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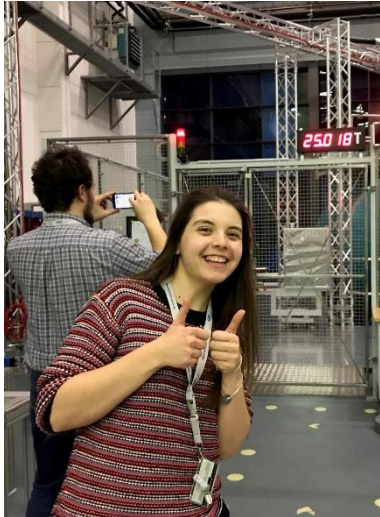
The normal state of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$

ELIZABETH BLACKBURN, ECRYS 2022, 2022-08-16



Acknowledgements

Emma Campillo



Ted Forgan

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Alex Holmes

Stephen Hayden

Johan Chang

Oleh Ivashko

Martin von Zimmermann



Ruixing Liang
Doug Bonn
Walter Hardy



Andreas Erb

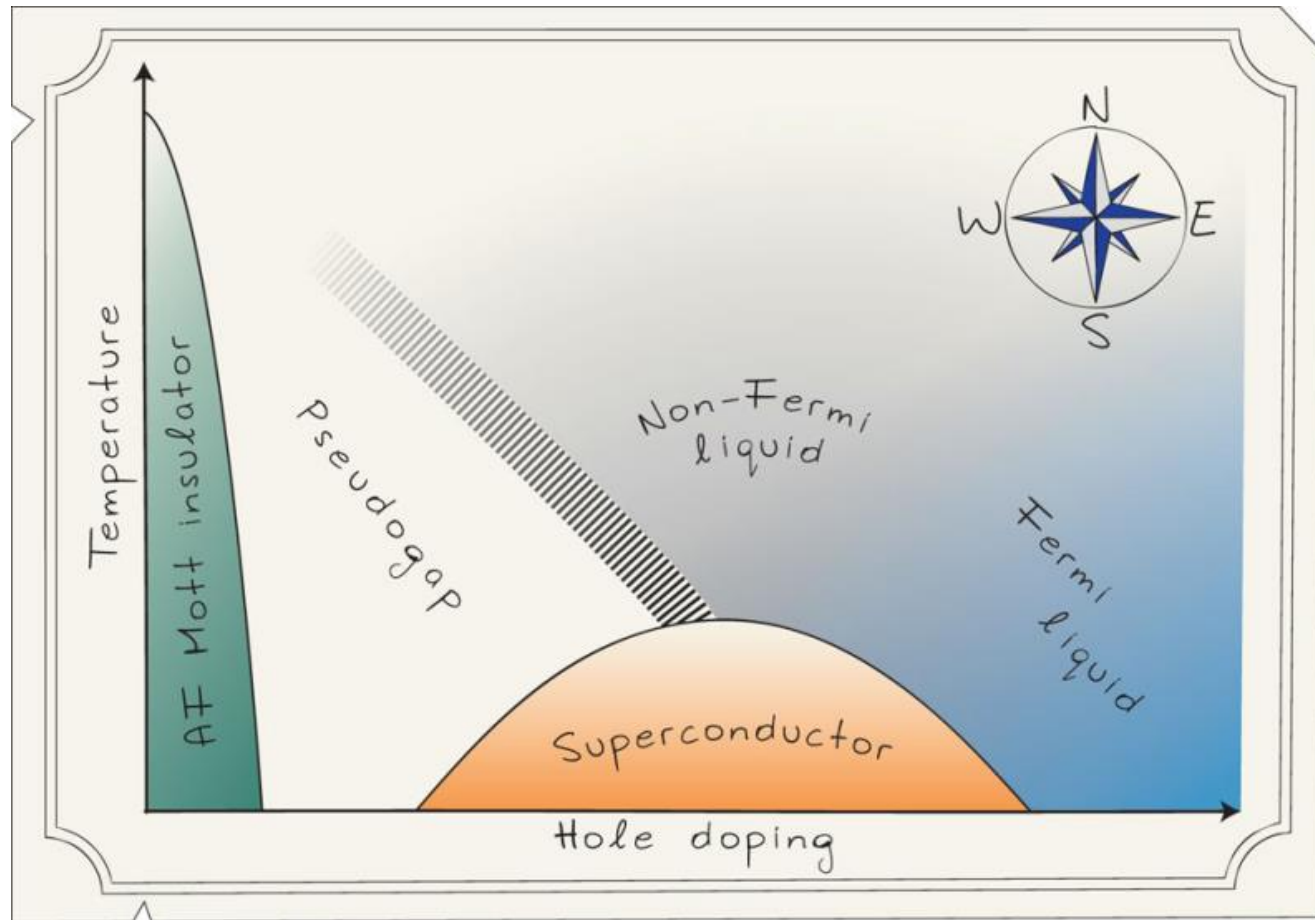
Outline – experimental data from YBCO

- Introduction to YBCO
- The vortex lattice at high magnetic fields
 - introducing the vortex lattice
 - how does it normally behave?
 - deviations from the London model
- Looking for a diffraction signature from the pair density wave
 - introducing the pair density wave
 - trying to find a diffraction signal

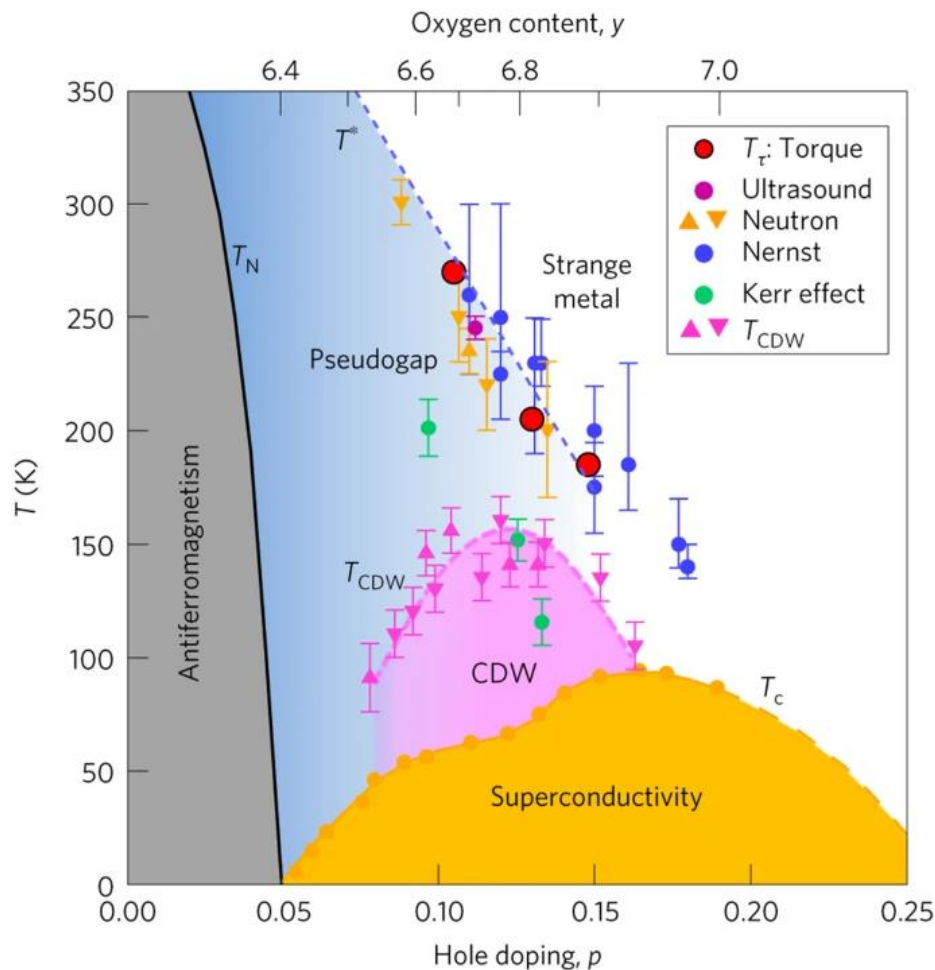
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Cuprate phase diagram

