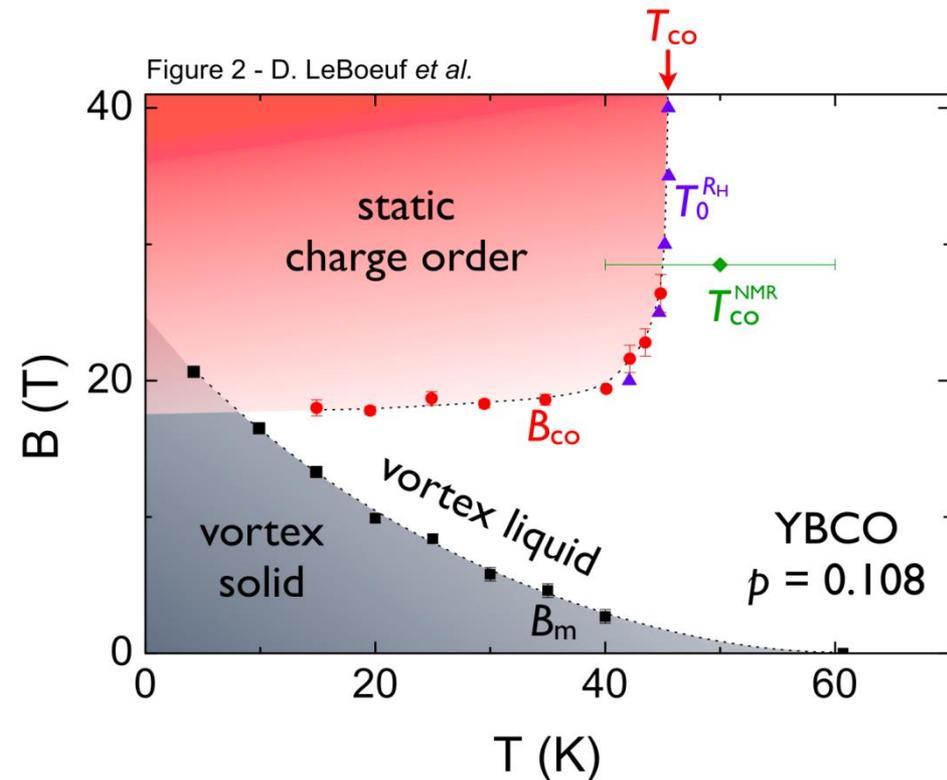
- Transport measurements
- NMR/NQR
- Quantum oscillations
- Kerr effect

FIG. 2 (color online). The Kerr effect of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$  crystal. The sample was first cooled to 4.2 K in a +4 T field. The field was turned off at 4.2 K, and measurements were taken while warming the sample. Note the large vortex contribution that disappears just before  $T_c = 65$  K. The inset shows the region above  $T_c$  with its zero baseline, indicating a finite Kerr signal that disappears at  $T_s = 155$  K. Dashed lines are guides to the eye.



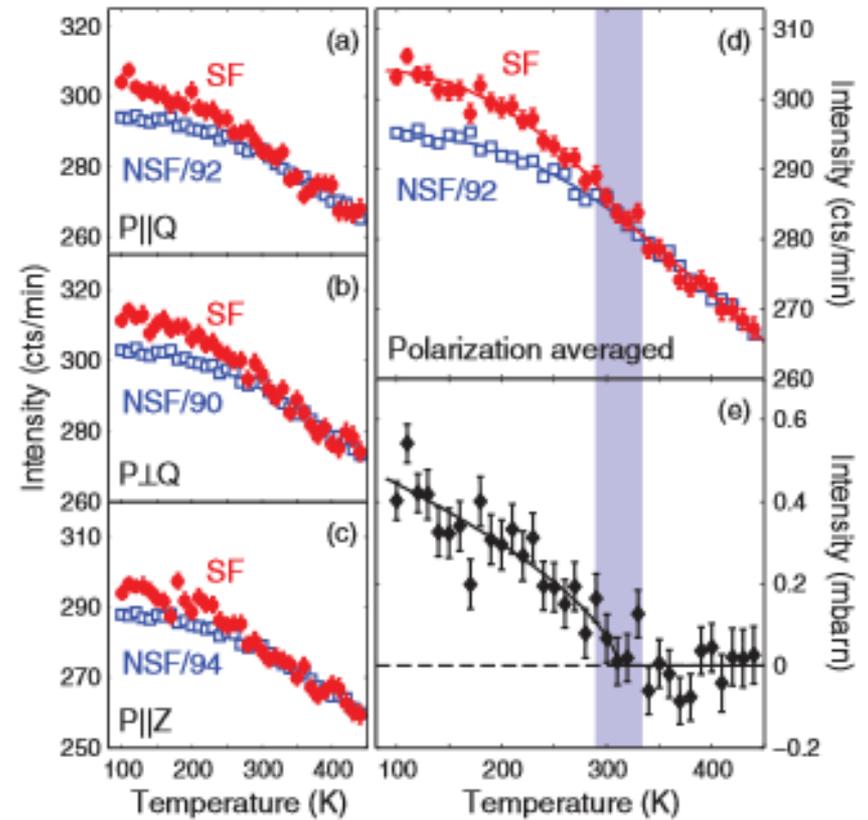
# Signs of something changing inside the PG region

- Transport measurements
- NMR/NQR
- Quantum oscillations
- Kerr effect
- Ultrasound



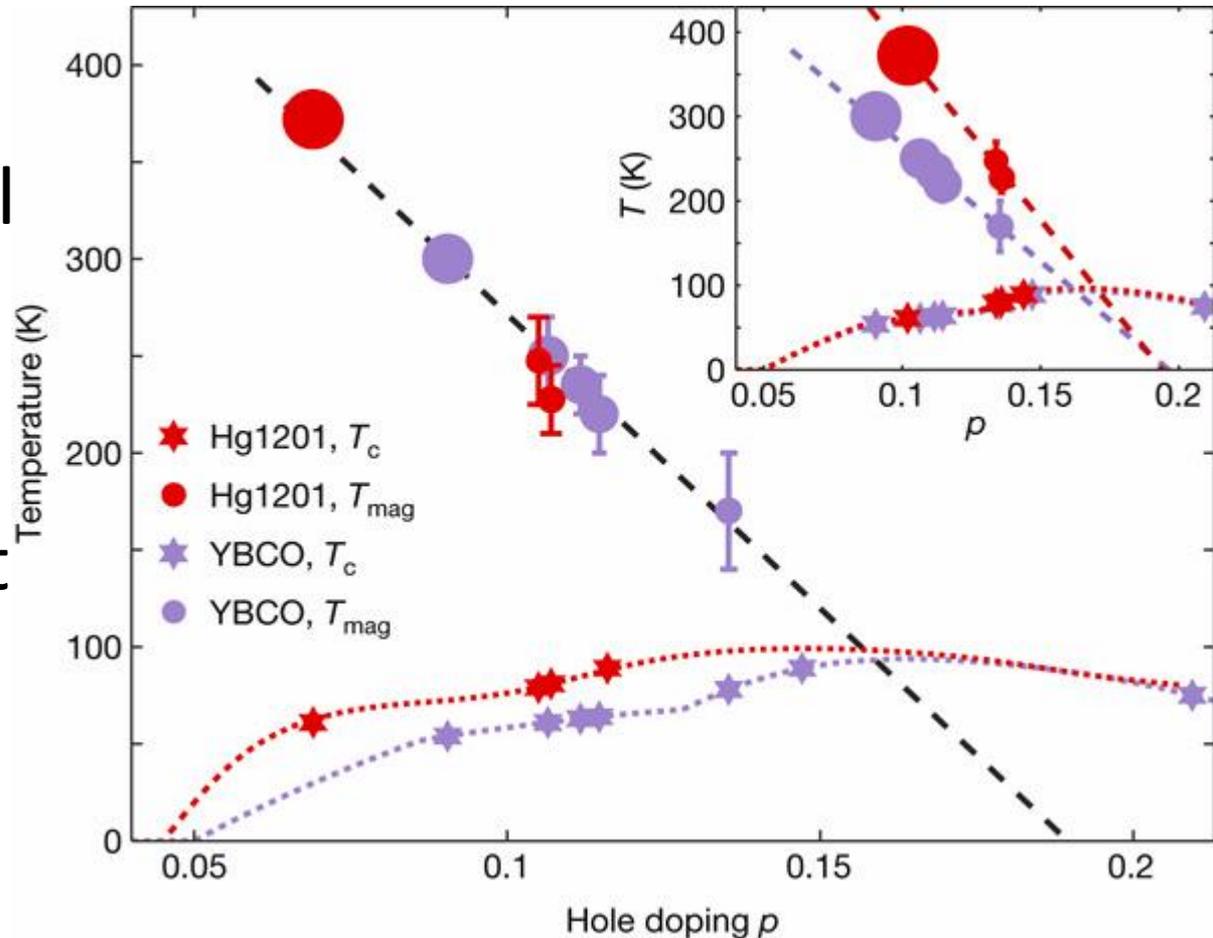
# Signs of something changing inside the PG region

- Transport measurements
- NMR/NQR
- Quantum oscillations
- Kerr effect
- Ultrasound
- Polarized neutron diffraction



# Signs of something changing inside the PG region

- Transport measurements
- NMR/NQR
- Quantum oscil
- Kerr effect
- Ultrasound
- Polarized neut

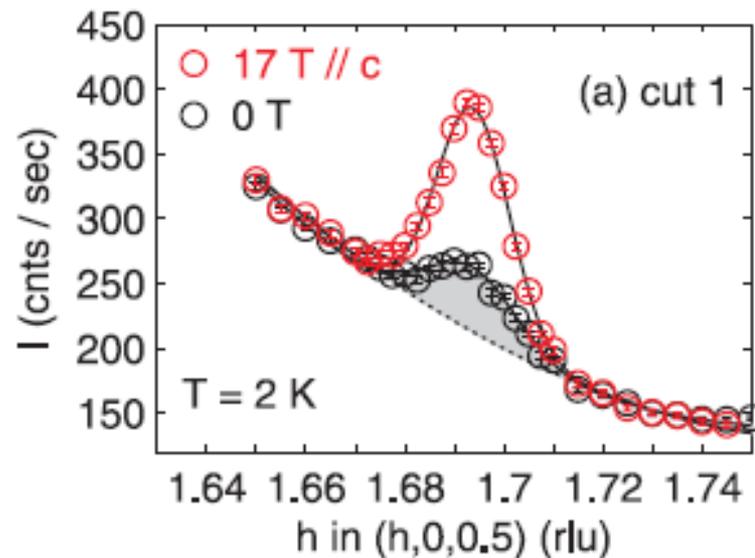


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- Transport measurements
- NMR/NQR
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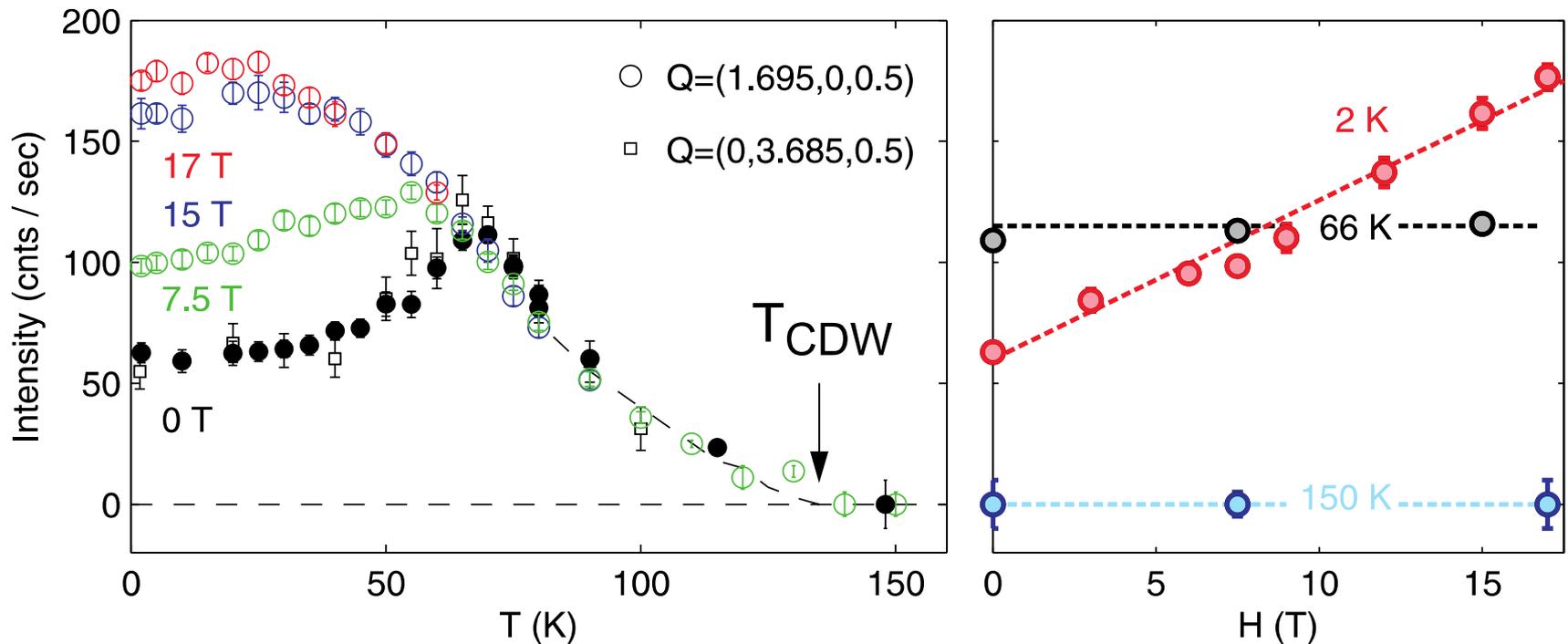
# What is changing?

The  $\text{YBa}_2\text{Cu}_3\text{O}_y$  family shows charge density wave order which competes with superconductivity



# What is changing?

The  $\text{YBa}_2\text{Cu}_3\text{O}_y$  family shows charge density wave order which competes with superconductivity



– Using high energy x-ray diffraction

- Chang *et al.*, Nature Physics (2012)
- Blackburn *et al.*, Phys. Rev. Lett. (2013)

– Using soft x-ray resonant scattering

- Ghiringhelli *et al.*, Science (2012)
- Achkar *et al.*, Phys. Rev. Lett. (2012)

# Direct Observations of CDWs - two techniques:

Our Collaboration: 'Hard' X-ray  
(100 keV) diffraction up to  $B = 17$  T

Diffraction signal arises  
from displacements of *all*  
atoms in the unit cell...

Large volume of  $\mathbf{Q}$ -space  
accessible – extra info.

Chang *et al.*, Nat. Phys. **8**, 871 (2012).

- o-VIII

Blackburn *et al.*, PRL **110**, 137004 (2013).

- o-II and o-III

Resonant Elastic X-ray Scattering:  
mainly 930 eV Cu  $L_3$  edge

Diffraction signal arises  
from spatial variation of  
Cu  $L$ -resonance energy

Small volume of  $\mathbf{Q}$ -space  
accessible – but site-specific

Ghiringhelli *et al.*, Science **337**, 821 (2012).

Achkar *et al.*, PRL **109**, 167001 (2012).

- o-III + origin of contrast discussion

Blanco-Canosa *et al.*, PRL **110**, 187001 (2013).

- o-II

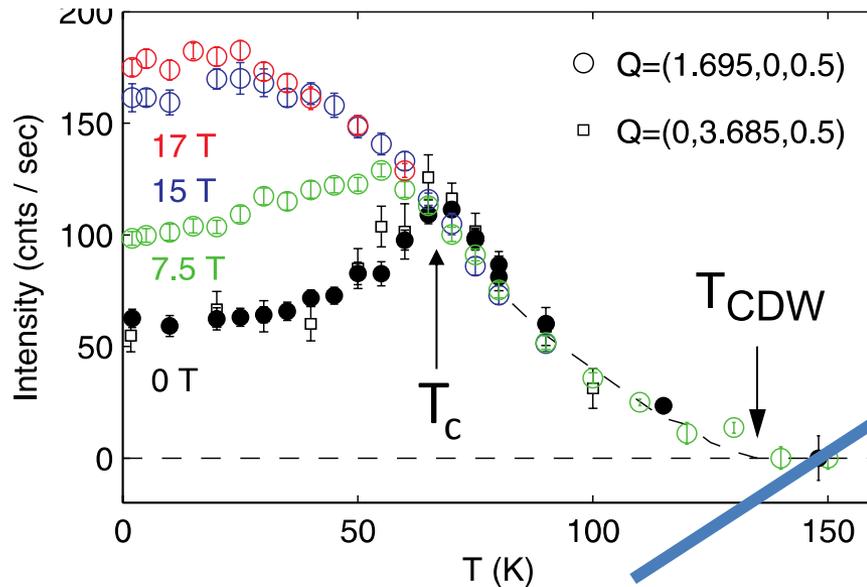
Similar results seen over a range of (under) dopings and for  
different Cu-O chain orderings (ortho-II, -III & -VIII)

# CDWs (and other lattice instabilities) are also seen in other cuprates!

- YBCO
- Bi2201 – Comin *et al.*, Science **343**, 390 (2014).
- Hg1201 – Tabis *et al.*, arXiv 1404.7658 (2014).
- Eu-LSCO – Ghiringhelli *et al.*, Science **337**, 821 (2012)
- LSCO – Christensen *et al.*, arXiv 1404.3192 (2014)
- ....