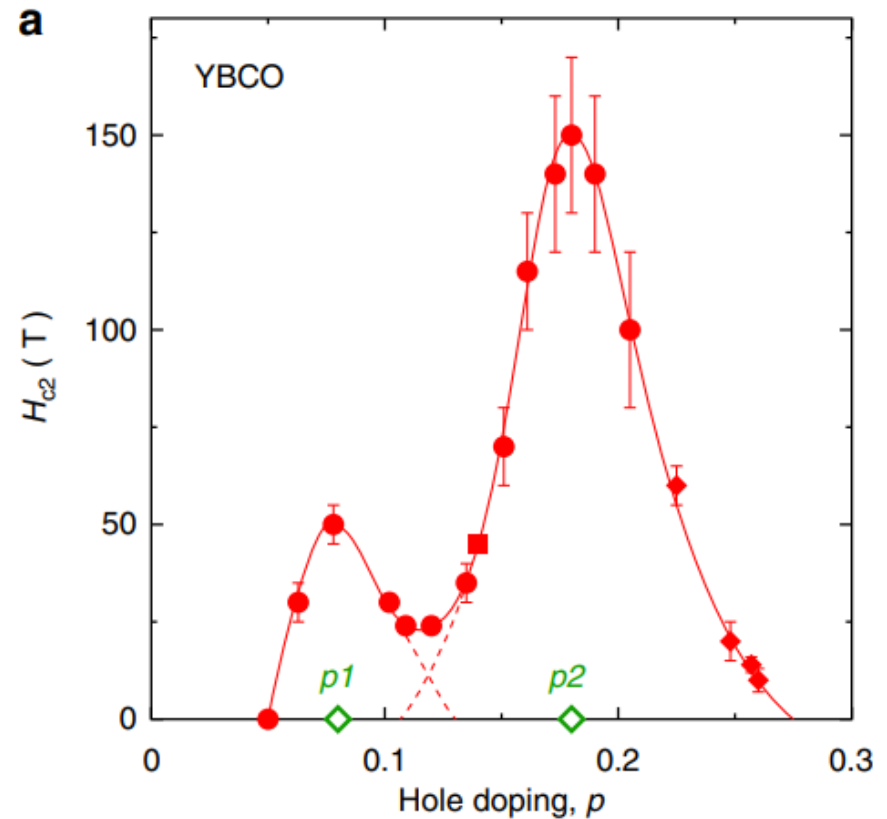


Electronic instabilities in the cuprates



Sato *et al.*, Nature Physics **13**, 1074 (2017)

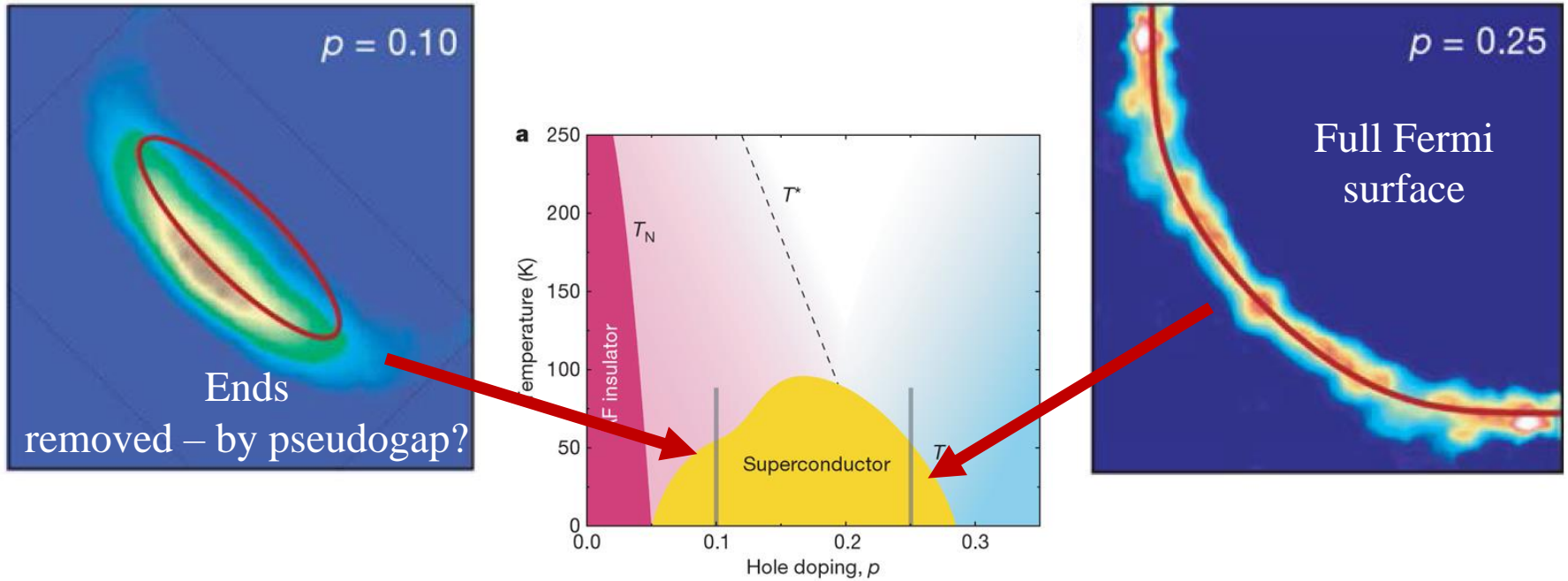
Grisonnanche *et al.*,
Nature Comms **5**, 3280 (2014)



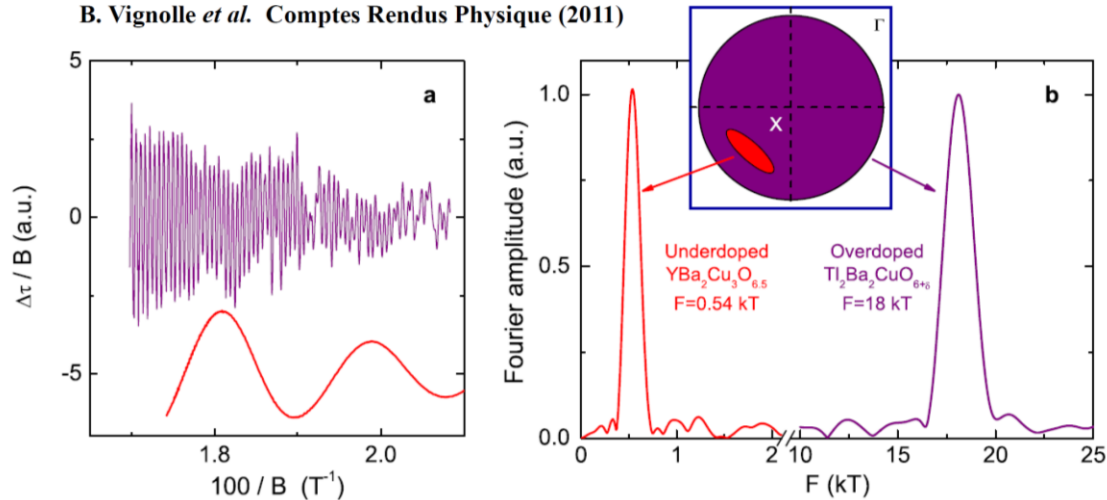
H_{c2} is defined as the onset of the vortex-solid phase as $T \rightarrow 0$, as measured from high-field resistivity data

Underdoping to overdoping

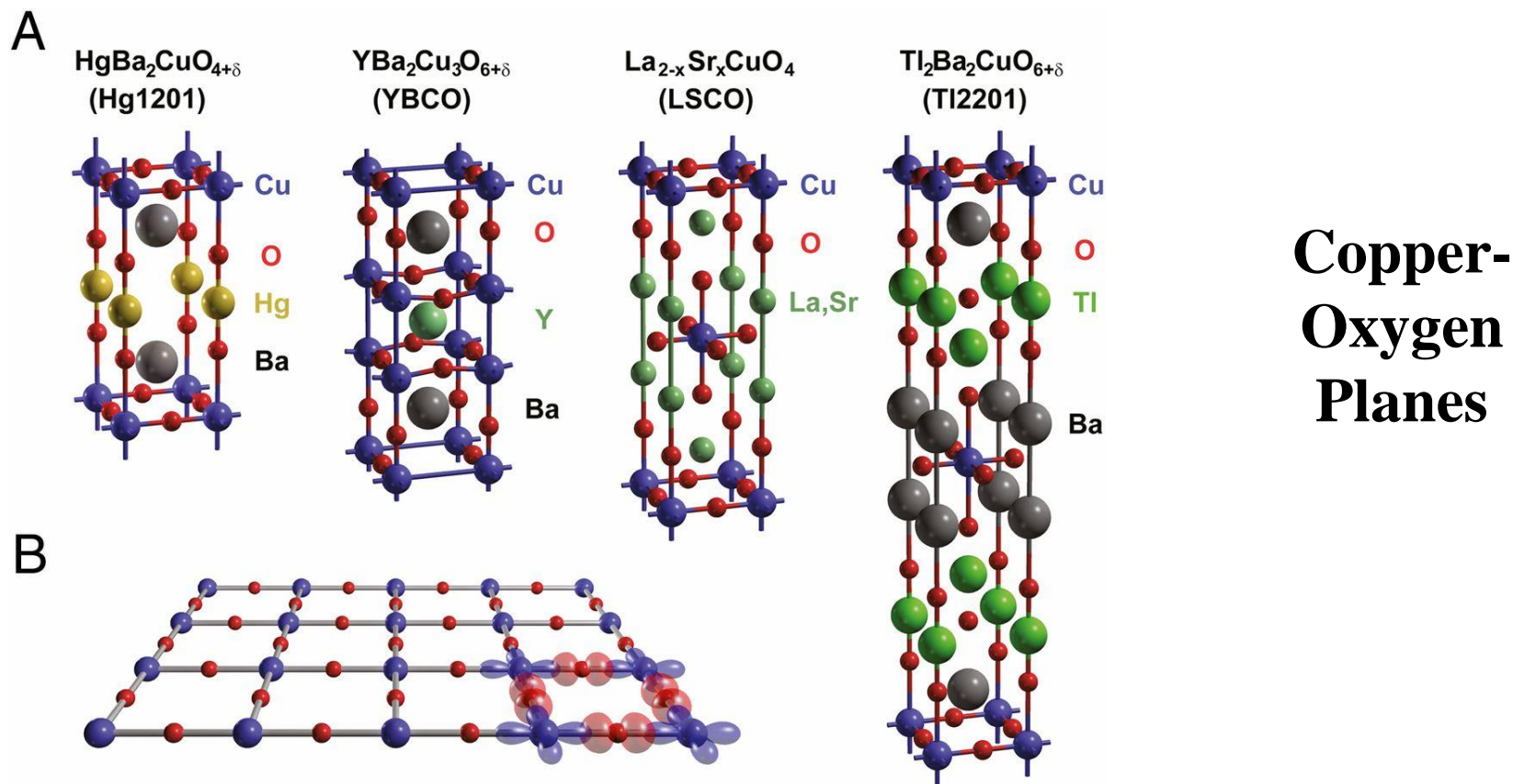
Doiron-Leyraud *et al.*, Nature (2007); Plate *et al.*, PRL (2005); Shen *et al.*, Science (2005)



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

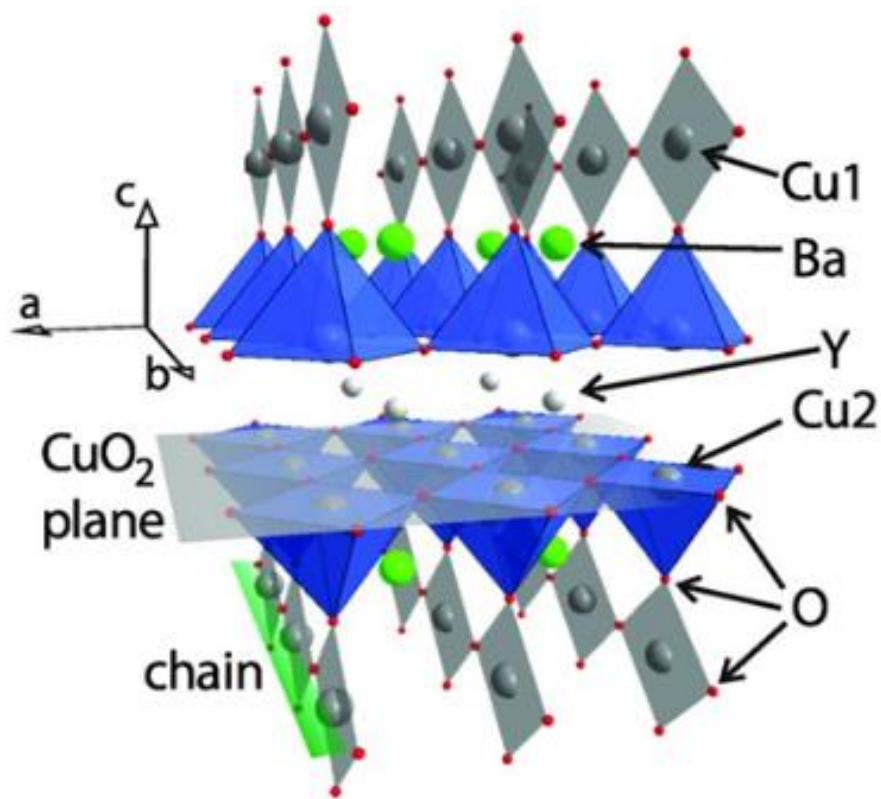


Introduction to $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ (YBCO)



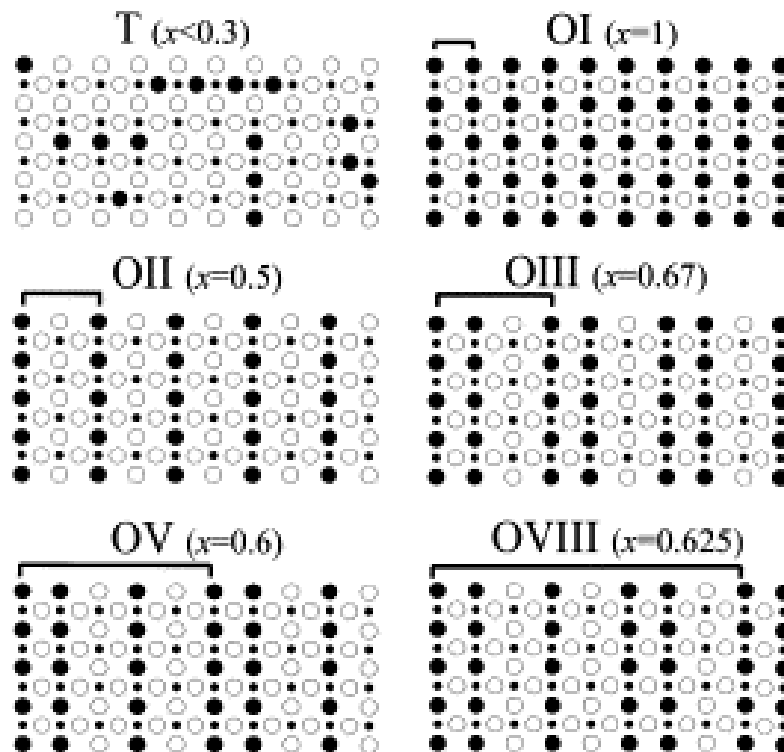
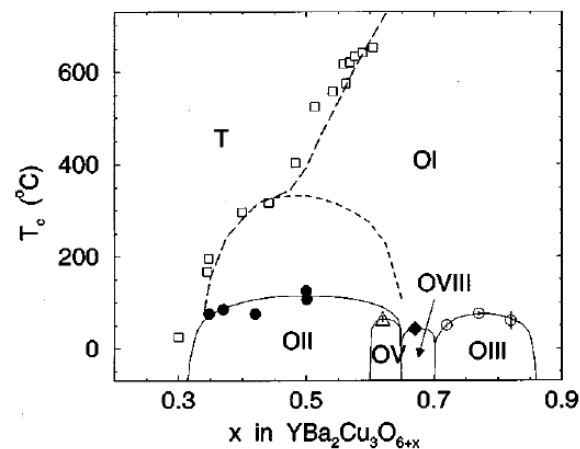
Barisic *et al.*, PNAS (2013)

Oxygen ordering in YBCO – the chains

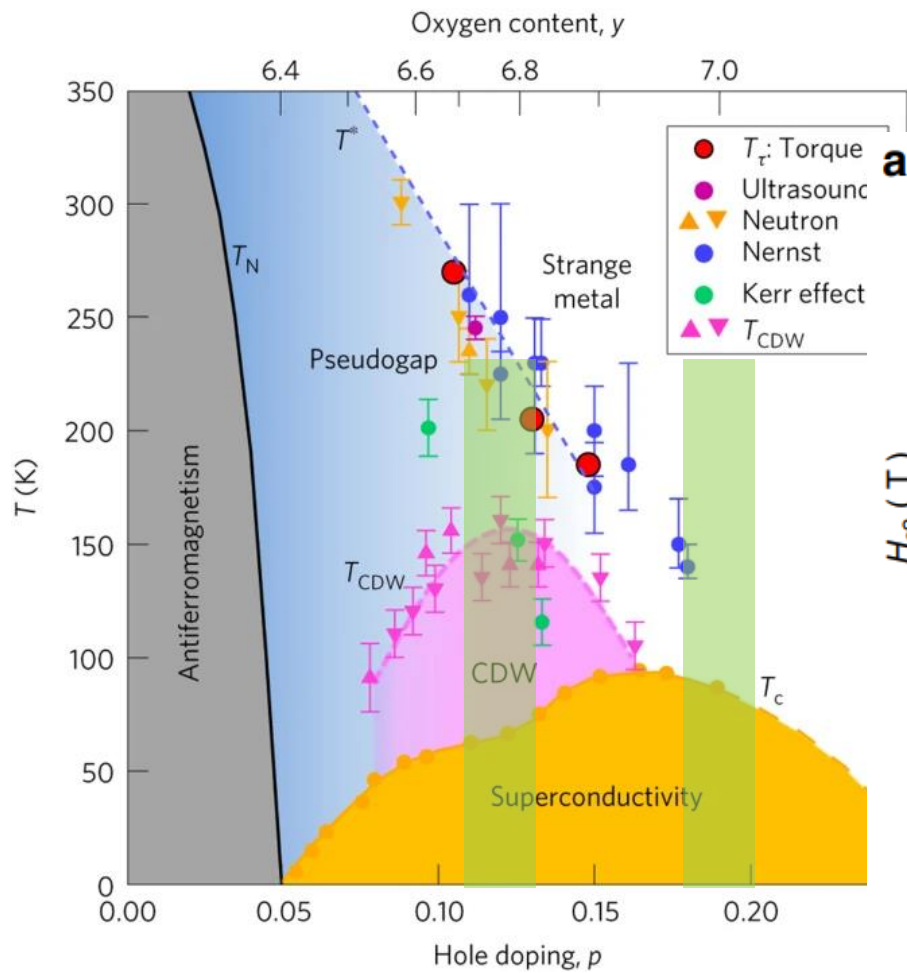


Ghiringhelli *et al.*, Science **337**, 821 (2012)

Andersen *et al.*,
Physica C **317**,
259 (1999).