**A general feature of the underdoped cuprates  
- can we link it to the other observations?**

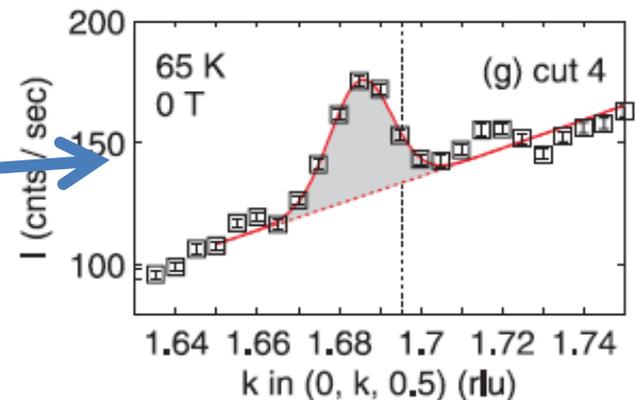
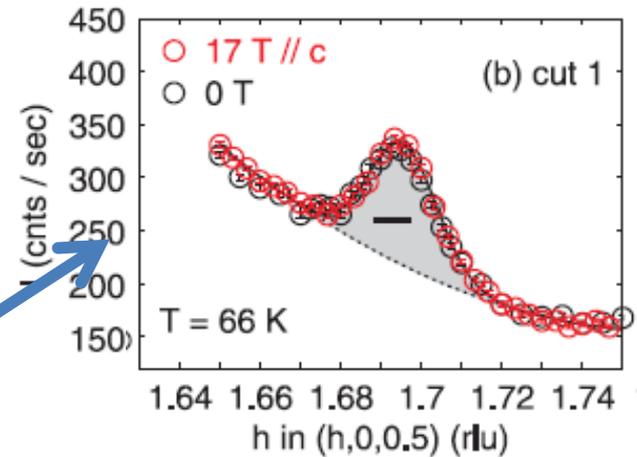
# Let's start with one compound, YBCO o-VIII



In  $\text{YBCO}_{6.67}$

$\mathbf{q}_1 = (0.305, 0, 0.5)$

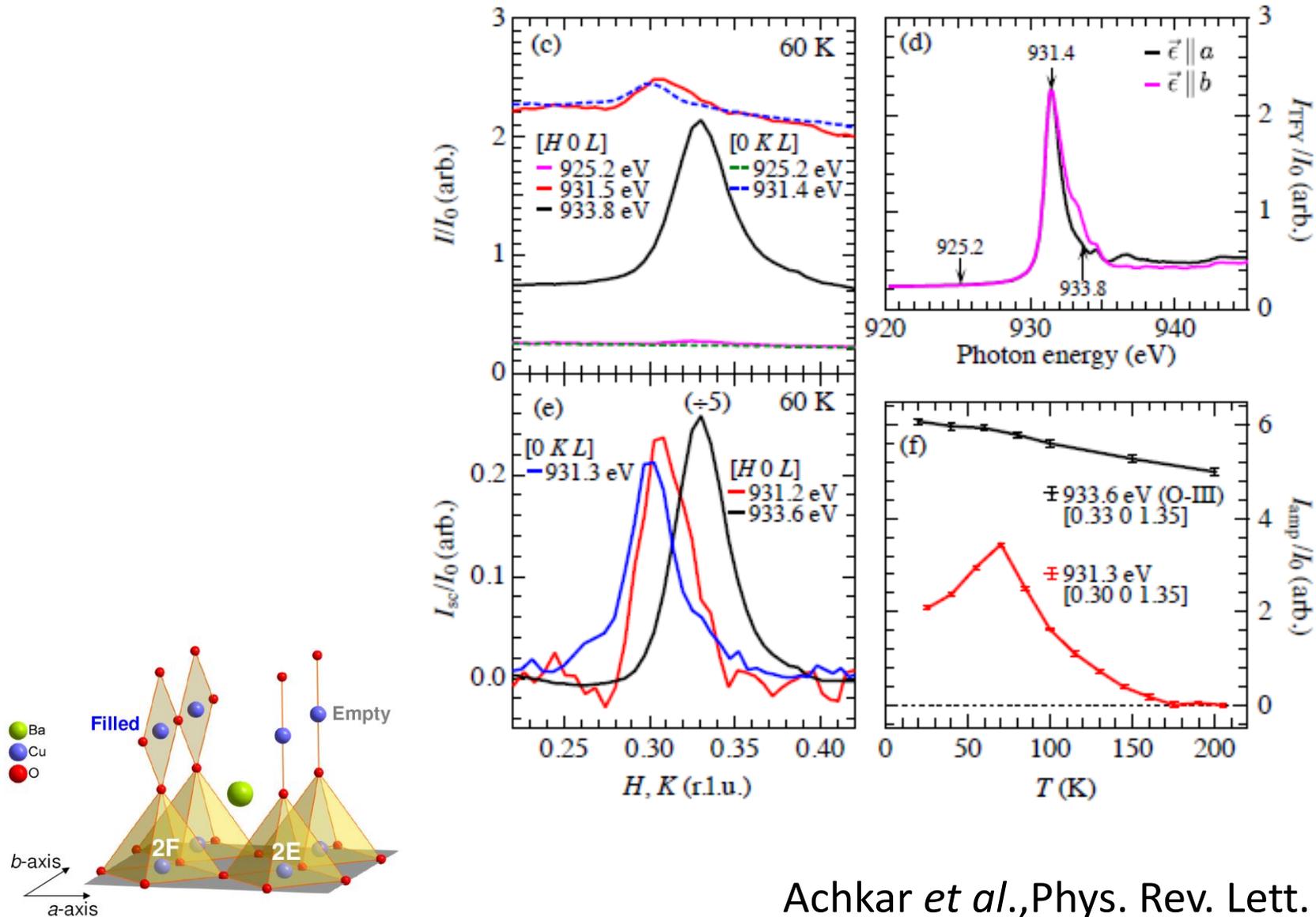
$\mathbf{q}_2 = (0, 0.314, 0.5)$



Similar but unequal  $\mathbf{q}$ -vectors along the  $\mathbf{a}$  &  $\mathbf{b}$  directions

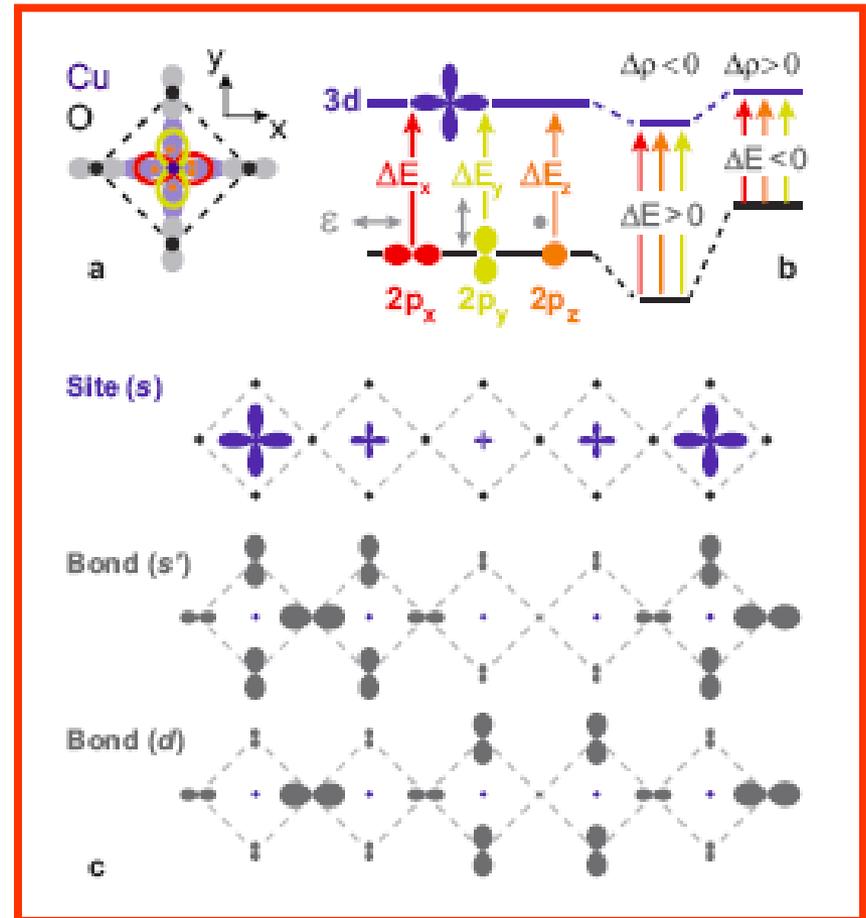
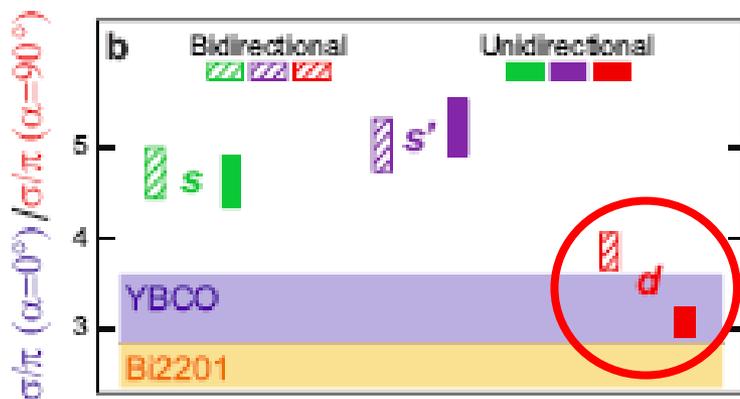
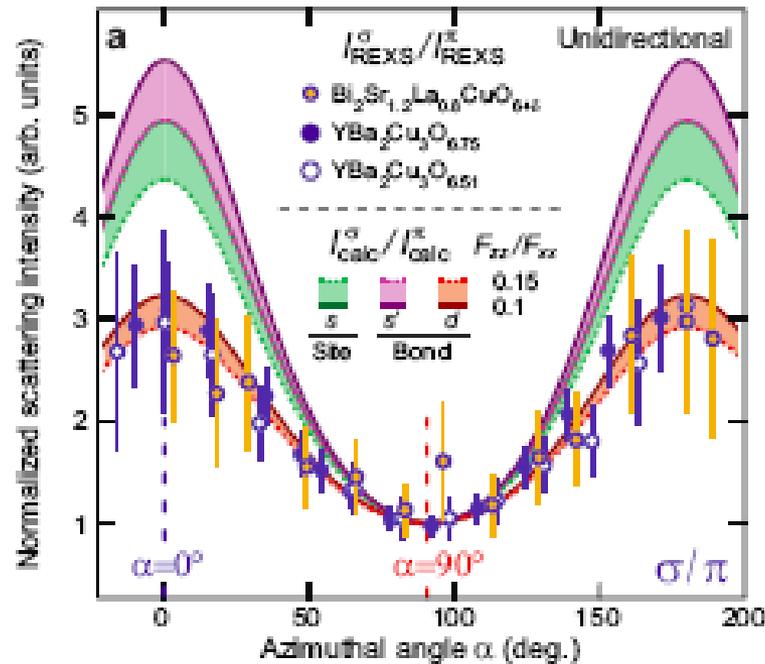
Adjacent cells along  $\mathbf{c}$  in antiphase

# Energy dependence in ortho-III YBCO



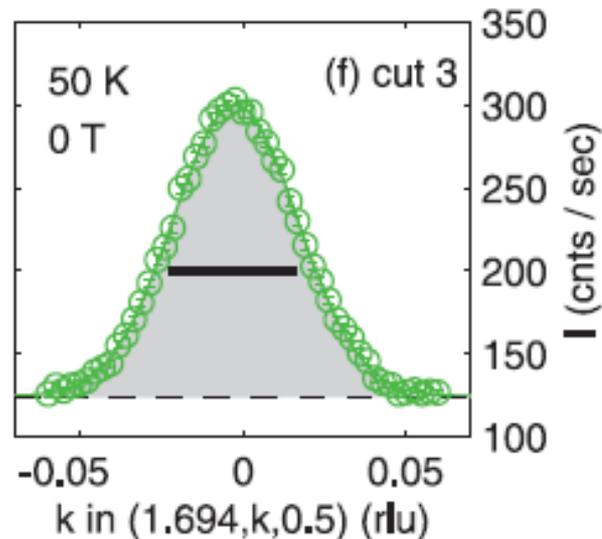
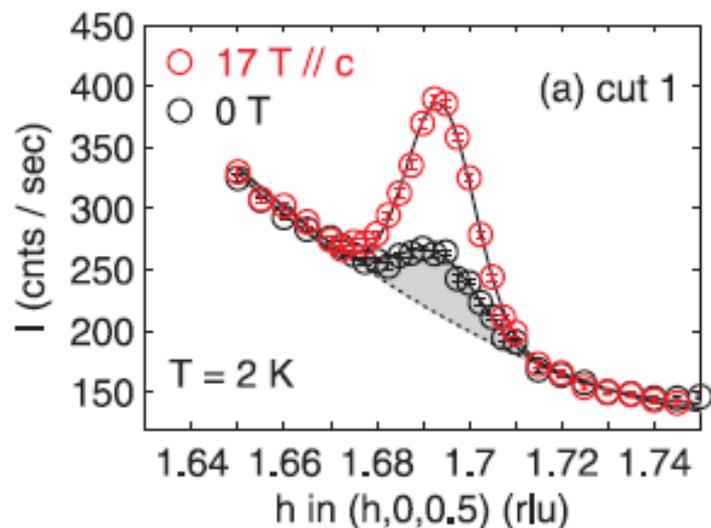
Achkar *et al.*, Phys. Rev. Lett. (2012).

# A bond density wave?



O-2p charge modulations

# Ortho-VIII example

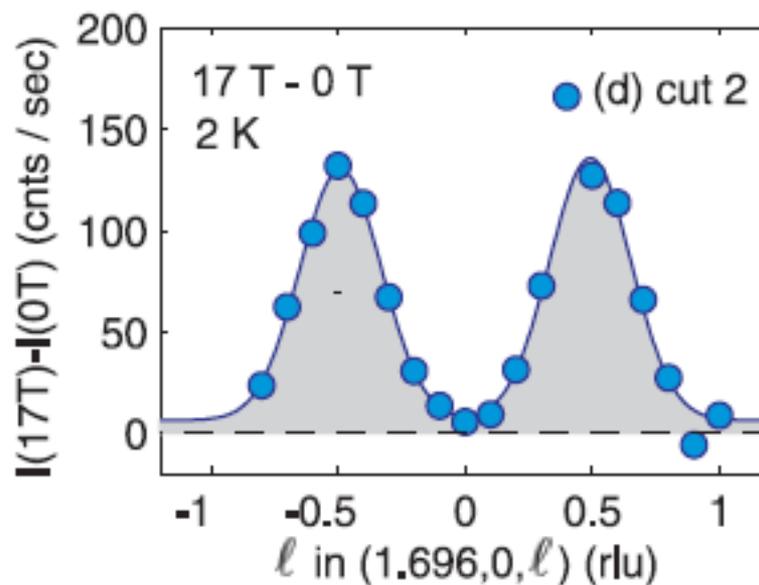


Correlation lengths:

$$\xi_a = 95 \pm 5 \text{ \AA}$$

$$\xi_c \approx 0.6 c$$

(Gaussian sigmas)



Lattice parameters:

$$a = 3.81 \text{ \AA}, b = 3.87 \text{ \AA}, c = 11.72 \text{ \AA}$$

# Origin of this scattering

atomic displacements vs charge modulation

$$\rho^u(x) = \frac{Ze}{a} [1 + uq \cos(qx)]$$

$$\rho^v(x) = \frac{2e}{a} [1 + \Sigma_{CDW} N(\epsilon_F) \cos(qx)],$$

$$\frac{I^u}{I^v} = \left( \frac{Zuq}{2\Sigma_{CDW} N(\epsilon_F)} \right)^2 \approx 600.$$