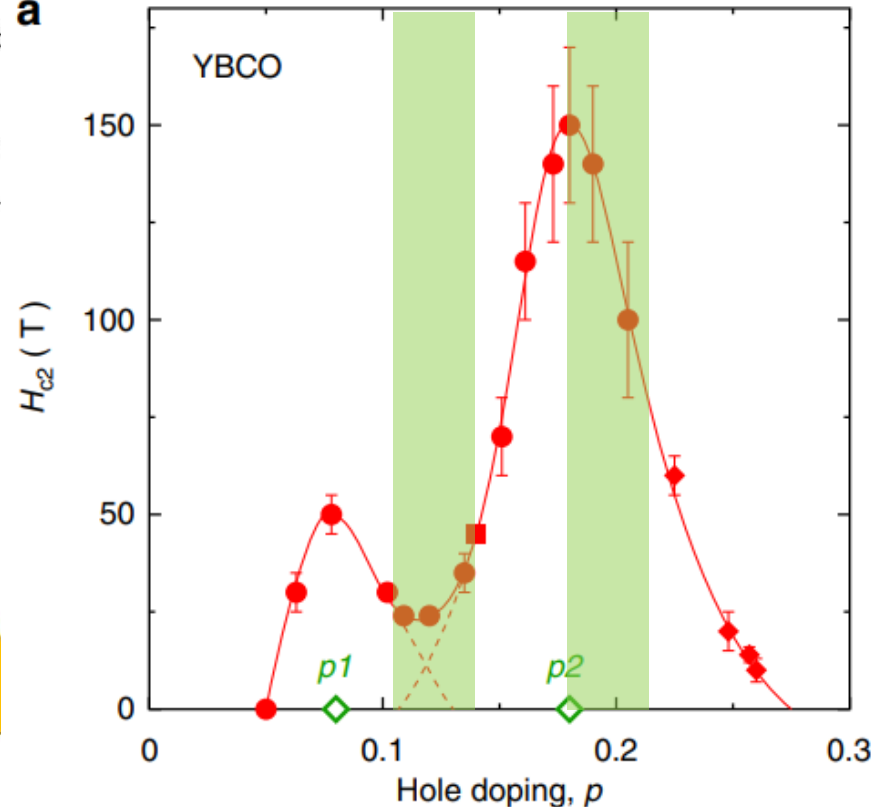


Electronic instabilities in the cuprates



Sato *et al.*, Nature Physics **13**, 1074 (2017)

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H_{c2} is defined as the onset of the vortex-solid phase as $T \rightarrow 0$, as measured from high-field resistivity data

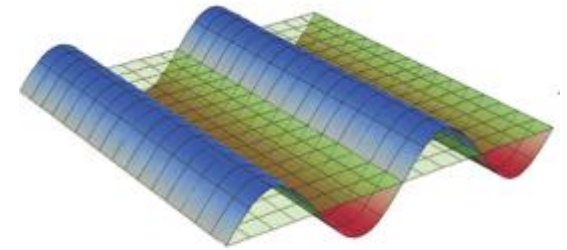
Outline – experimental data from YBCO

- Introduction to YBCO
- **Looking for a diffraction signature from the pair density wave**
 - introducing the pair density wave
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What are pair density waves?

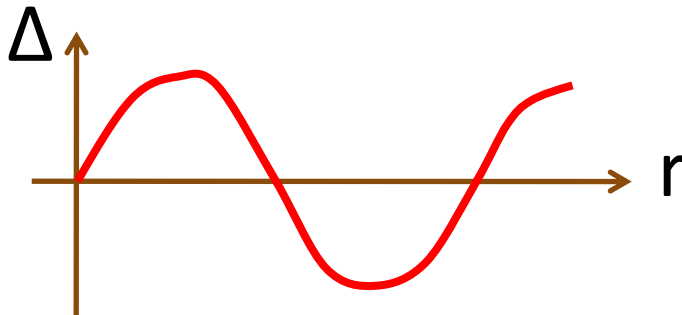
A pair density wave is a superconducting state in which the order parameter varies periodically as a function of position in such a way that its spatial average vanishes.

Agterberg *et al.*, Annu. Rev. CMP **11**, 231 (2020)



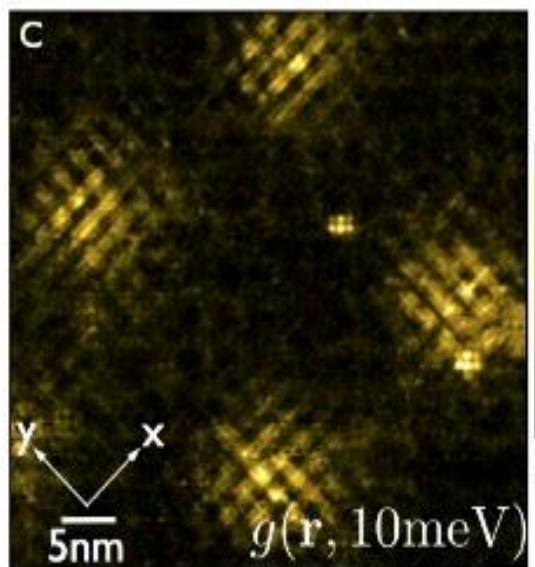
a) FFLO superconductor

The PDW state does not necessarily break time-reversal symmetry

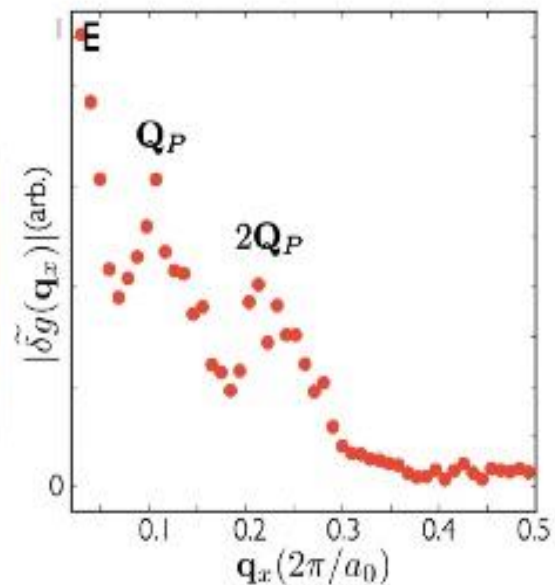


STM data – the PDW seen in field

STM (differential tunnelling conductance)



Amplitude Fourier transform



S. D. Edkins *et al.*, Science **364**, 976 (2019).

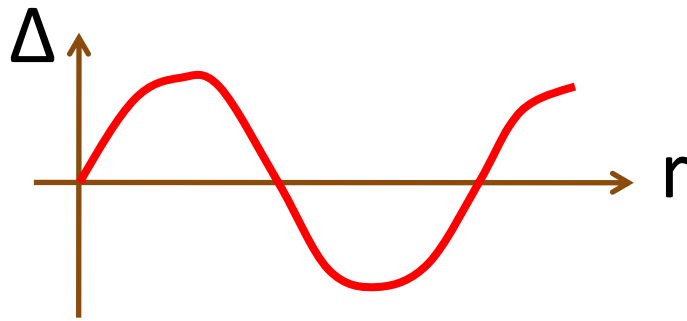
The right hand plot is obtained from data measured at 8.25 T, with the 0 T data subtracted.

What can we see with X-rays?

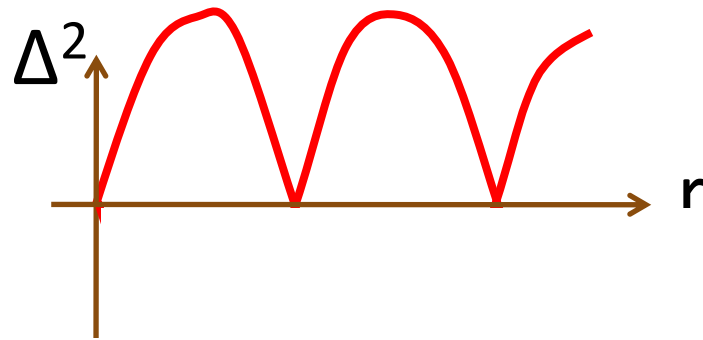
For the charge density wave, the X-rays are scattered by the electrons, and so we are sensitive to spatial variation in the electron density.

The high energy X-rays are more sensitive to (induced) atomic displacements than purely charge displacements.

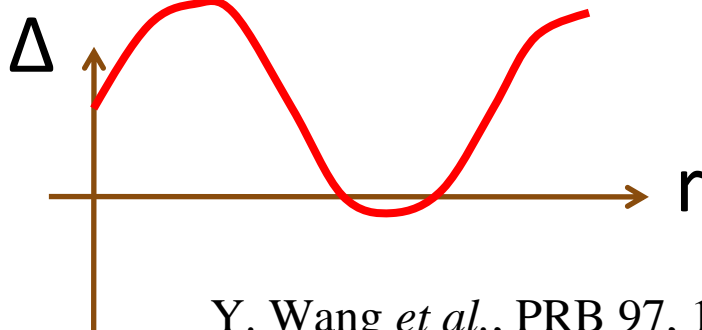
→ not directly sensitive to the pair density wave



$$\rho_e(r) \propto |\Delta(r)|^2$$



$$\rho_e(r) \propto \Delta_1^2 \sin^2(qr) \quad 2Q_{\text{PDW}}$$



Uniform SC OP

PDW OP

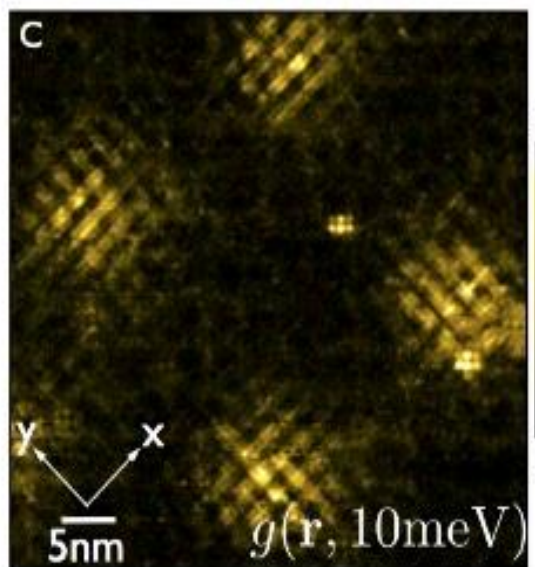
$$\rho_e(r) \propto (\Delta_0^2 + 2\Delta_0\Delta_1 \sin(qr) + \Delta_1^2 \sin^2(qr))$$

Q_{PDW}

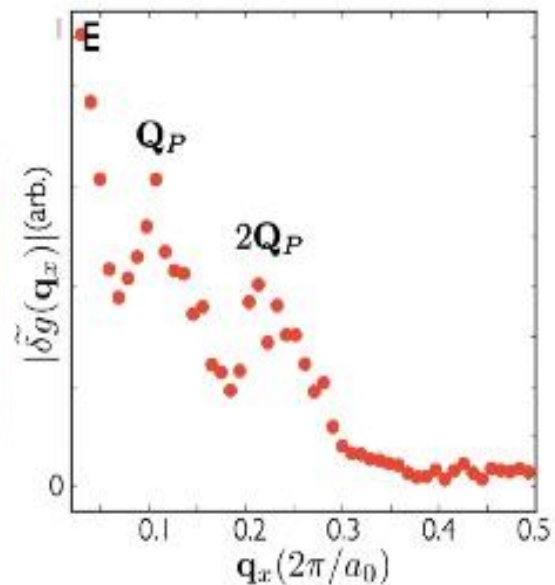
$2Q_{\text{PDW}}$

STM data – the PDW seen in field

STM (differential tunnelling conductance)



Amplitude Fourier transform

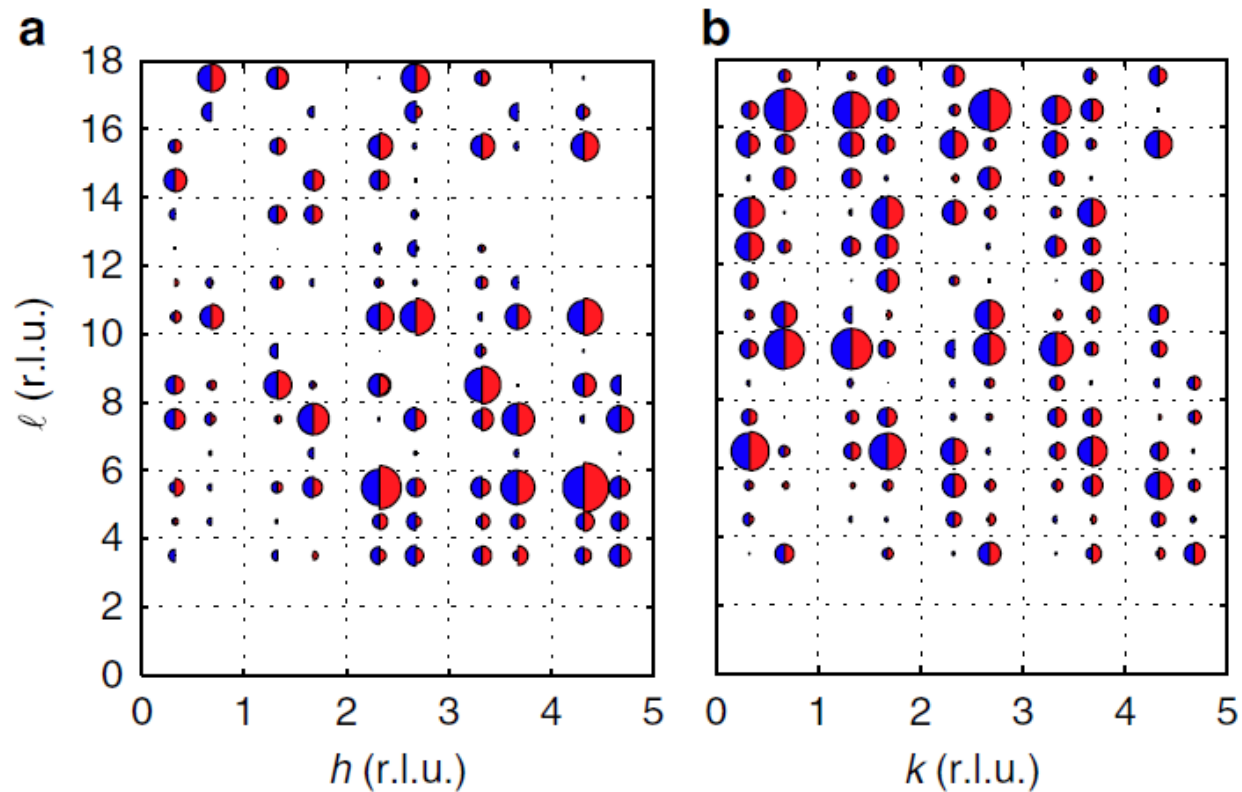


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The right hand plot is obtained from data measured at 8.25 T, with the 0 T data subtracted.

Where to look in reciprocal space?

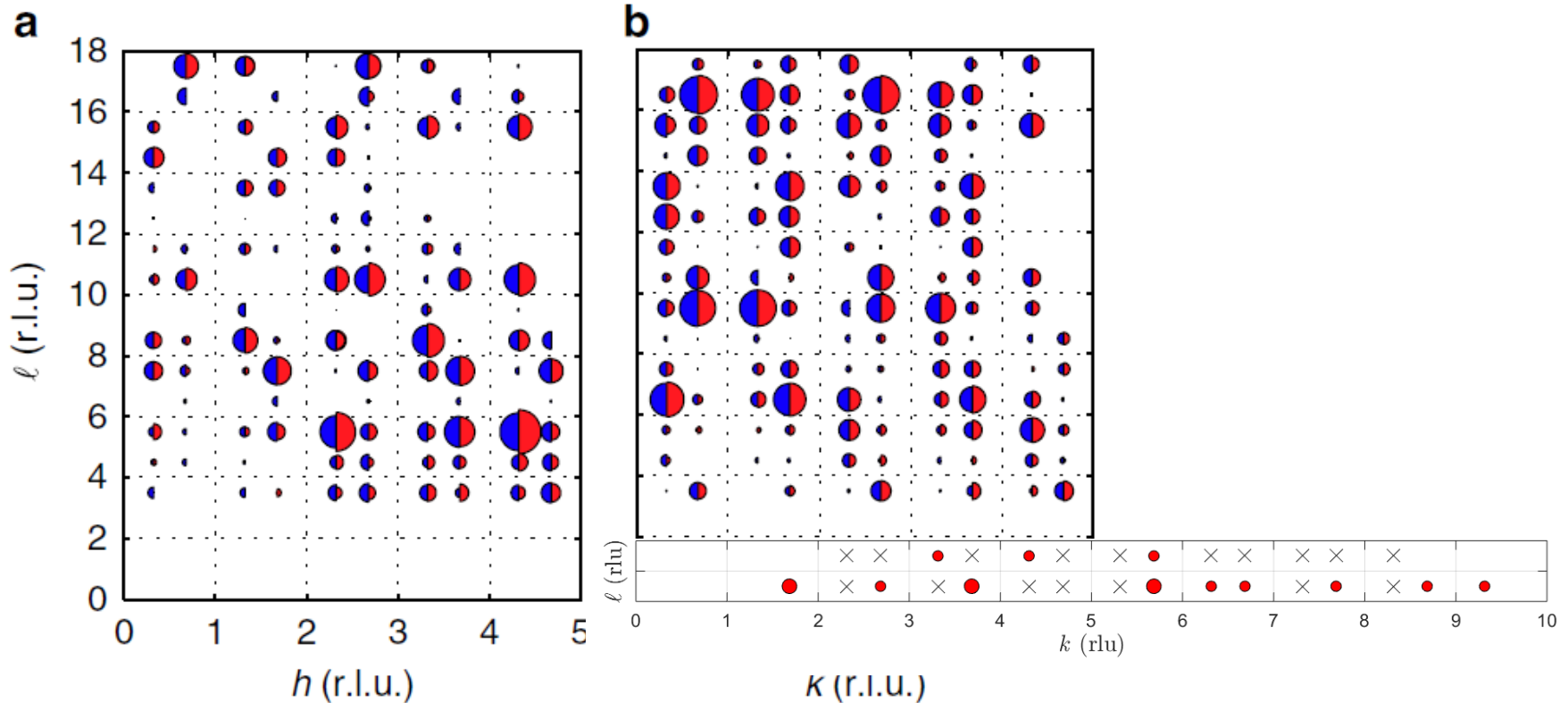
The CDW satellites in ortho-II (data, fit) @ 0 T



Forgan *et al.*, *Nature Comms* **6**, 10064 (2015).