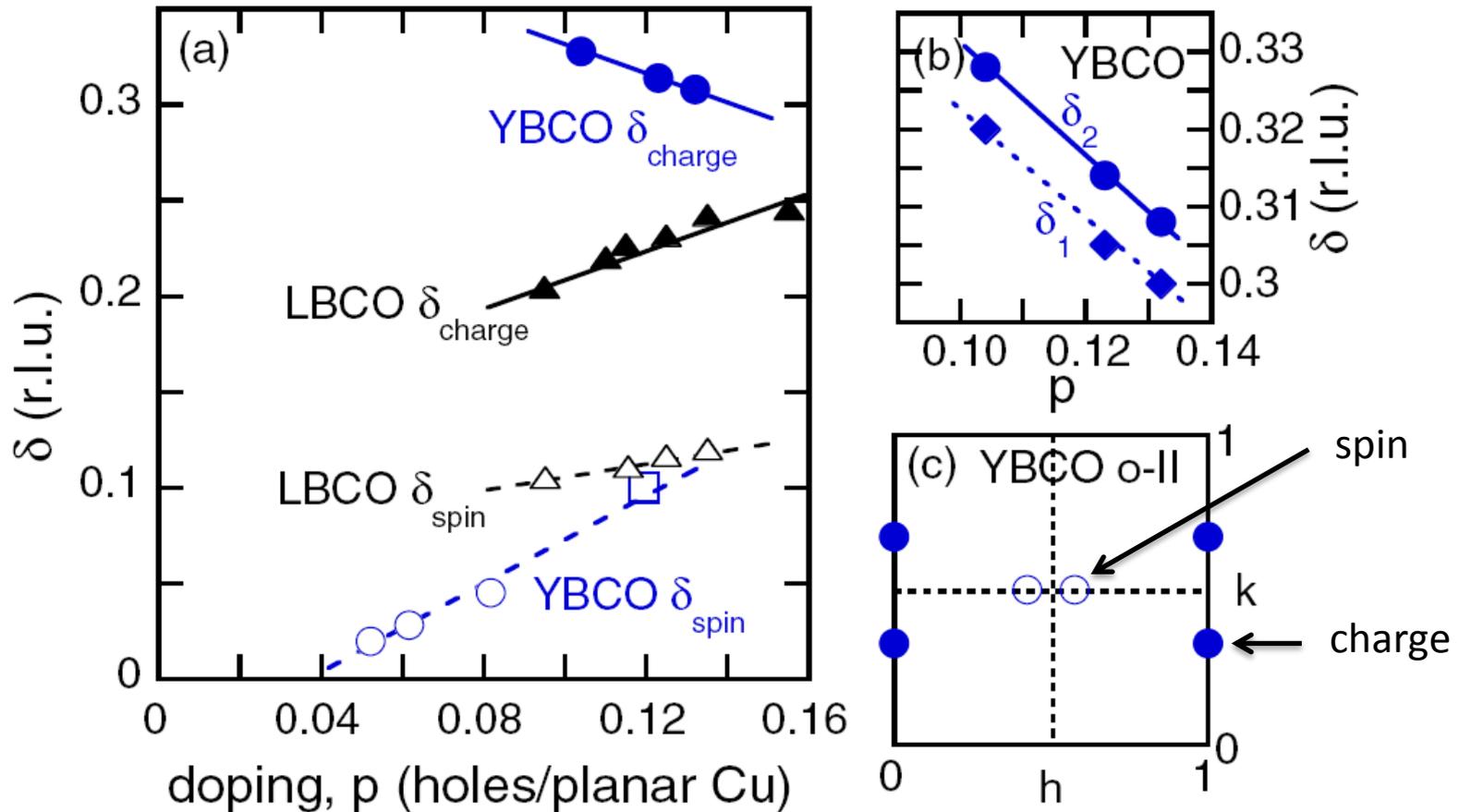
estimated:  $u/a \sim 8 \times 10^{-4}$

measured  $u/a \sim 7 \times 10^{-4}$

$$u = \left( \Sigma_{CDW}^2 N(\epsilon_F) / M\omega_q^2 \right)^{1/2} \approx 0.003 \text{ \AA}.$$

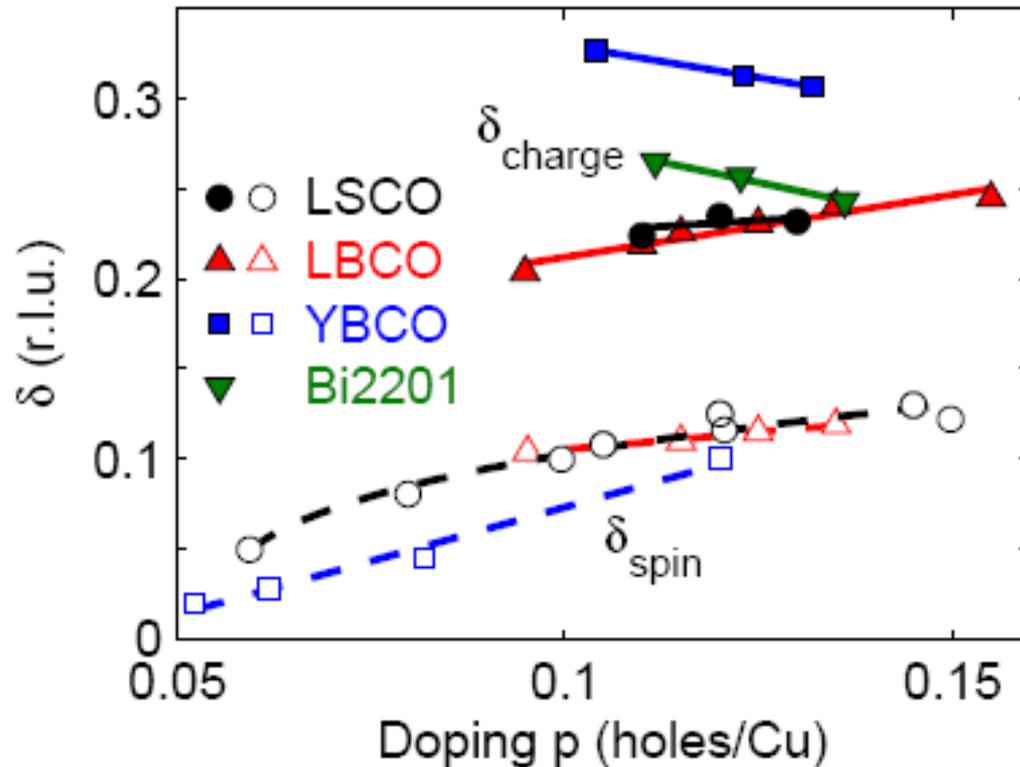
net charge / unit cell  
(CDW amplitude) is  
 $\sim 10^{-3} e$ , => not a Cu  
valence modulation

# Spin and charge wavevectors



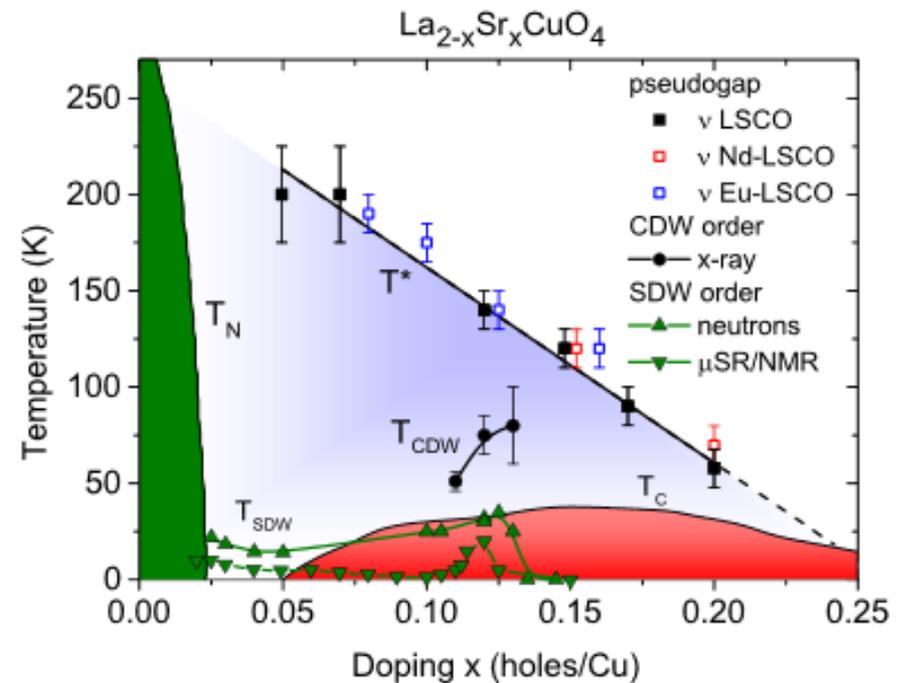
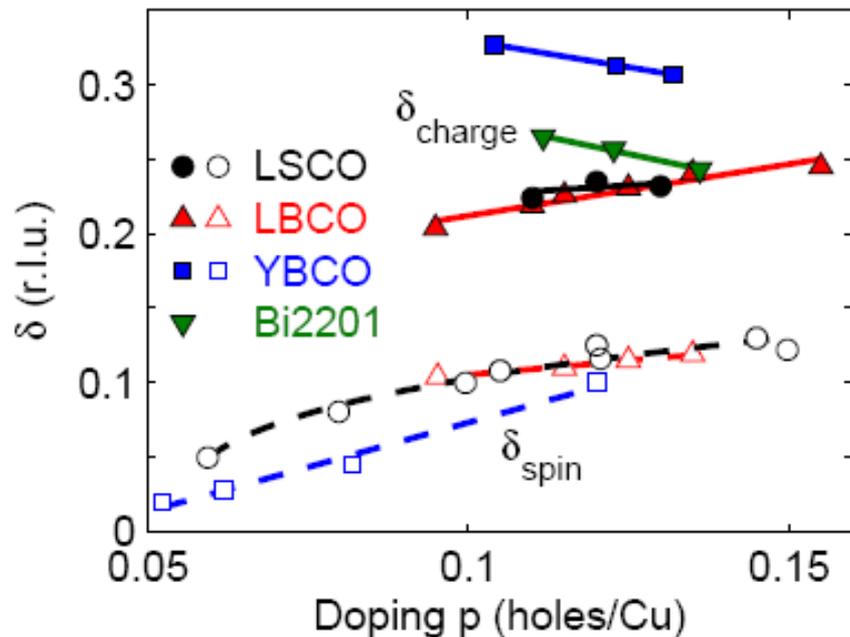
$$\delta_{\text{charge}} \neq 2\delta_{\text{spin}}$$

# Spin and charge wavevectors – updated a little...



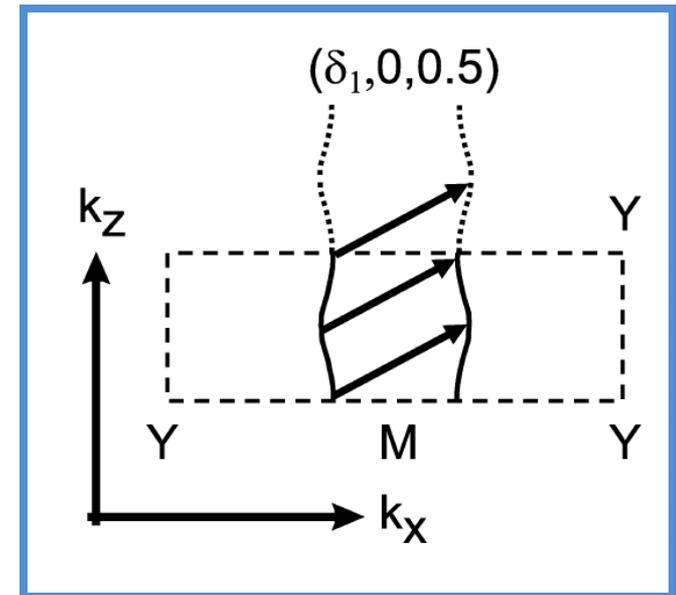
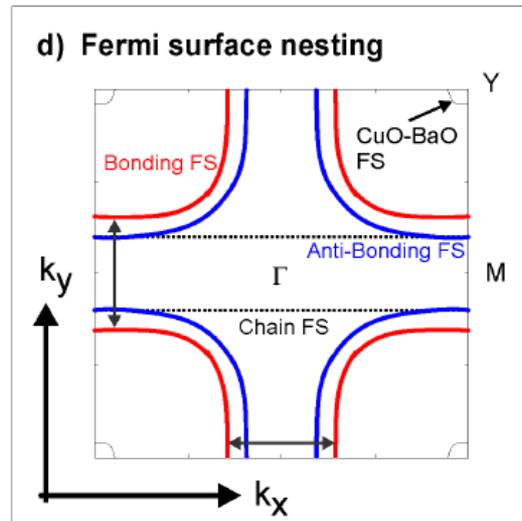
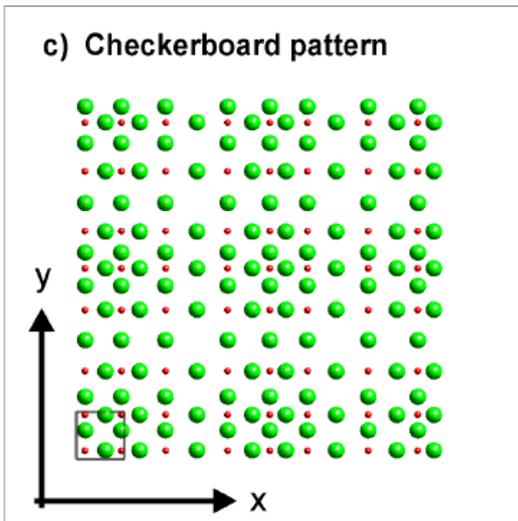
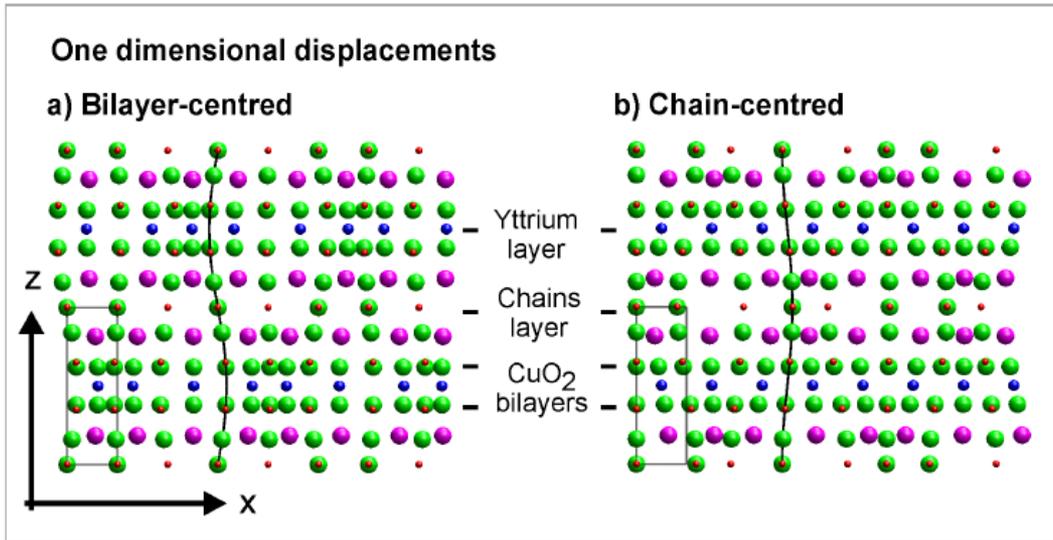
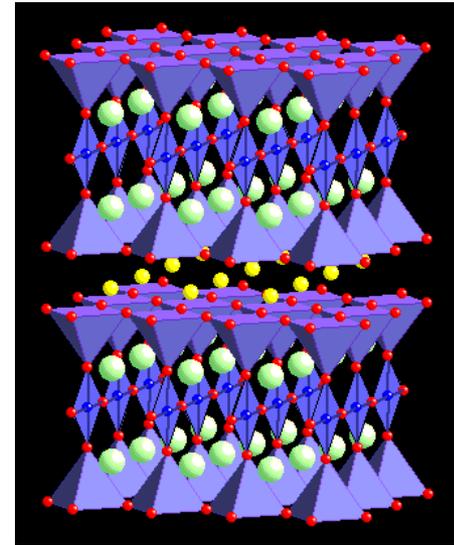
Open points: spin order or strong spin fluctuations at  $(\frac{1}{2} + \delta_{\text{spin}}, \frac{1}{2})$   
Closed points: CDW peaks at  $(\delta_{\text{charge}}, 0)$