Where to look in reciprocal space?

The CDW satellites in ortho-II (data, fit) @ 0 T

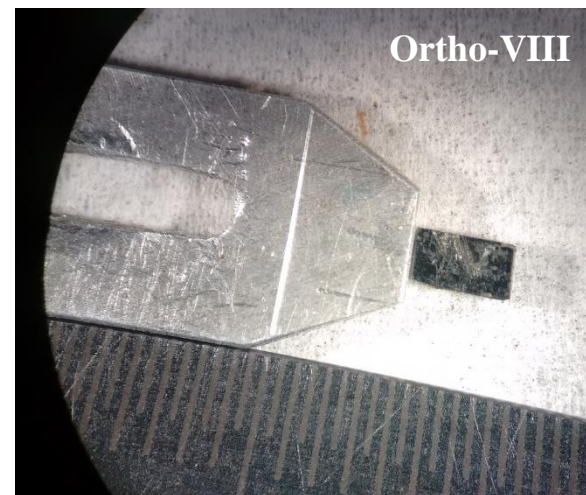
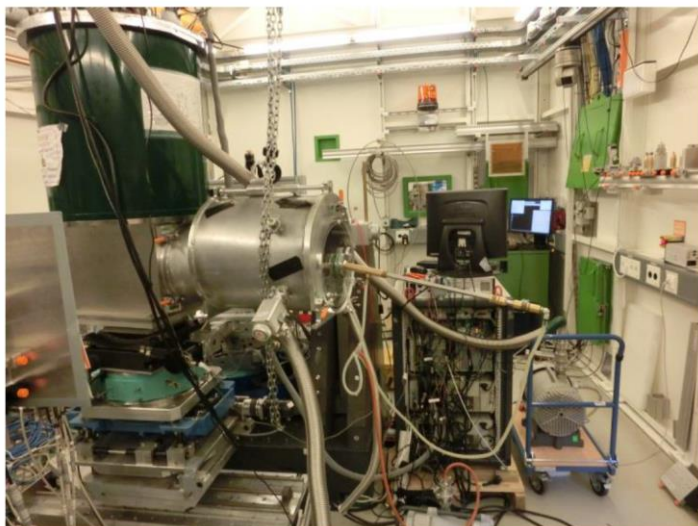


Forgan *et al.*, *Nature Comms* **6**, 10064 (2015).

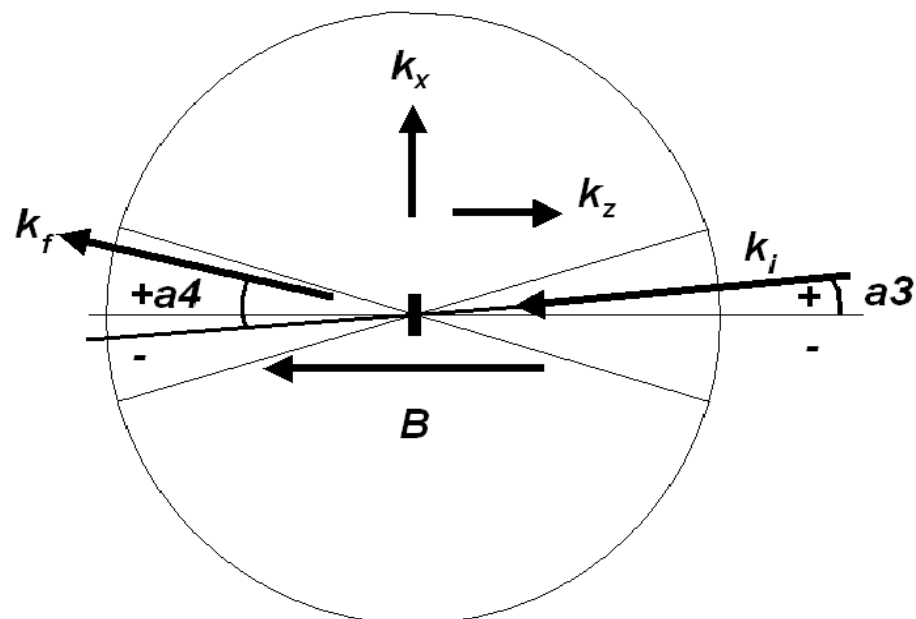
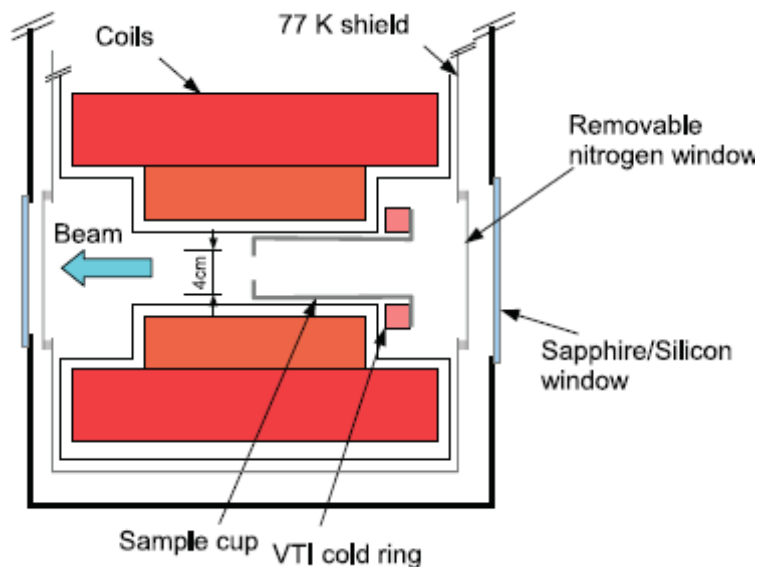
- good CDW signal
- weak CDW signal and/or background issues
- ✕ no clear CDW signal

We also need high field

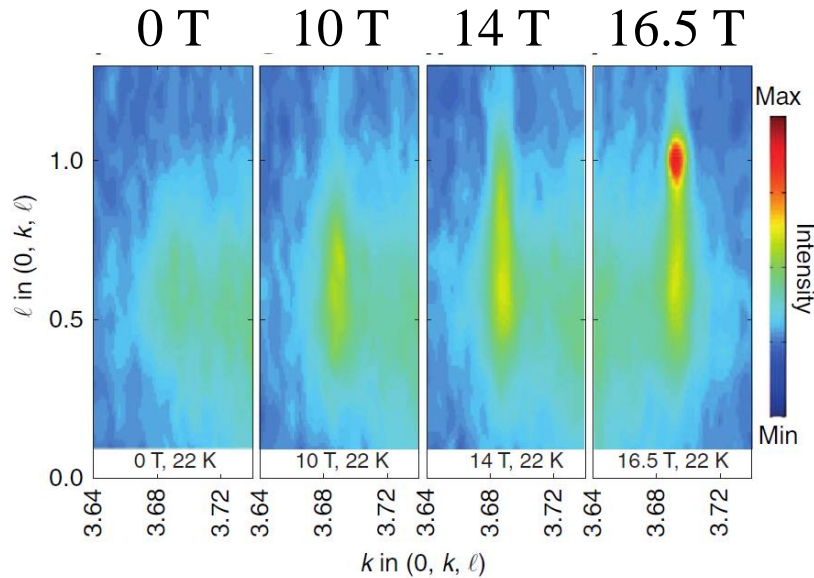
P07 @ PETRA



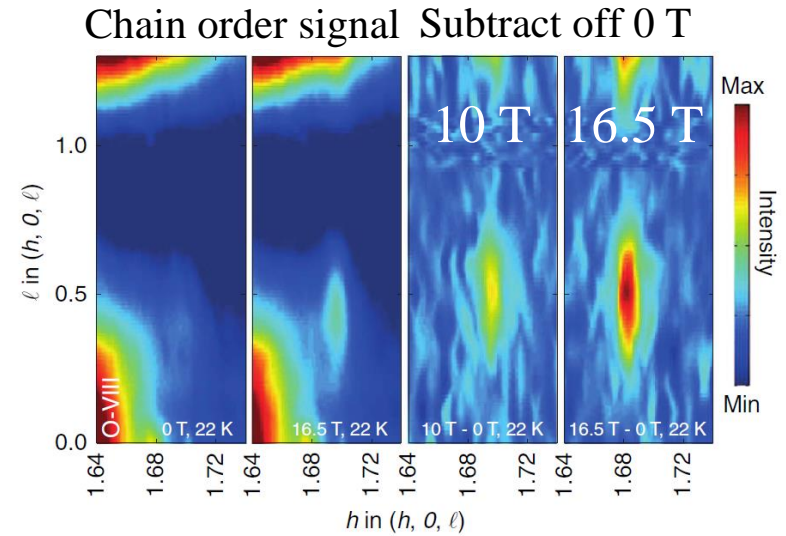
Liang, Bonn, Hardy



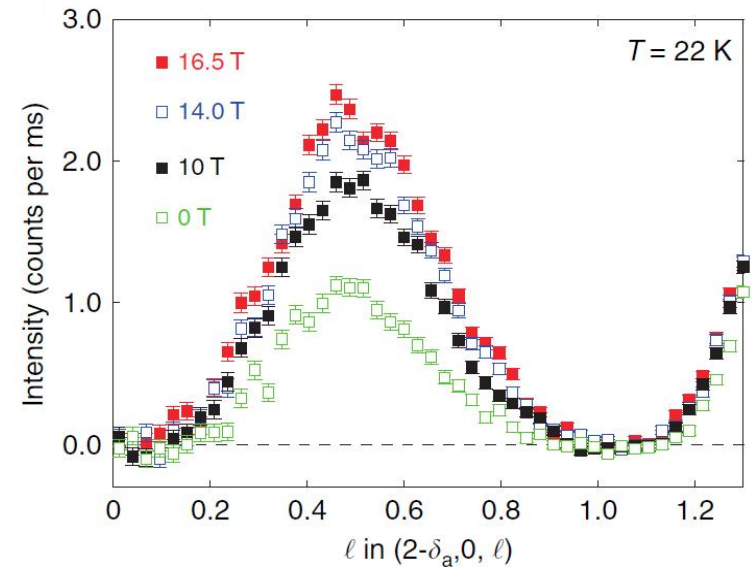
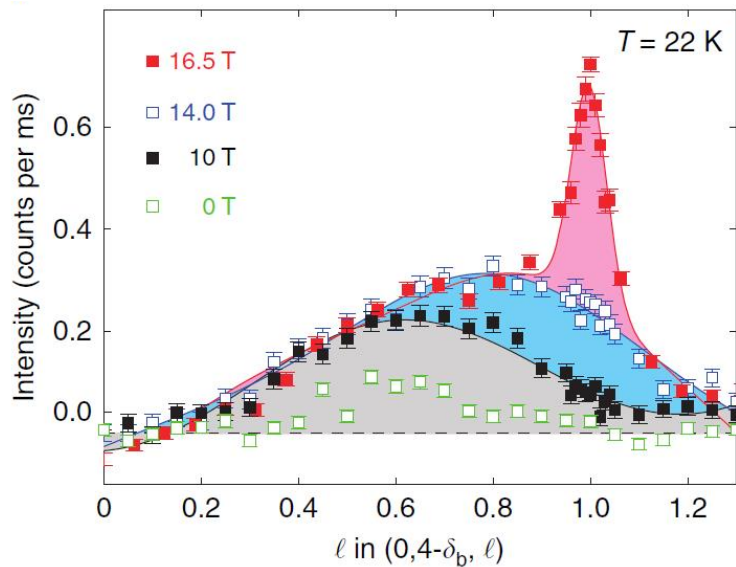
CDW order in a large B field



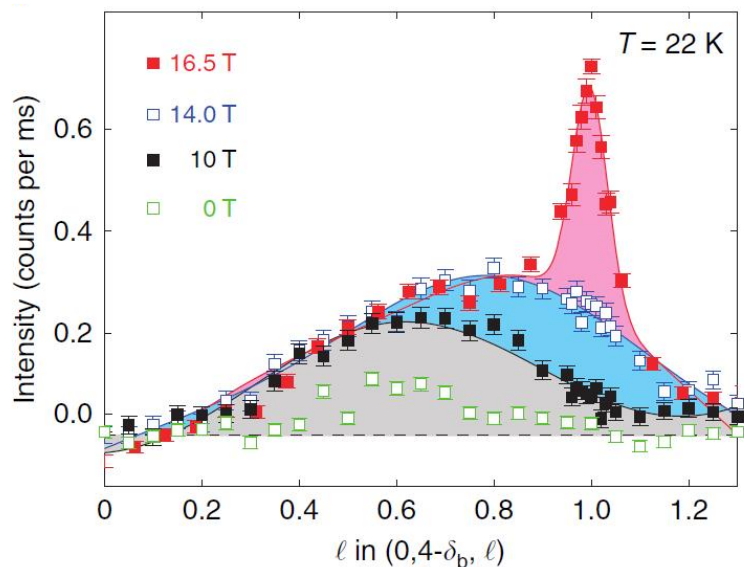
Chang *et al.*, Nature Comms **7**, 11494 (2016).



Now the q_a part



CDW order in a large B field



Chang *et al.*, Nature Comms **7**, 11494 (2016).

Correlation lengths (0 T):

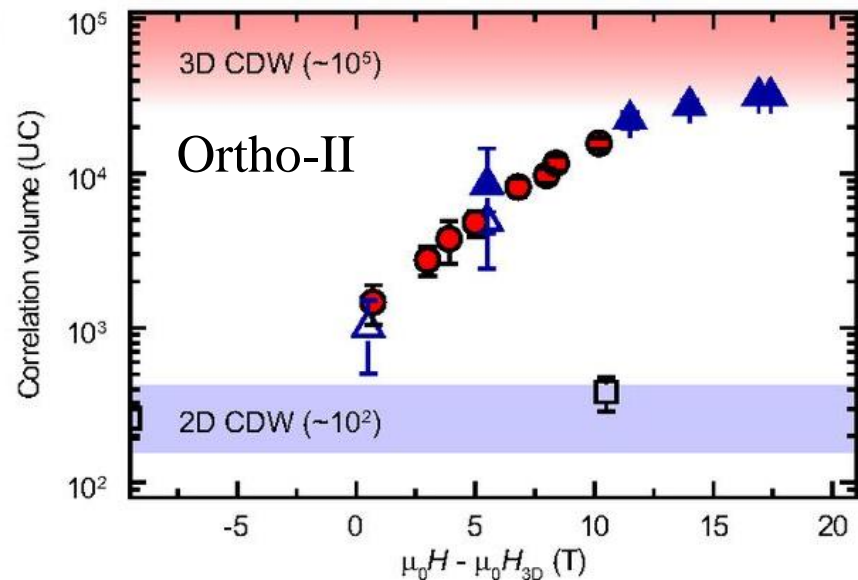
$$\xi_a = 95 \text{ \AA}$$

$$\xi_c \approx 0.6 c$$

Correlation lengths (16 T):

$$\xi_a = 310 \text{ \AA}$$

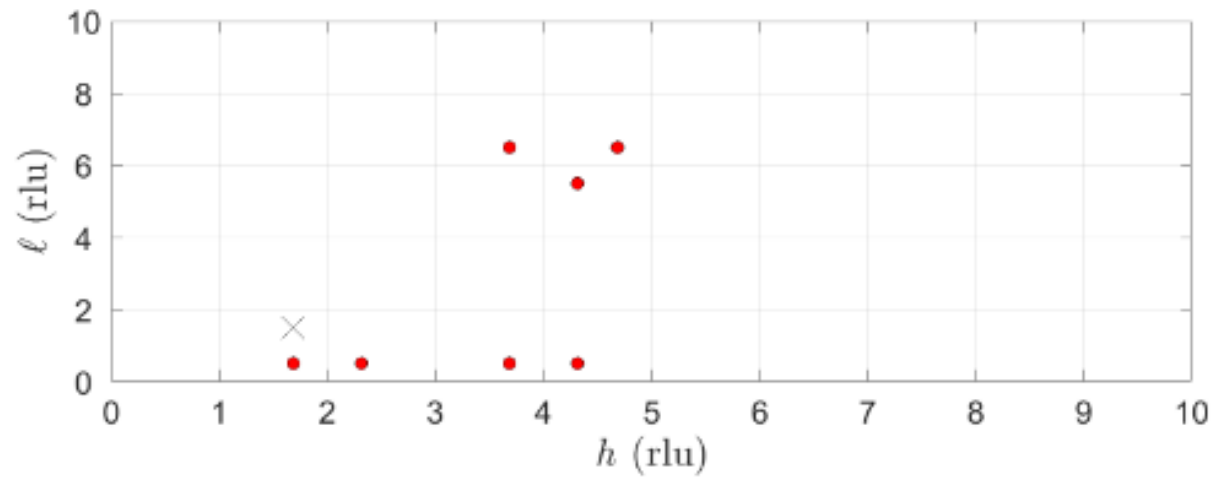
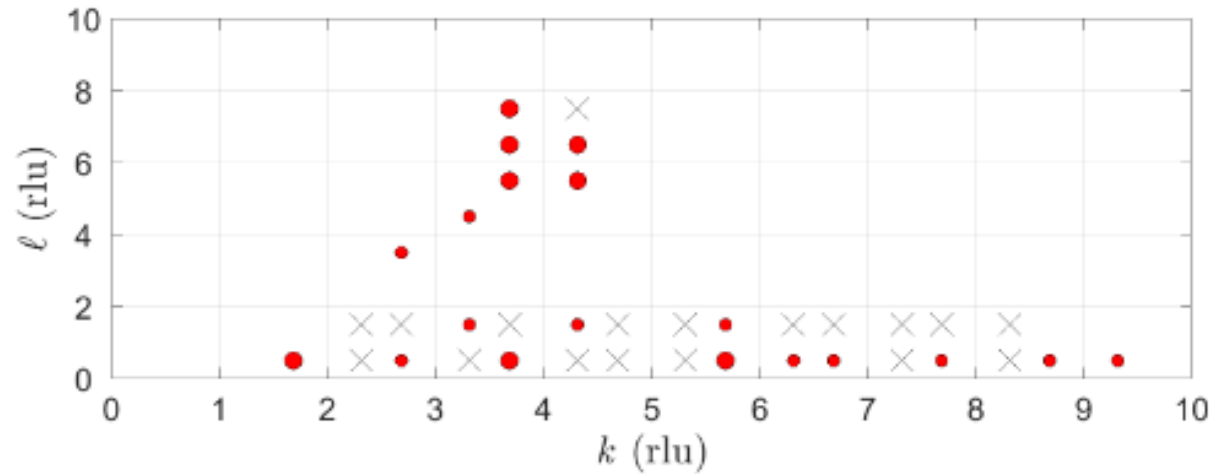
$$\xi_c \approx 4 c (47 \text{ \AA})$$



Jang *et al.*, PNAS **113**, 14645 (2016).