# Spin and charge wavevectors – updated a little...

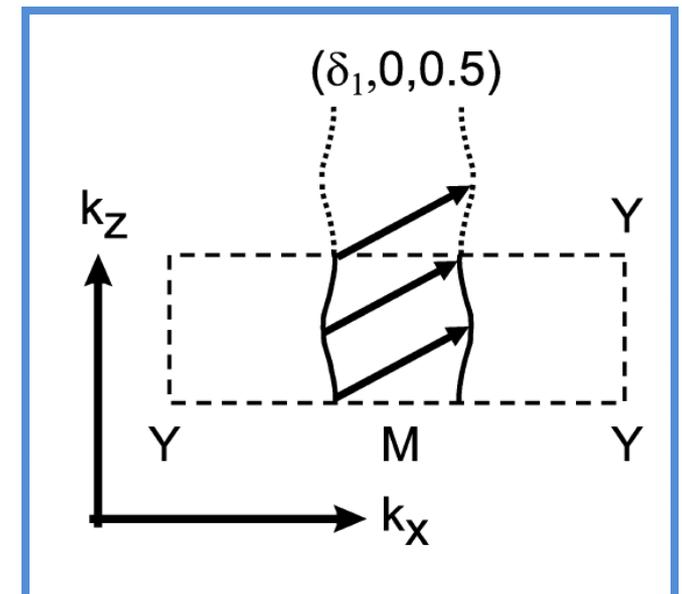
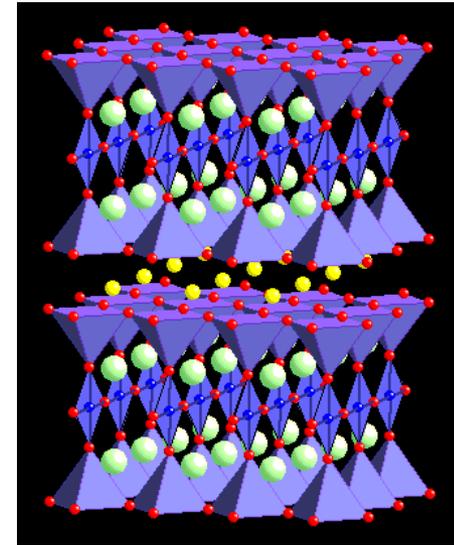
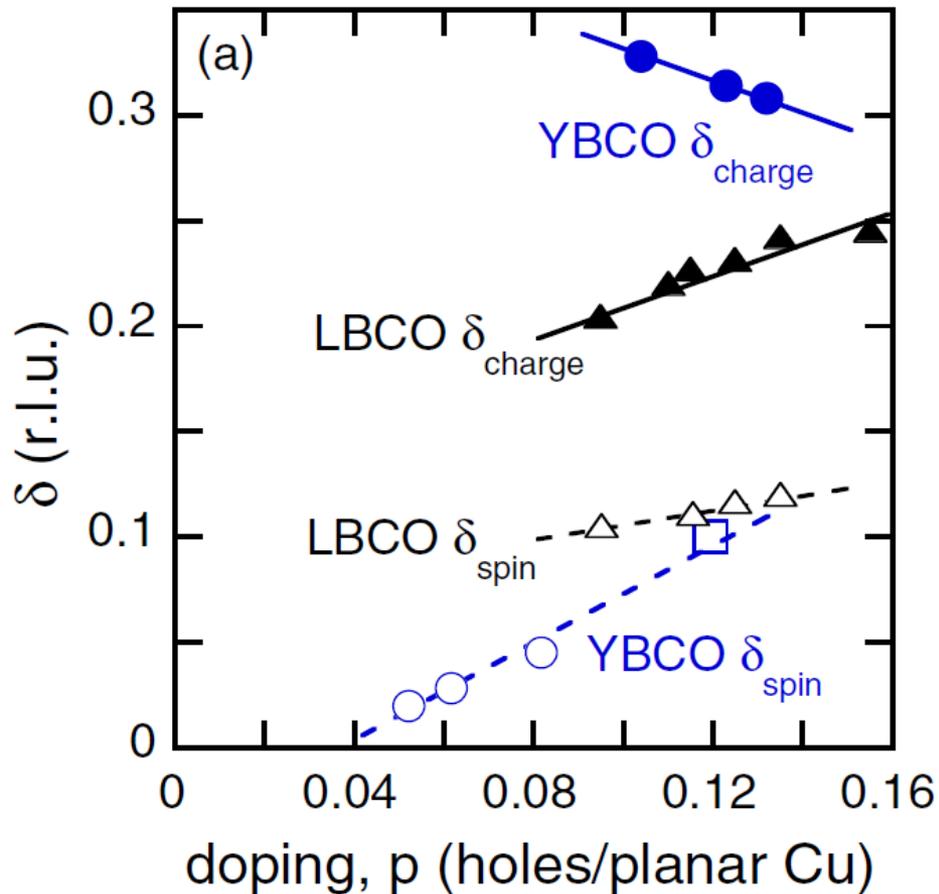


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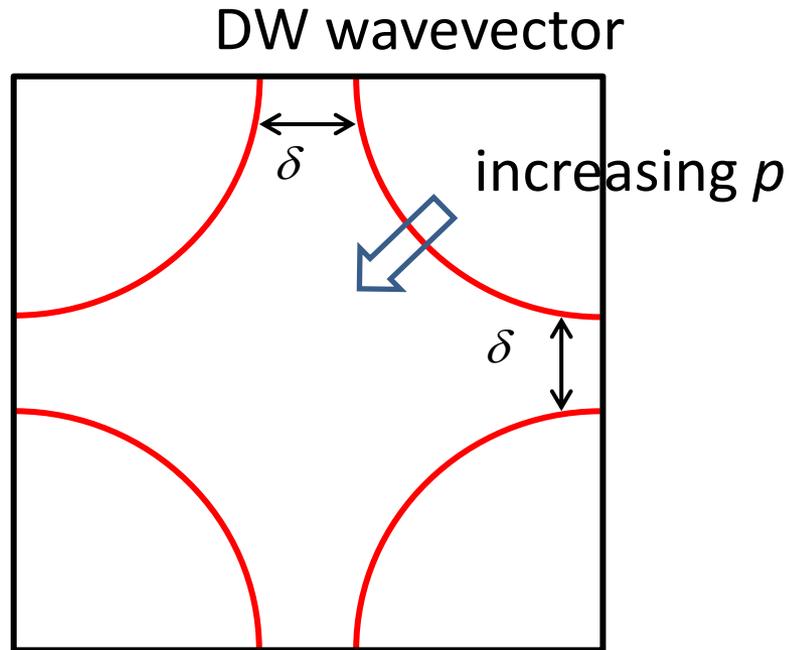
# Modelling the CDW



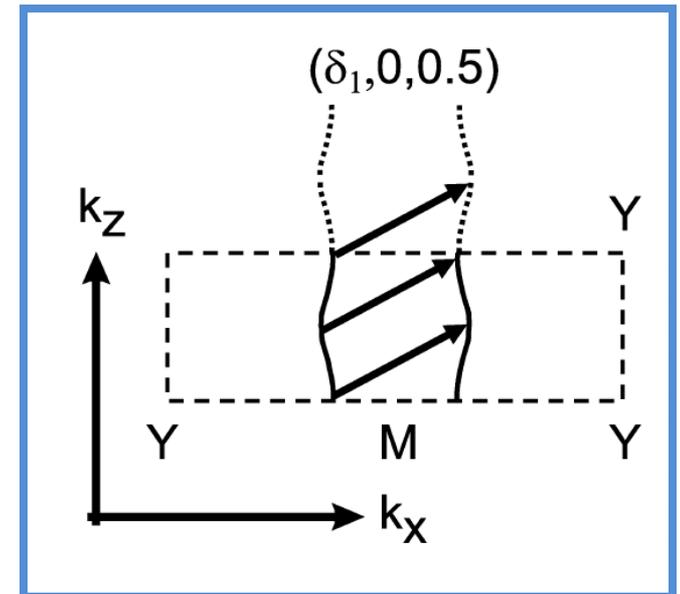
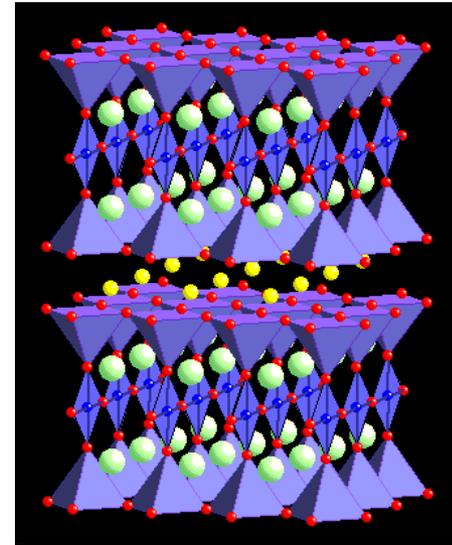
# Modelling the CDW



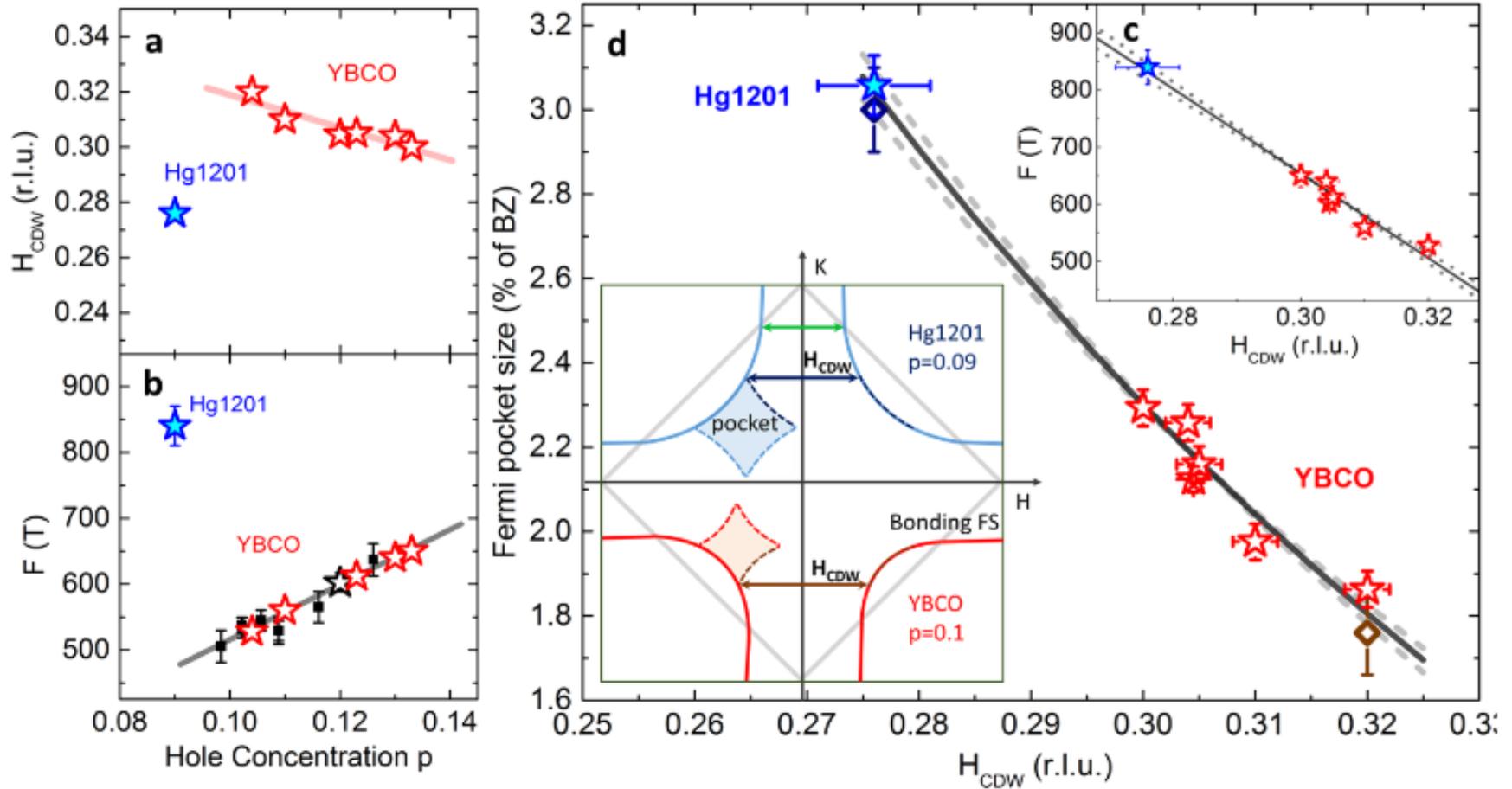
# Modelling the CDW



→ Fermi surface effects

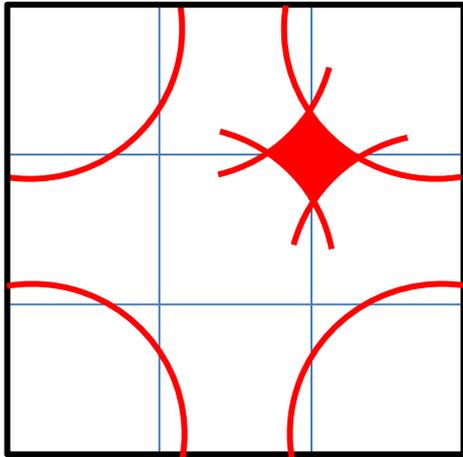


# Links to the Fermi surface



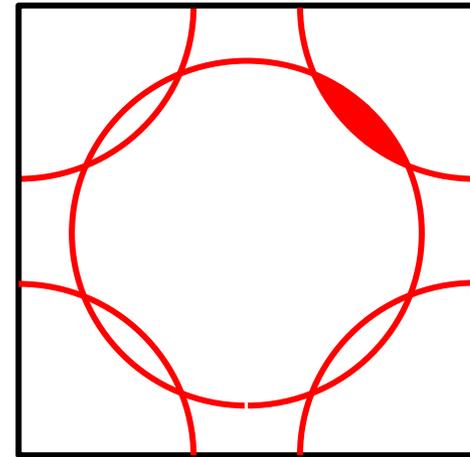
# 2D suggestions for Fermi surface reconstruction

Charge Density Wave



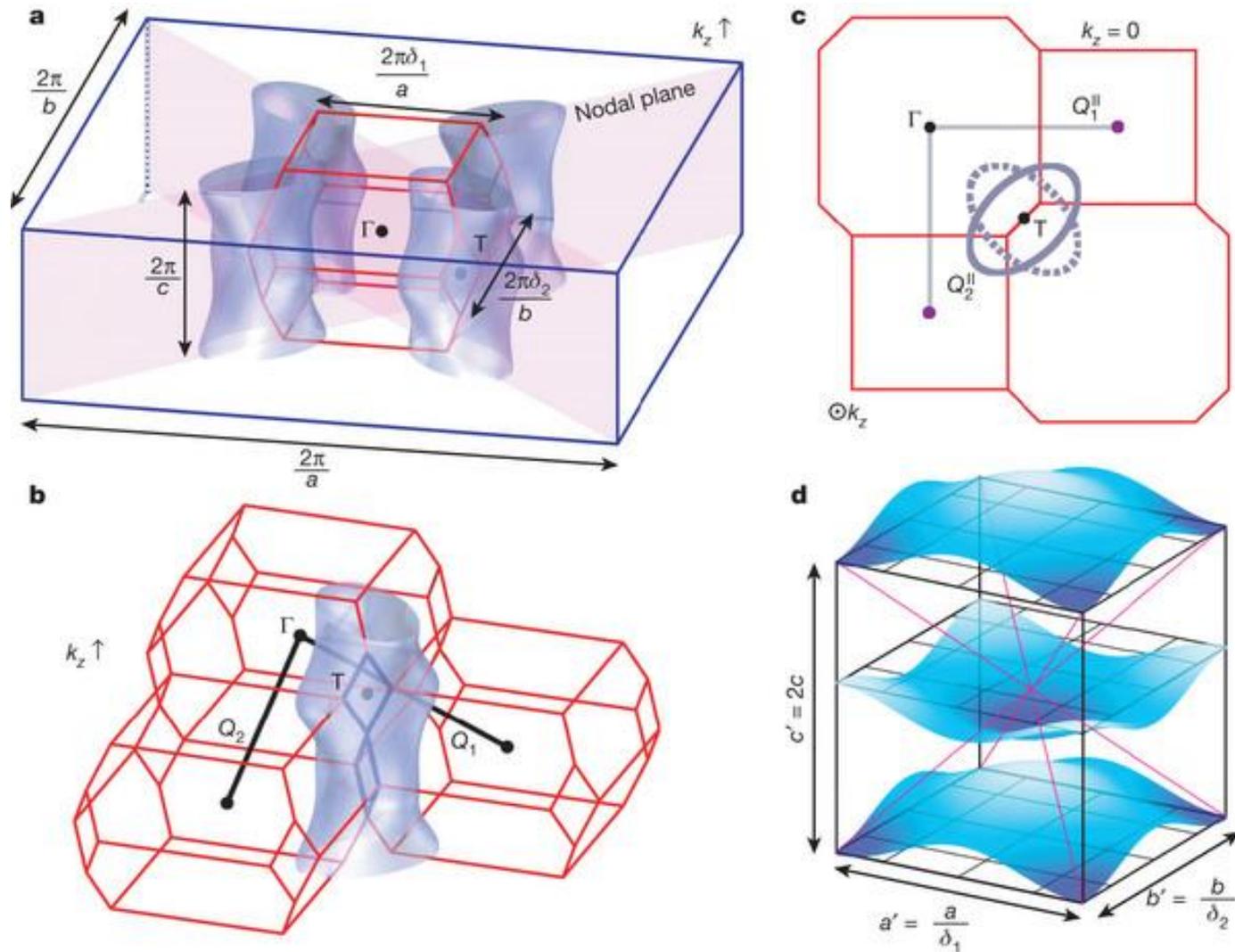
gives an electron pocket  
(N.B. this is a 2d picture of  
3d reconstruction by CDW)

“Antiferromagnetic”

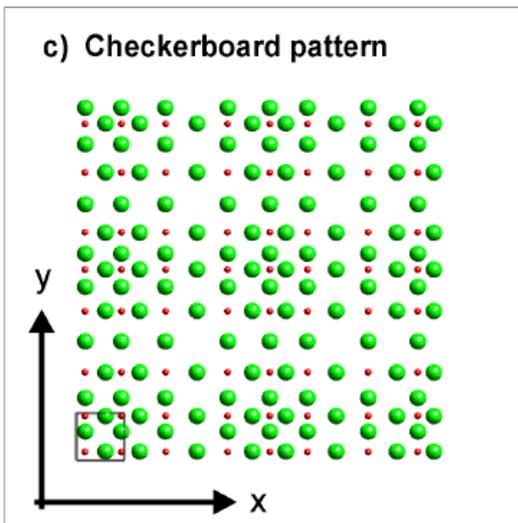
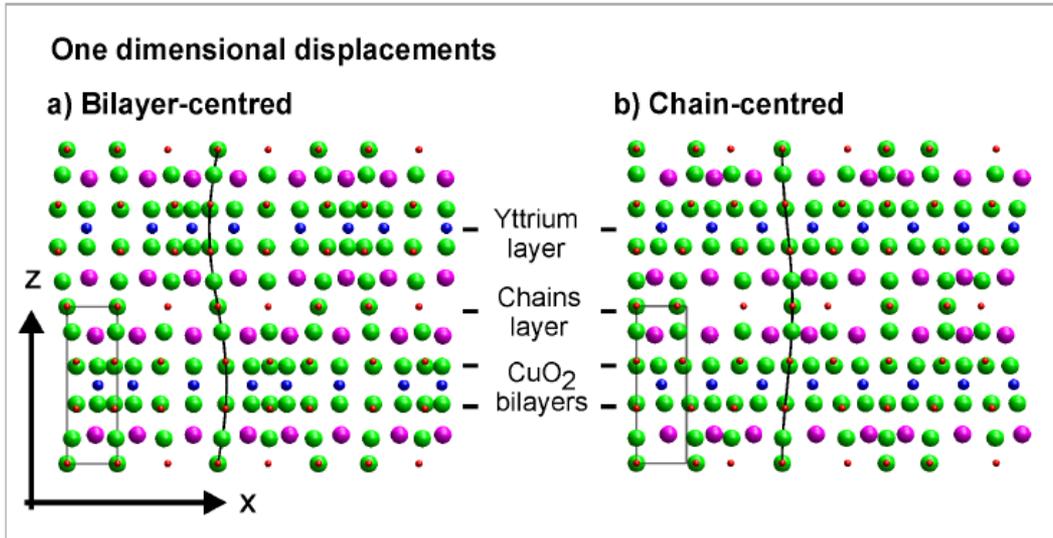


looks a bit like  
the ARPES/STM signals  
gives a hole pocket –  
disagrees with Hall data

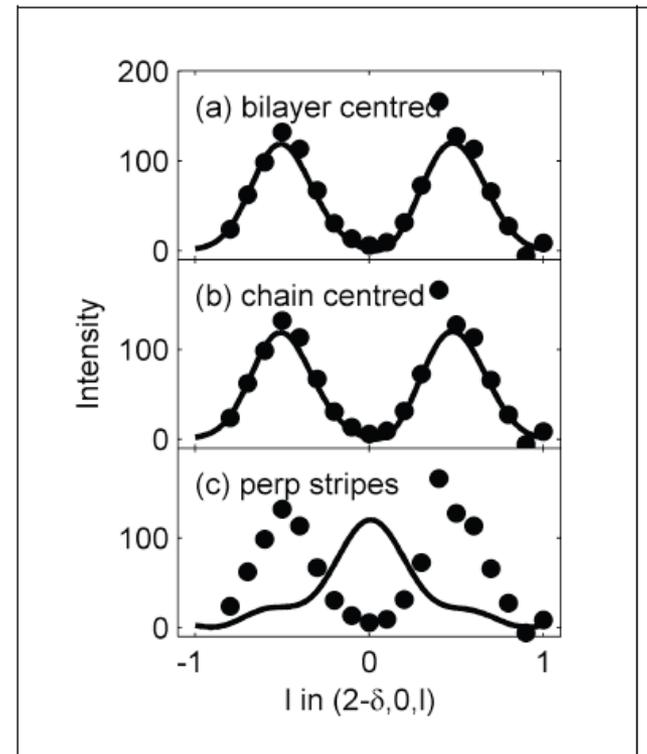
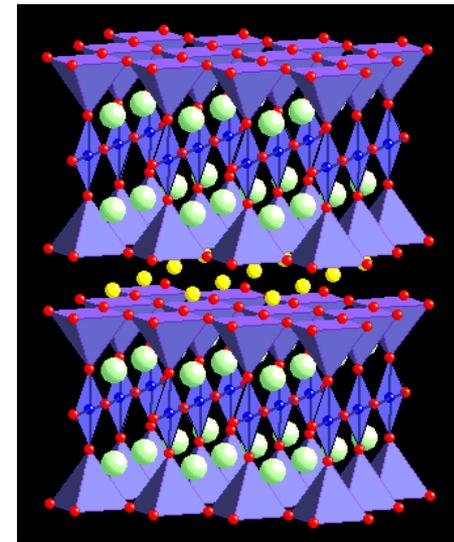
# The Fermi surface – quantum oscillation data



# Modelling the CDW

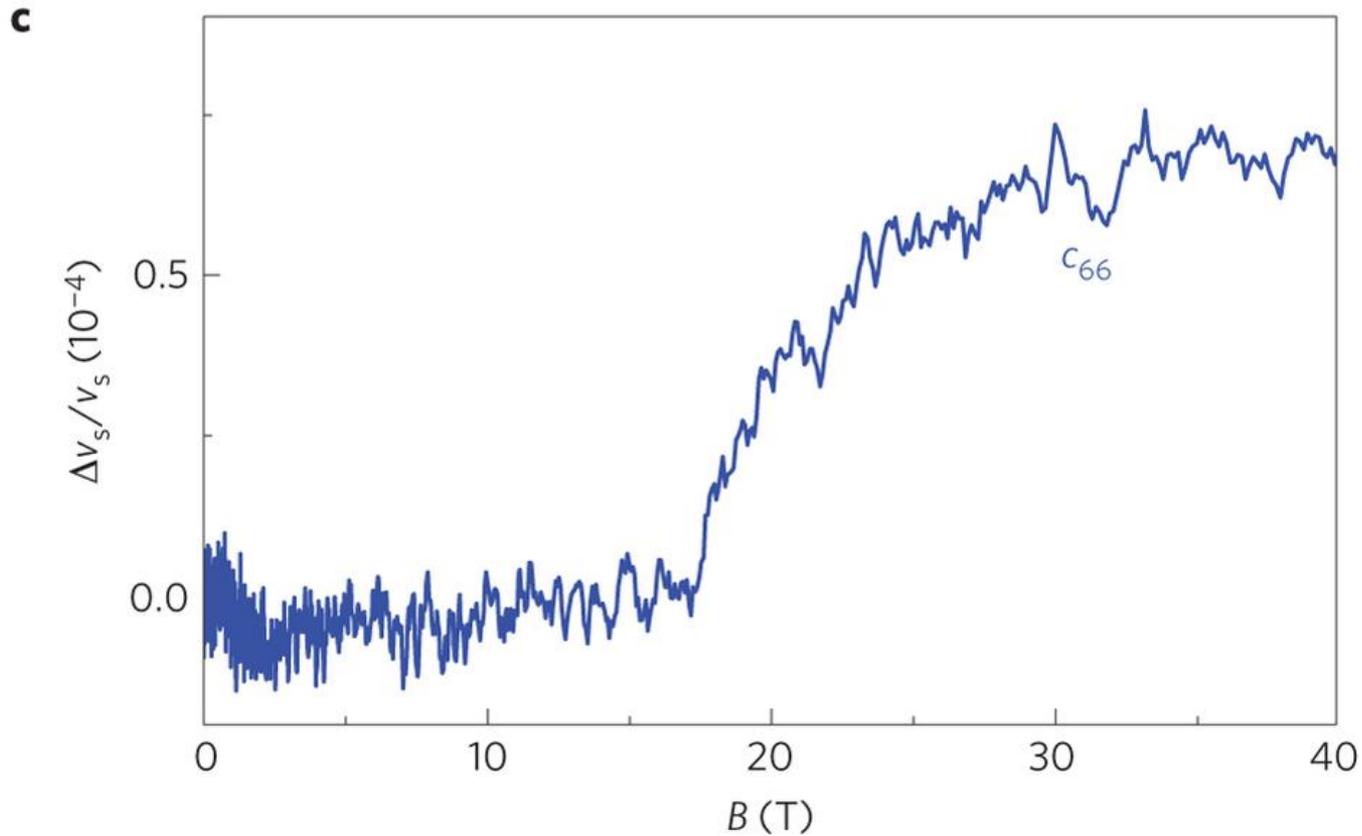


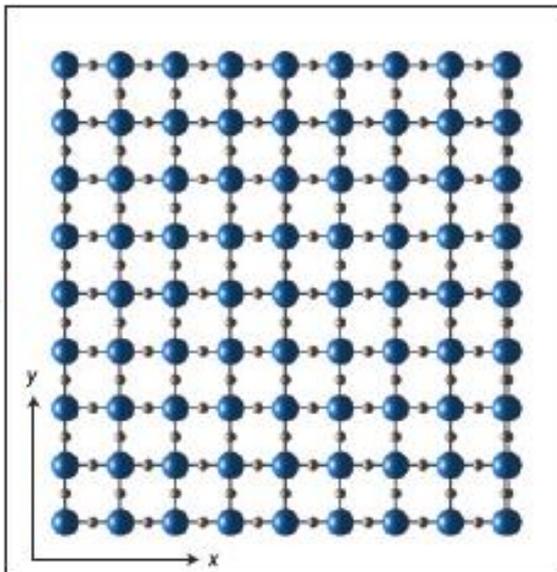
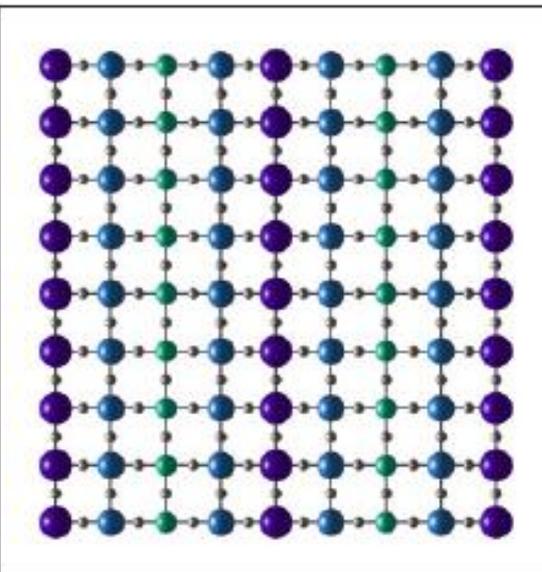
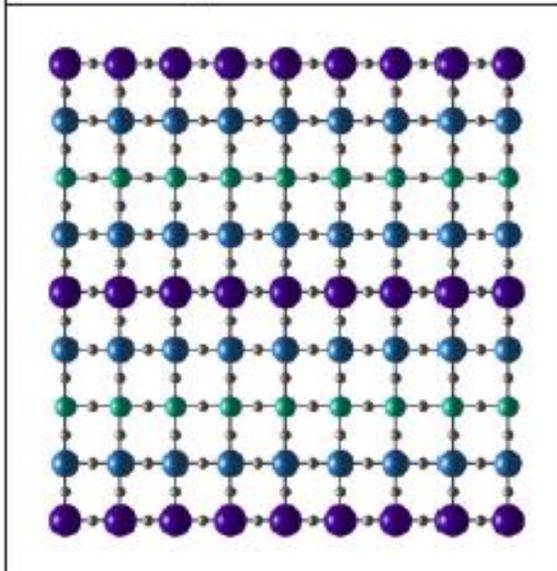
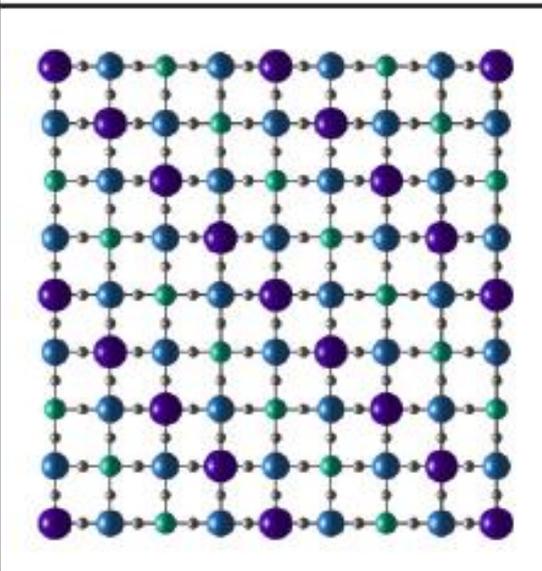
Is it single-q or double-q?



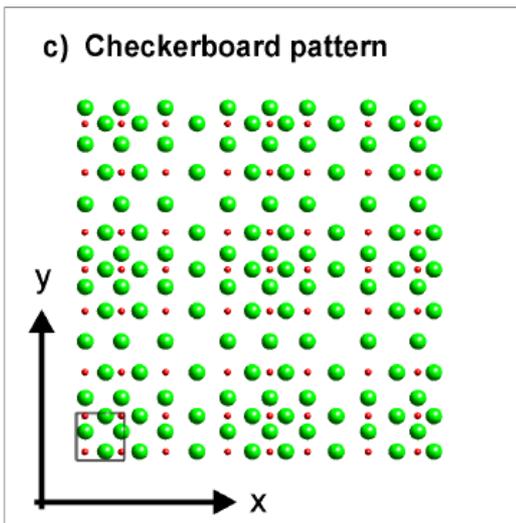
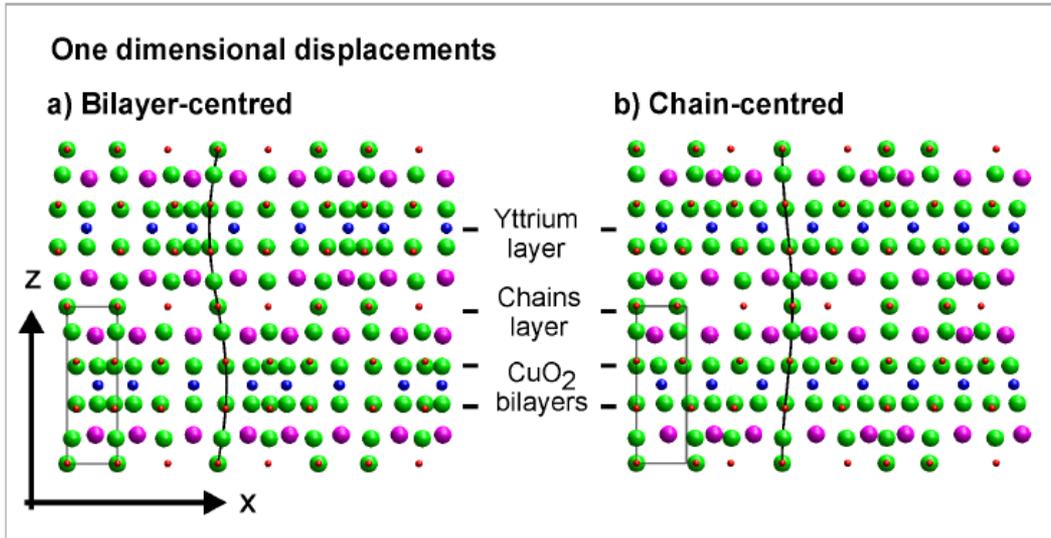
# Ultrasound Studies

ortho-II

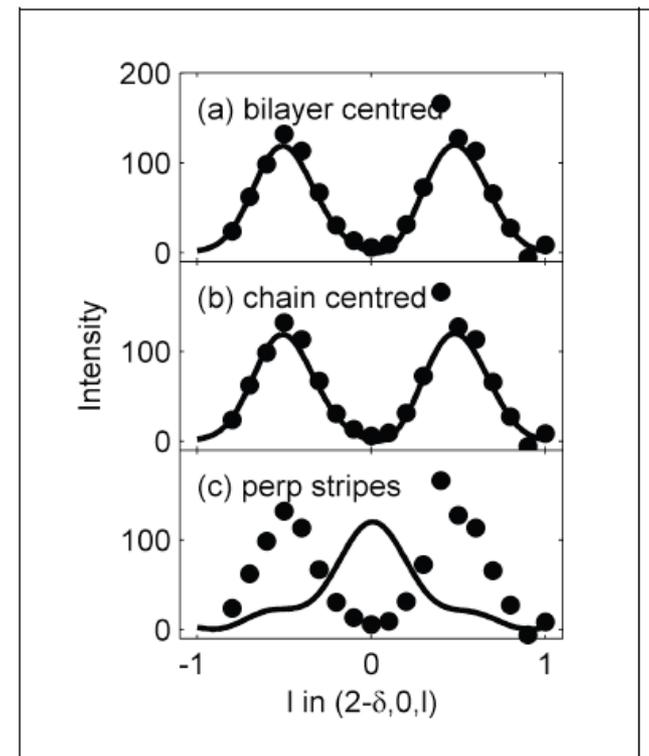
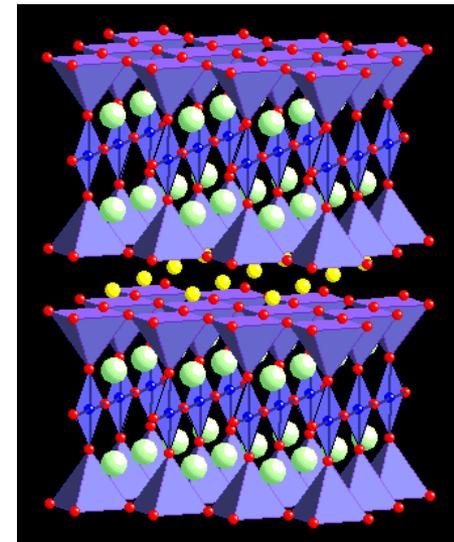


$C_{11}$  $c_{11}$  $c_{44}$  $C_{44}$  $C_{55}$  $c_{55}$  $c_{66}$  $C_{66}$ 

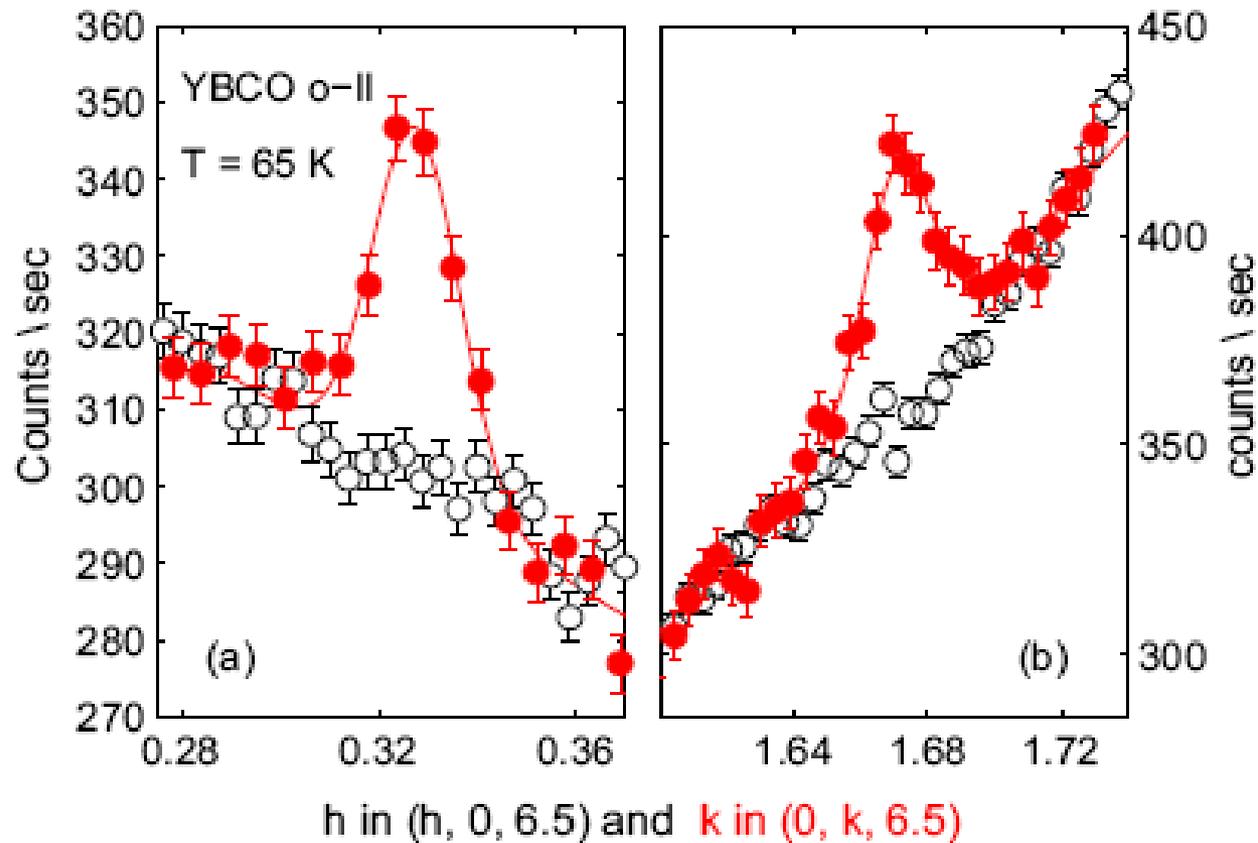
# Modelling the CDW



Is it single-q or double-q?

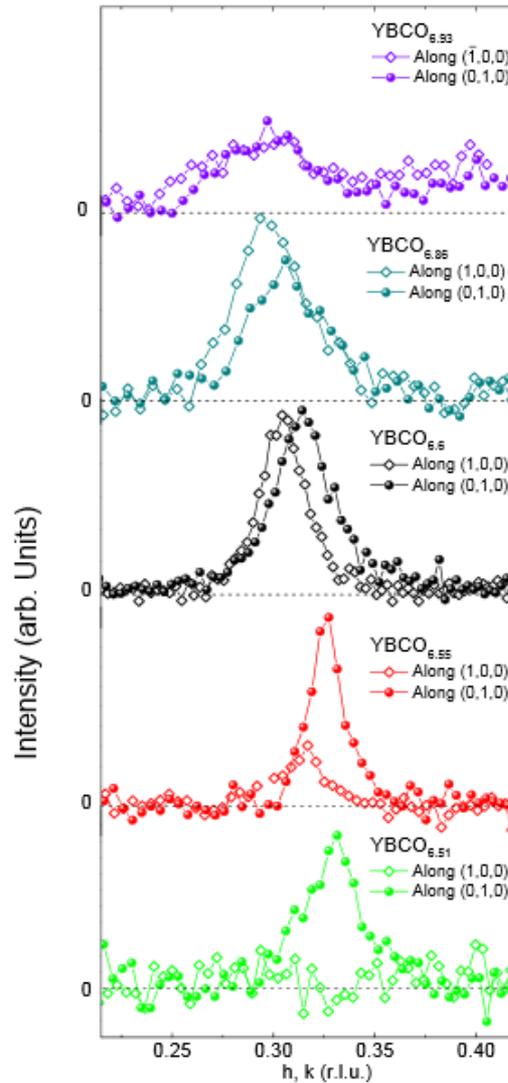


# Differences between $q_a$ and $q_b$



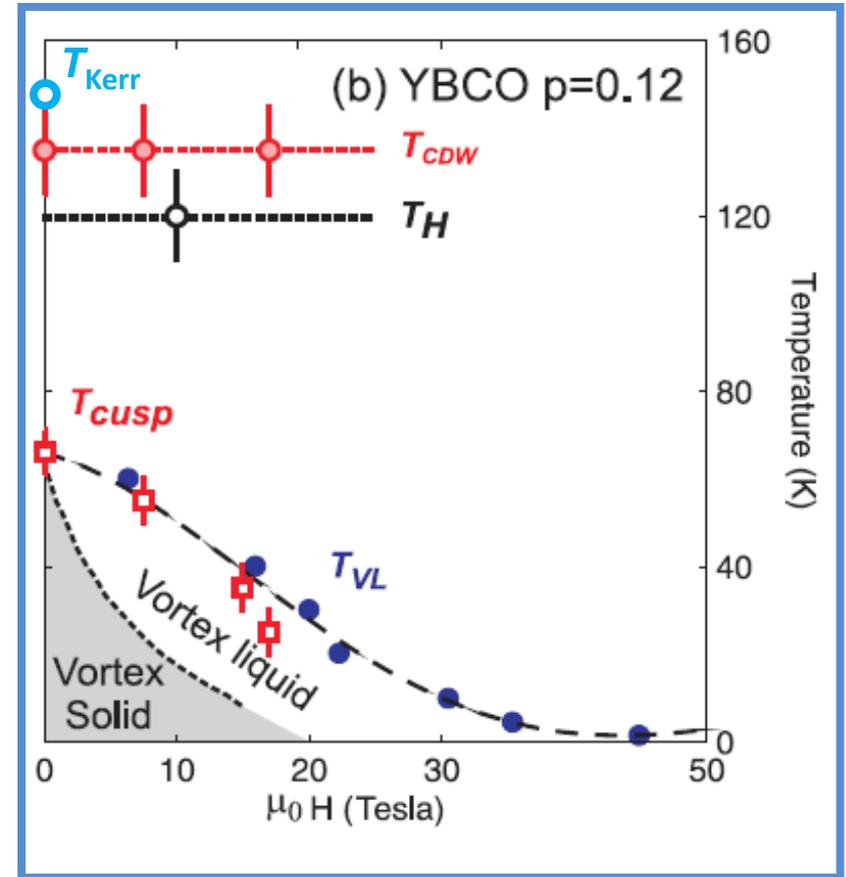
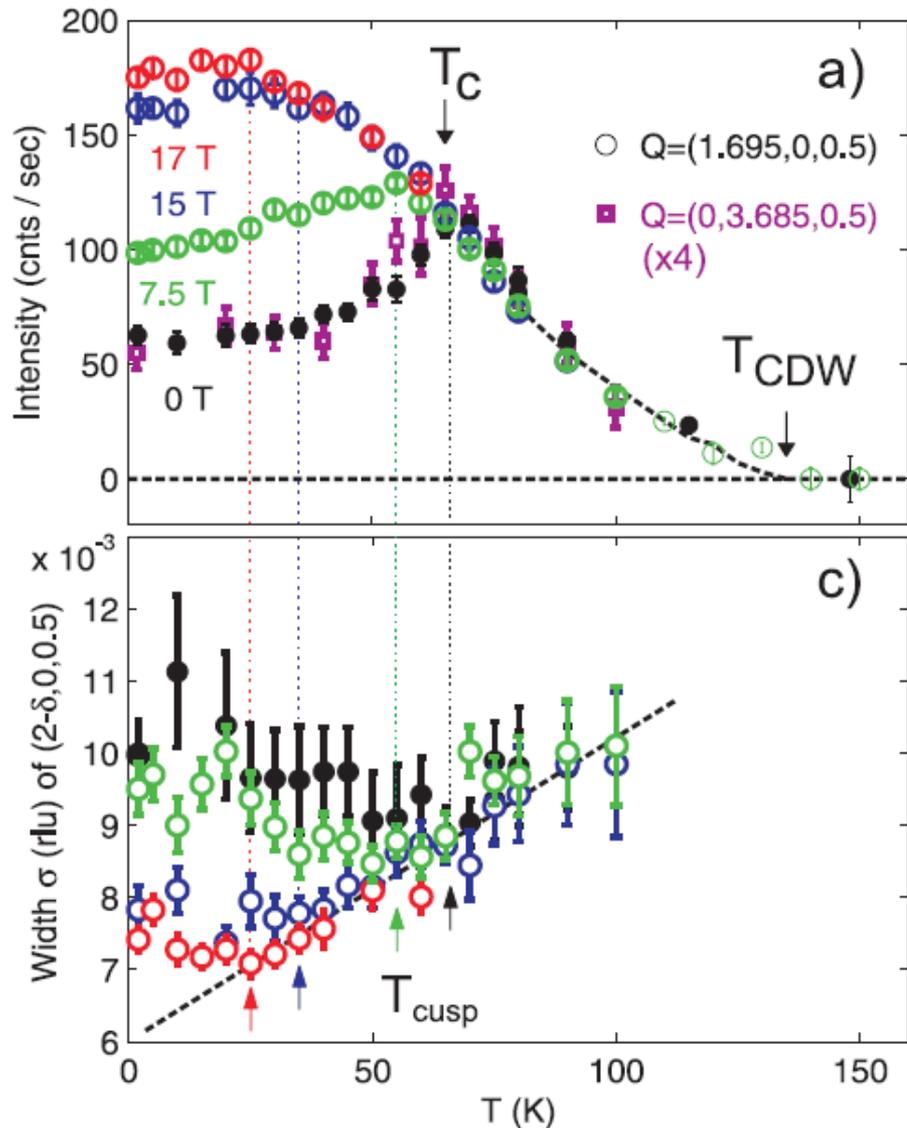
It is therefore likely that the lattice response is driven by the  $\text{CuO}_2$  planes, which determine the  $\mathbf{q}$ .

# Differences between $q_a$ and $q_b$



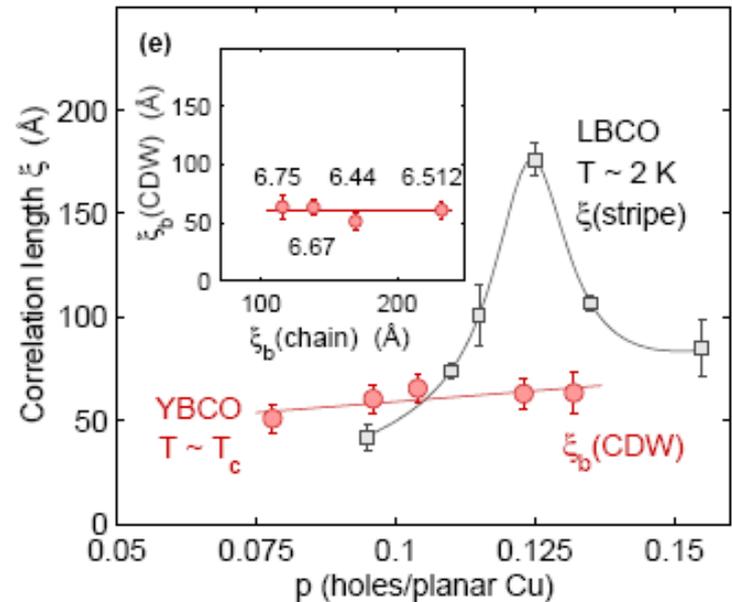
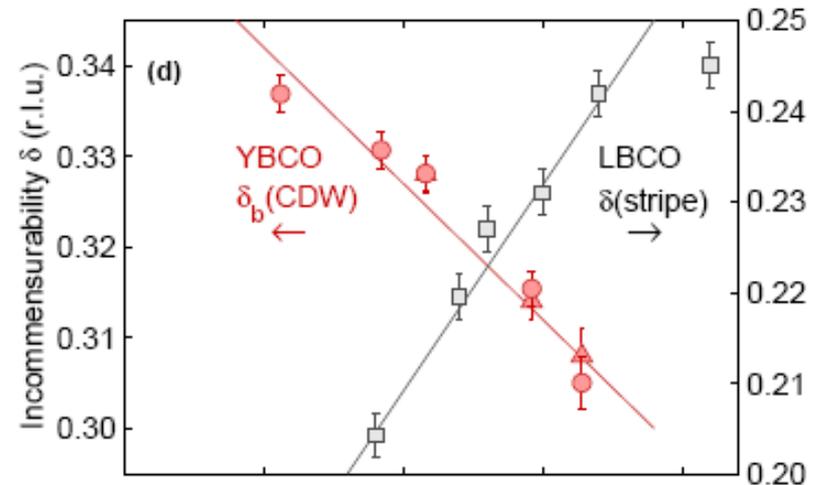
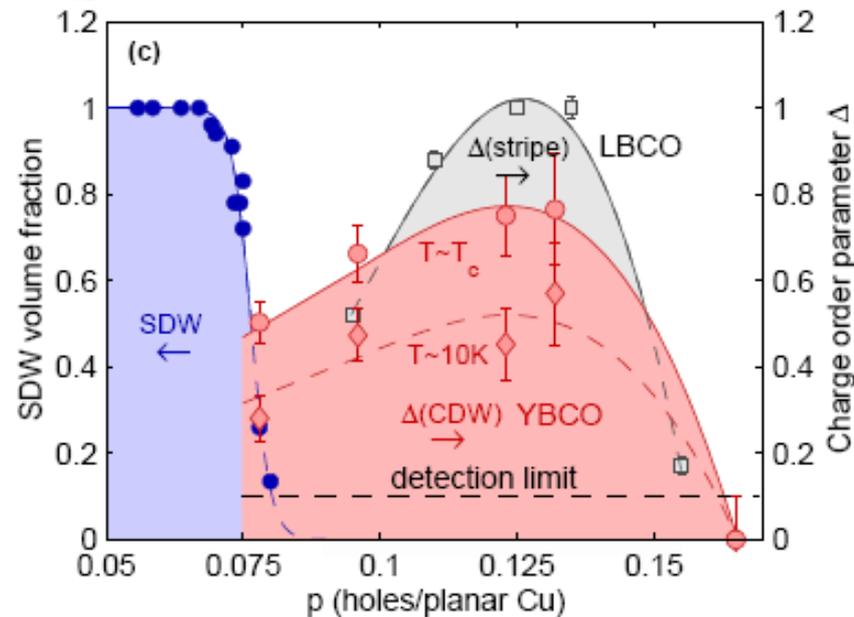
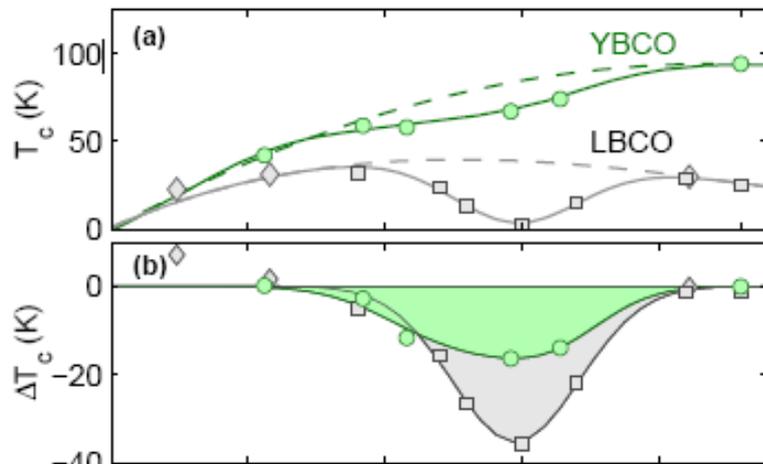
Blanco-Canosa *et al.* arXiv 1406.1595 (2014).

# Crossover temperature as f(B)

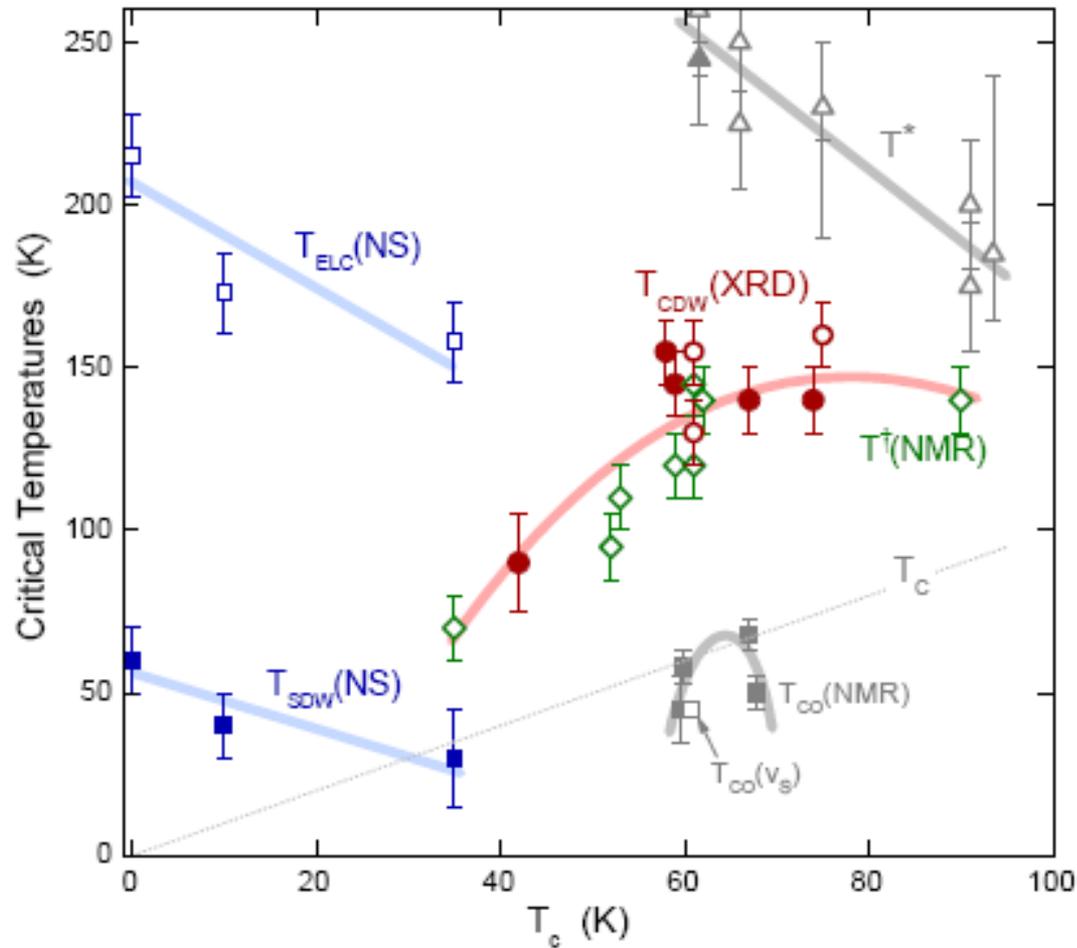


$T_{VL}$  and  $T_{VS}$  from  
LeBoeuf *et al.*, PRB **83**, 054506 (2011).

# Examining the doping dependence



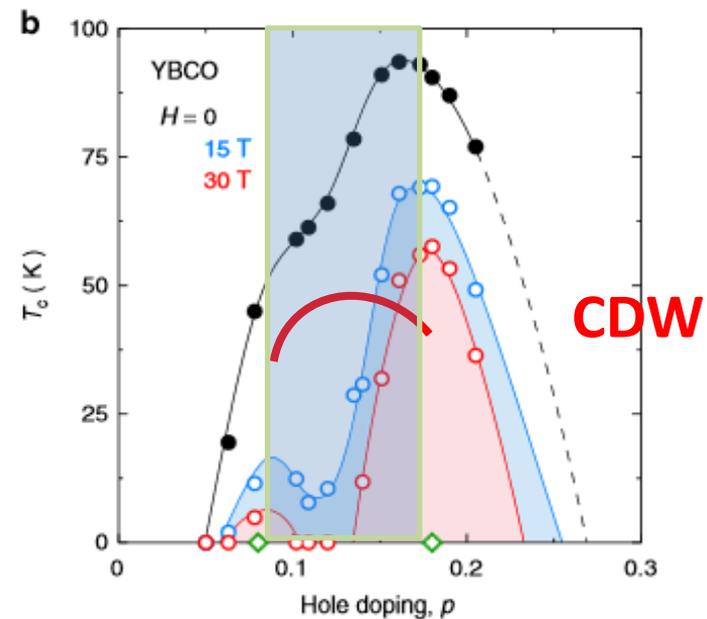
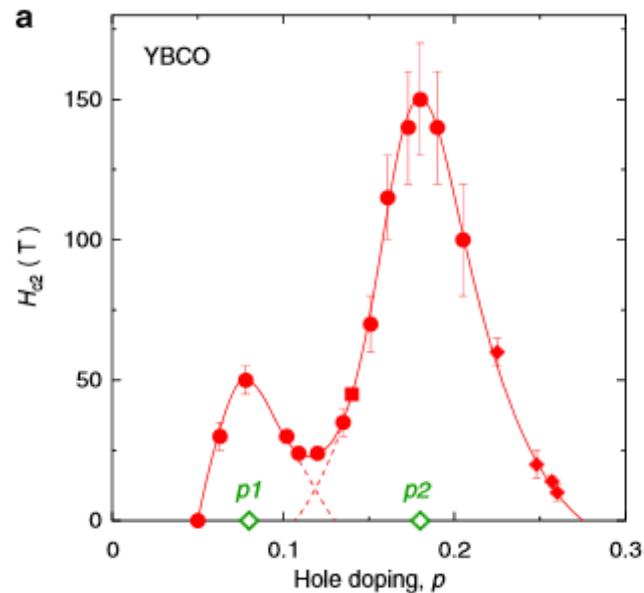
# Examining the doping dependence



$T^\dagger$  = broad maximum in  $1/(T_1T)$  from planar  $^{63}\text{Cu}$  NQR/NMR

# Studying the critical field in YBCO

- Two superconducting domes?

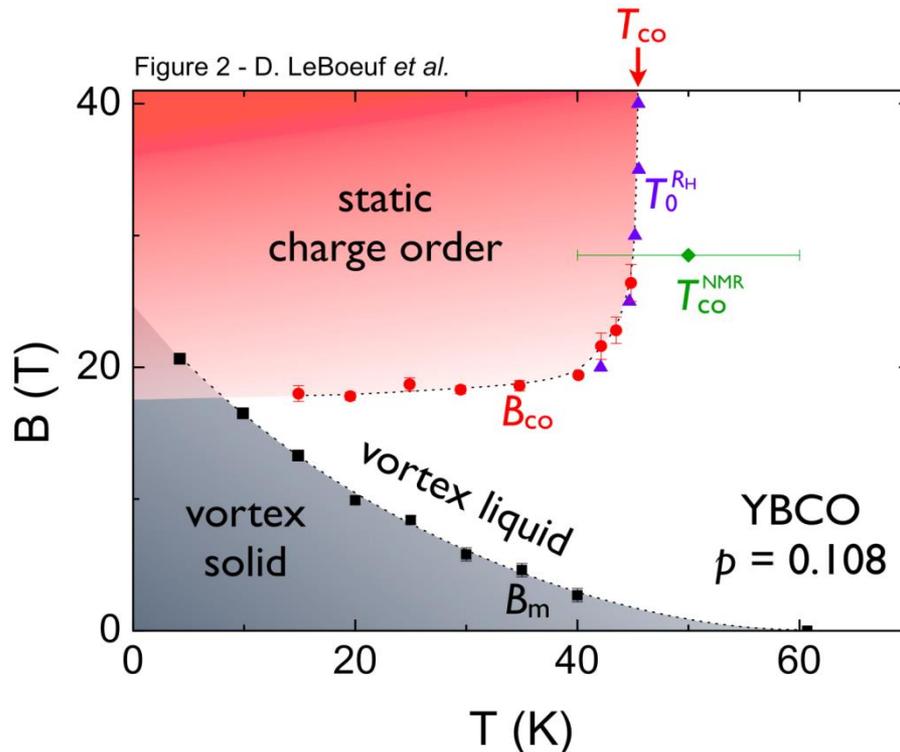


# Signs of something changing inside the PG region

- Transport measurements
- NMR/NQR
- Quantum oscillations
- Kerr effect
- Ultrasound
- Polarized neutron diffraction

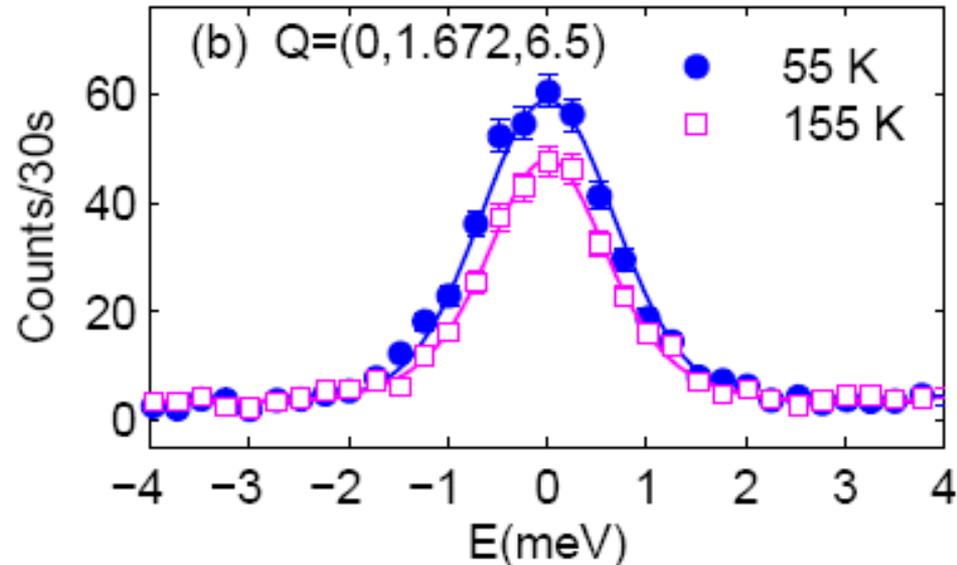
# Time/Energy Scales of CDW

Probe	$E_{\text{probe}}$	$T_{\text{CO}}(\text{K})$	B(T)
NMR <sup>8</sup>	$1.5 \mu\text{eV}$	50	28.5
ultrasound <sup>10</sup>	$0.6 \mu\text{eV}$	44.8	26.4
100 keV x-ray diffraction <sup>4</sup>	$\sim 1 \text{ keV}$	155(10)	0
IXS (this work)	$1.5 \text{ meV}$	150(40)	0



# Can we improve these measurements with using inelastic x-ray scattering?

Lifetime



Energy at which the charge response is probed.

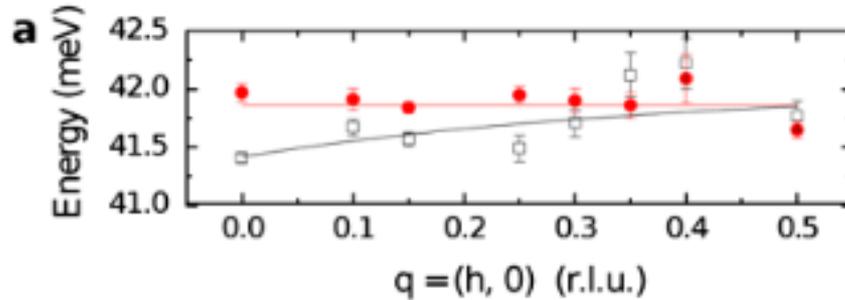


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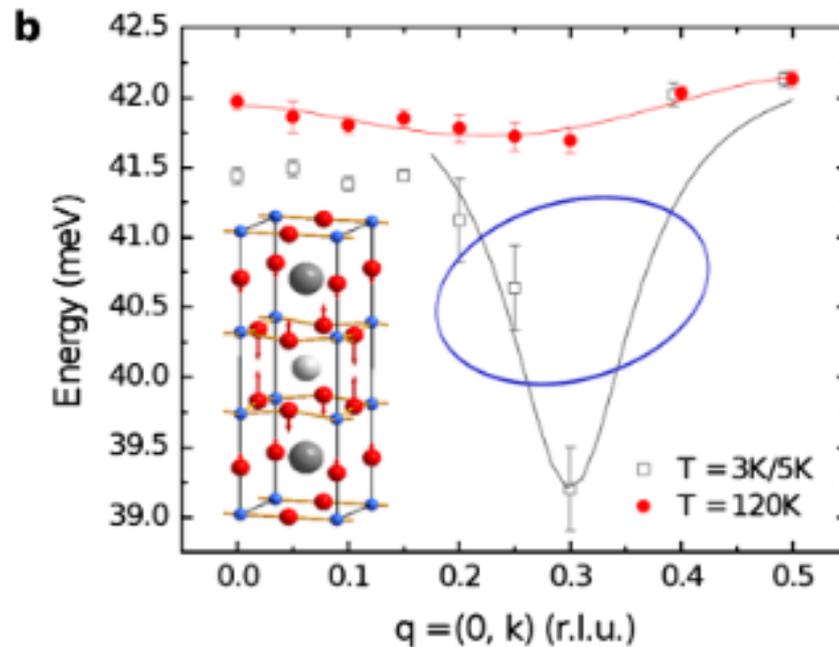
Energy resolution of the instrument.

# What about phonons?

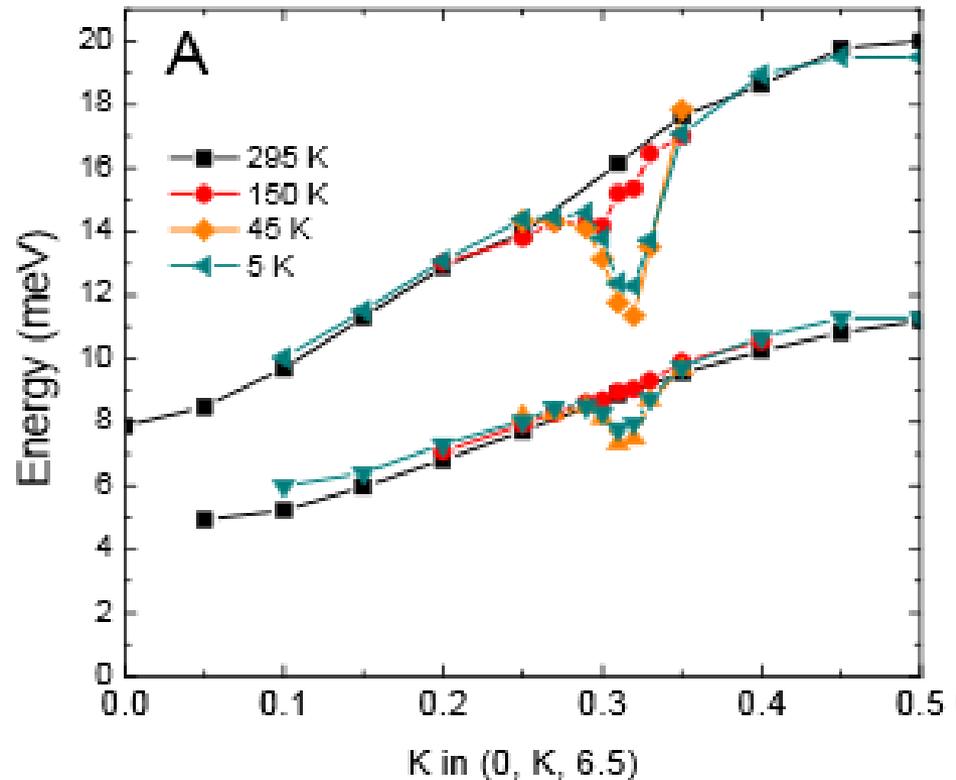
Cu-O bond bending phonon @  $\sim 40$  meV (YBCO7)



Softens at  $k = 0.3$ ,  
but not at  $h = 0.3$

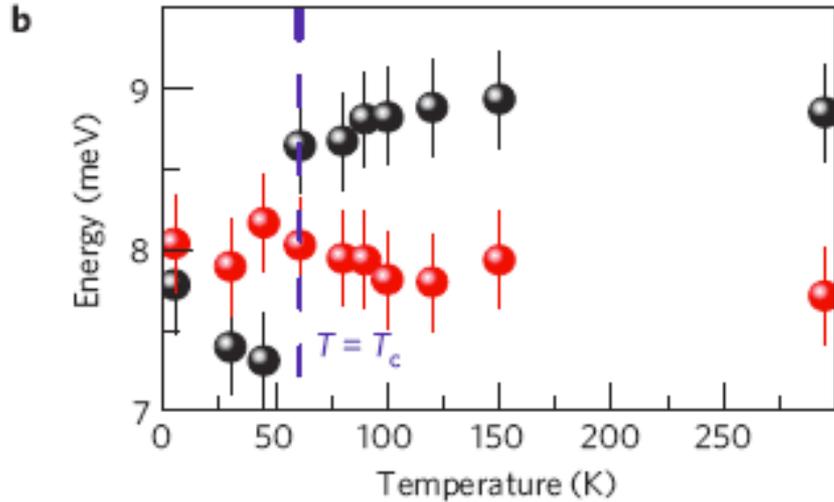


# Associated Phonon Anomalies – ortho-VIII



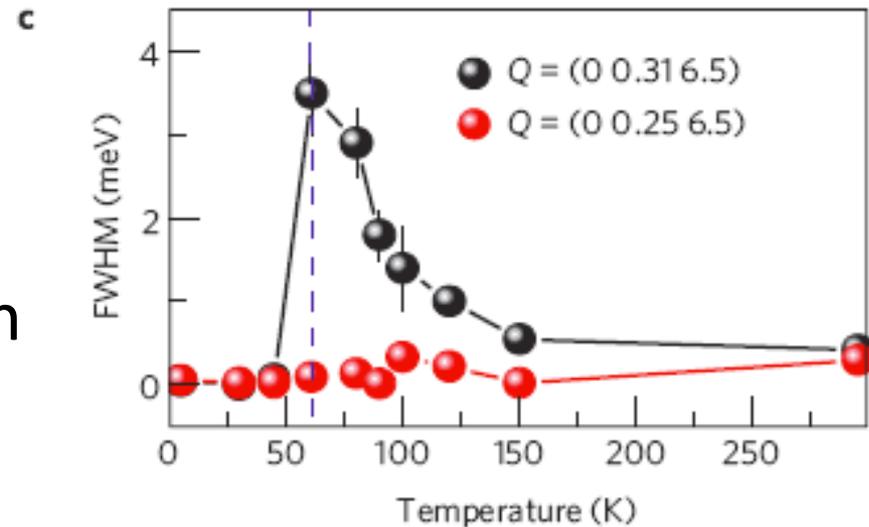
Almost purely transverse acoustic mode

# Associated Phonon Anomalies – ortho-VIII

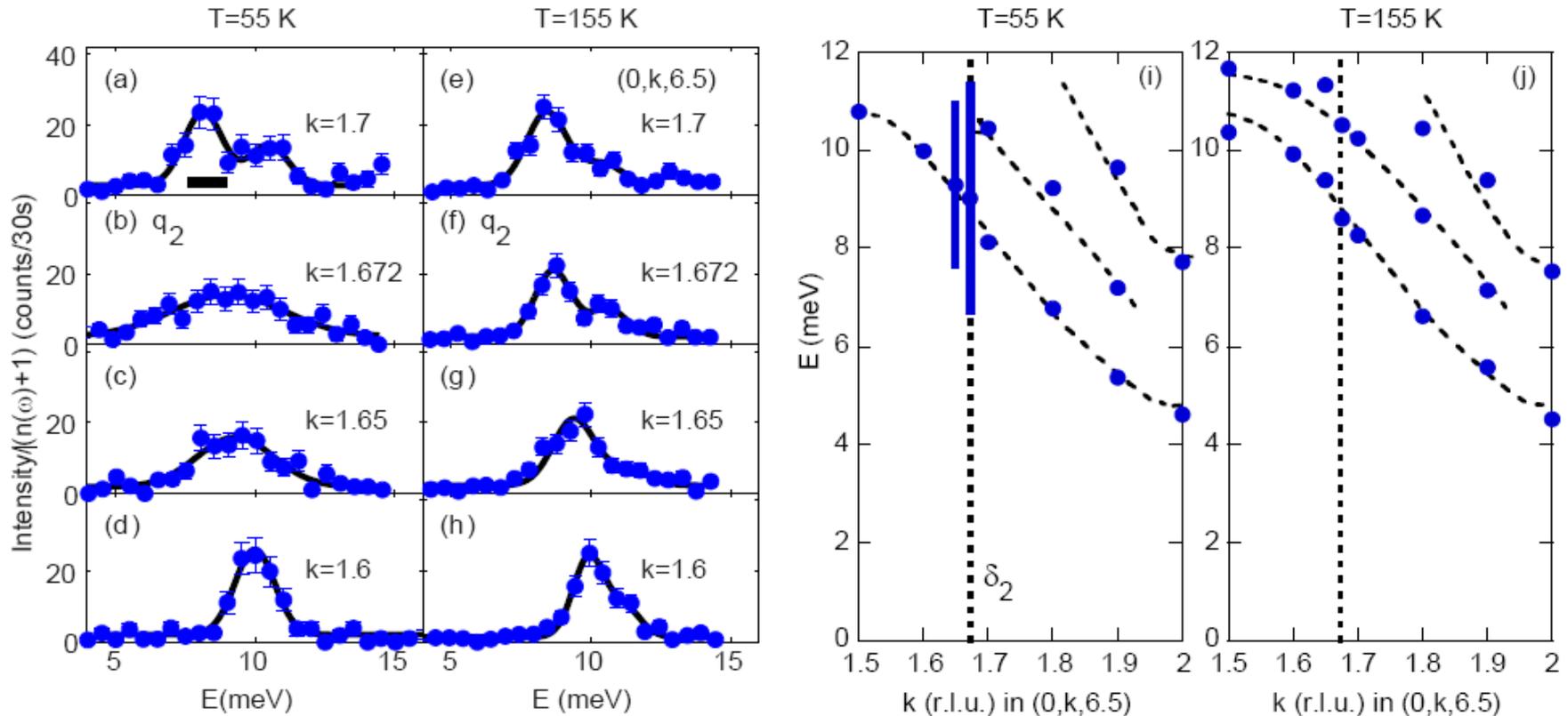


Mode Energy

Phonon Linewidth

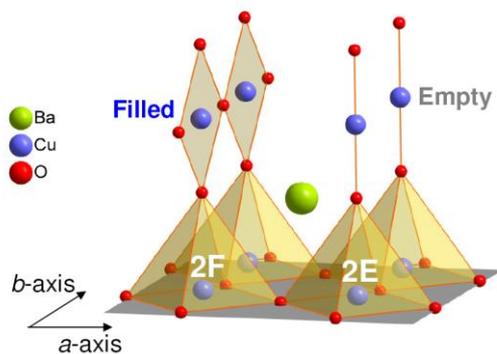
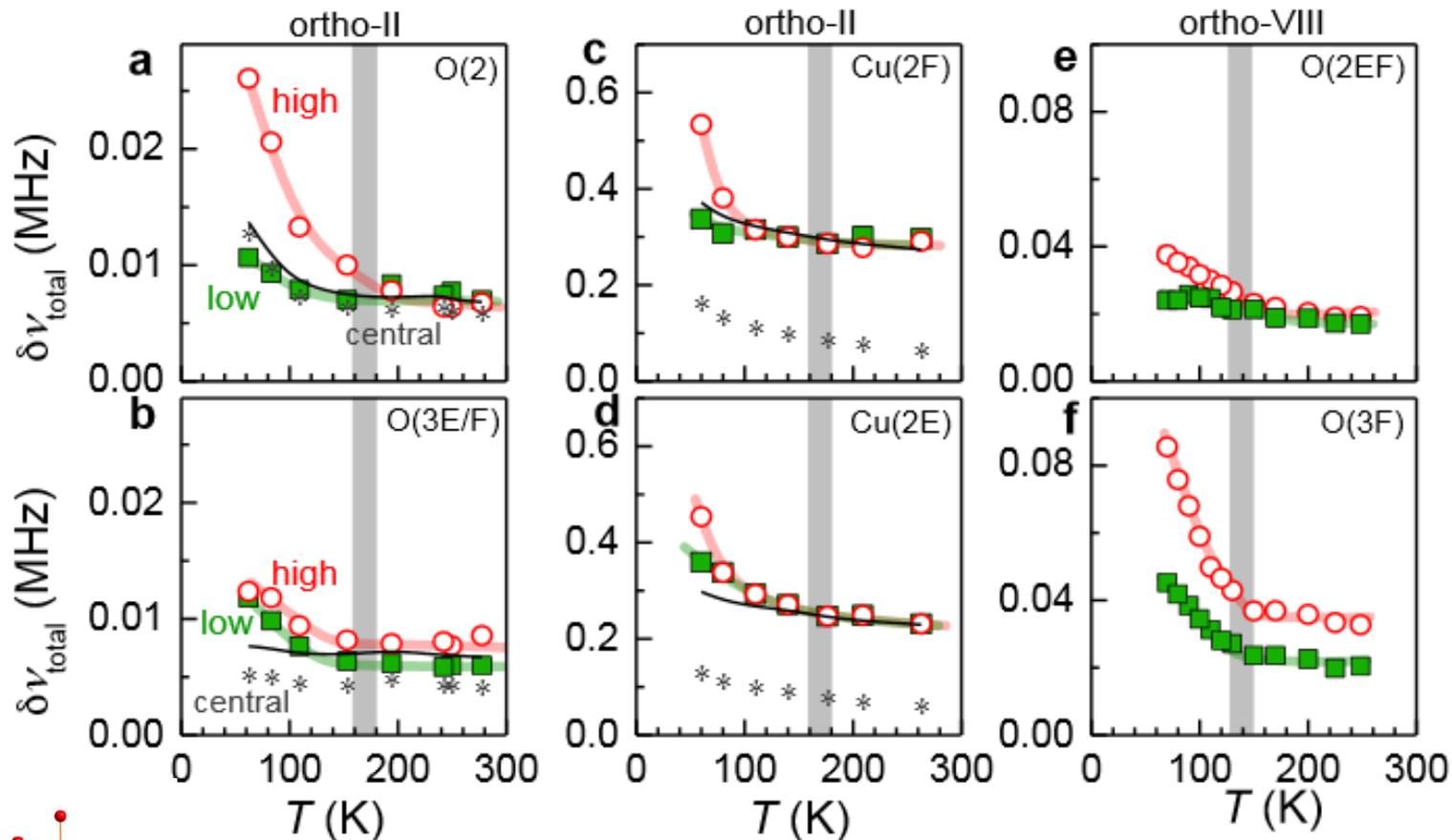


# Associated Phonon Anomalies – ortho-II



Measured at a mixed mode, thought to be primarily transverse acoustic

# BUT – does this match the NMR data?



**Evidence of static charge order in the pseudogap state.**

# BUT – does this match the NMR data?

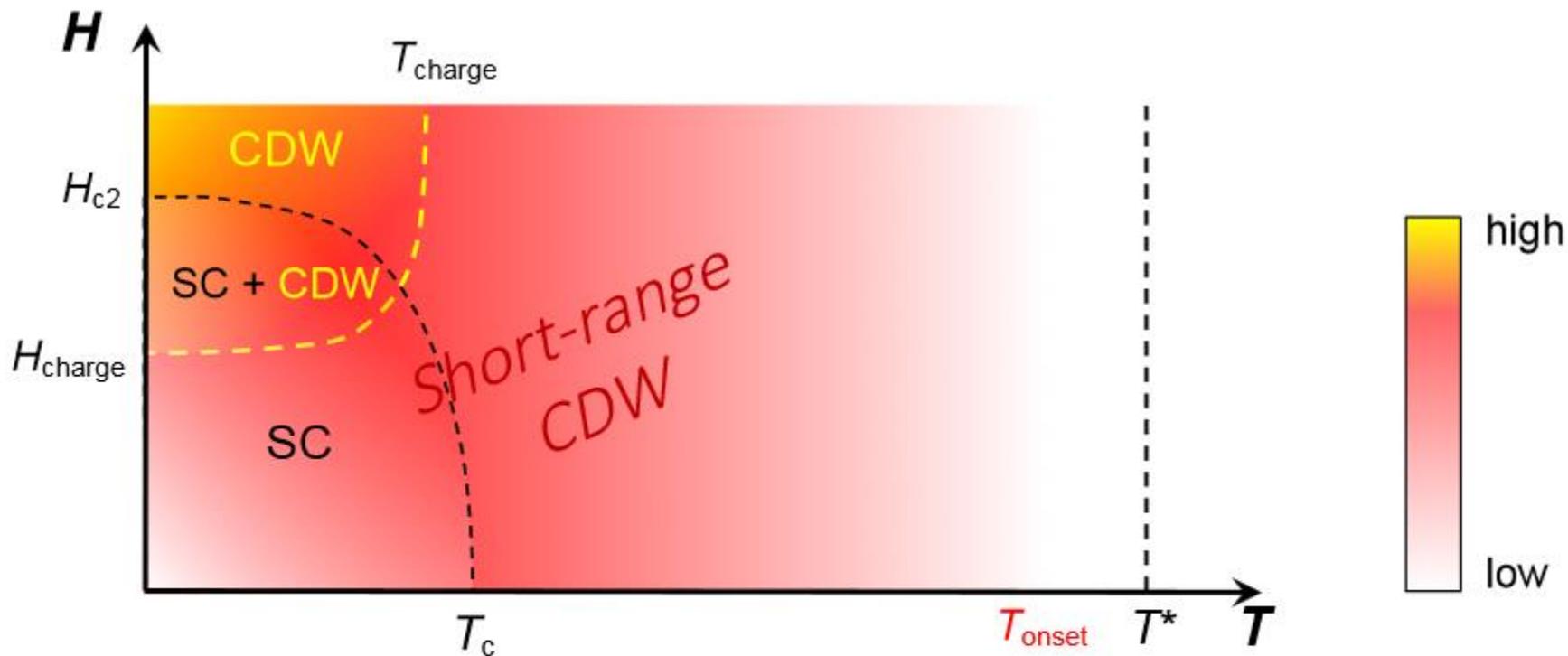
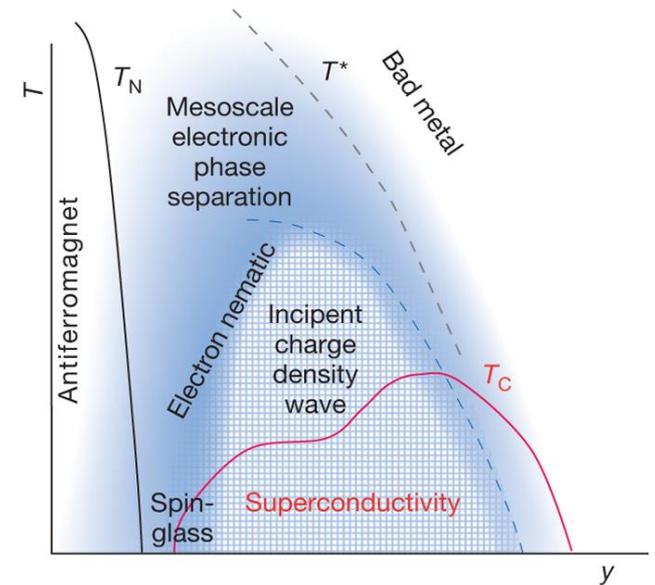


Figure 4 |  $H$ - $T$  phase diagram of charge-ordered  $\text{YBa}_2\text{Cu}_3\text{O}_y$ .

# Summary



Fradkin & Kivelson  
Nature Physics (2012)

- The  $\text{CuO}_2$  planes are prone to an instability before becoming superconducting.
- The CDW appears to be able to motivate the FS reconstruction.
- What does it have to do with the pseudogap?