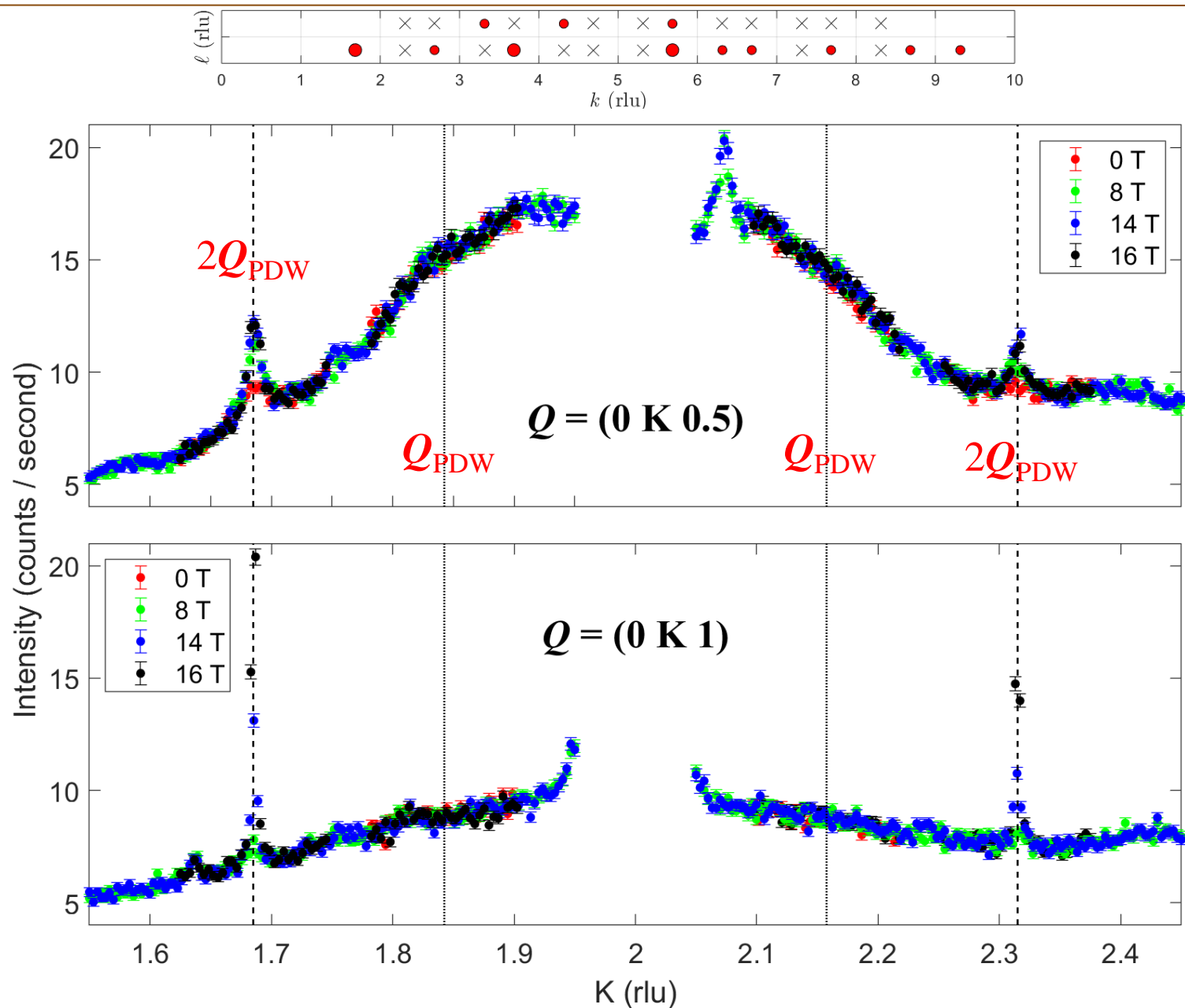


Where to look for the PDW in Q space?



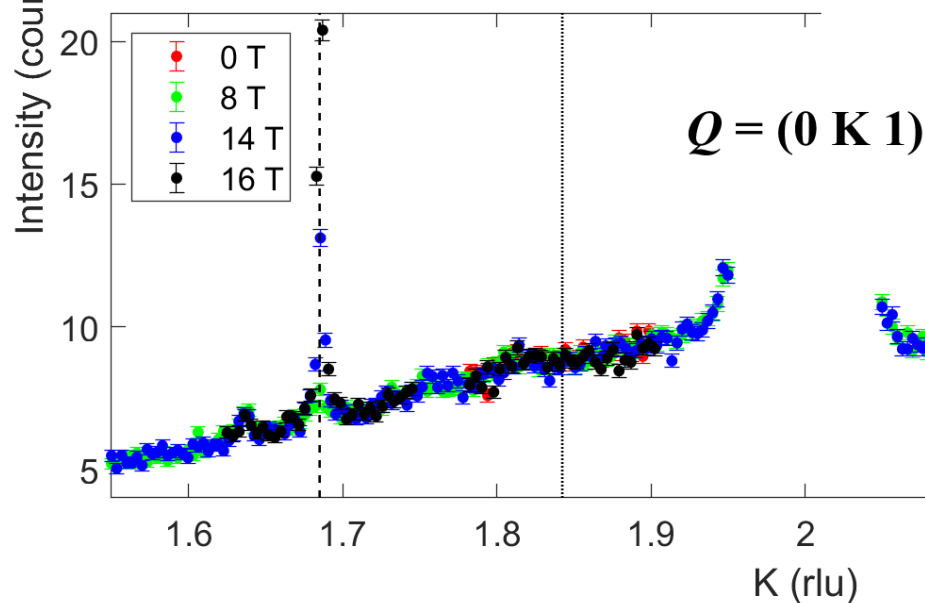
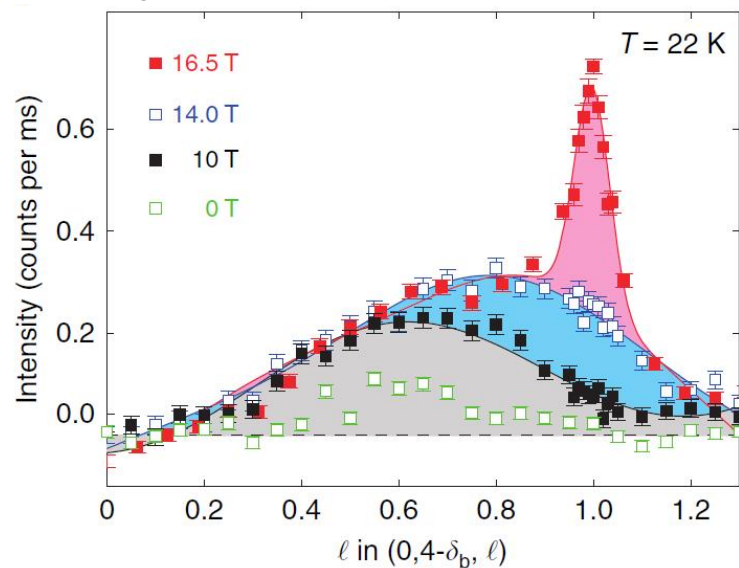
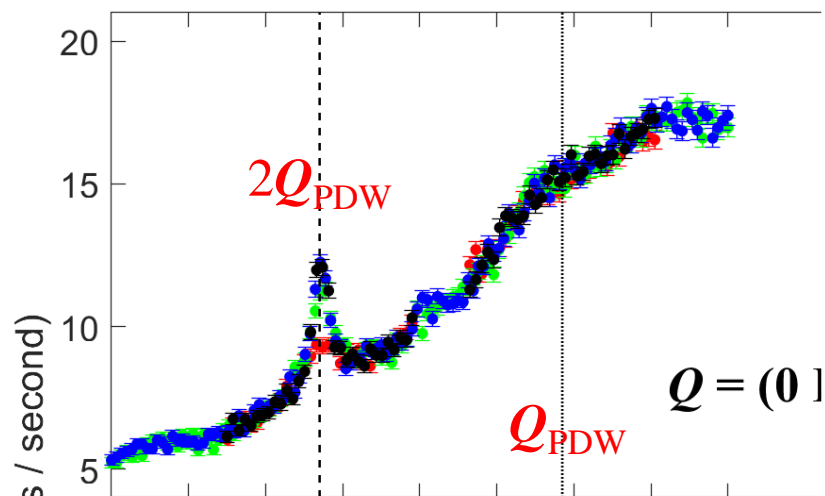
- good CDW signal
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Example data at (0 K 0.5) and (0 K 1) – 3 K

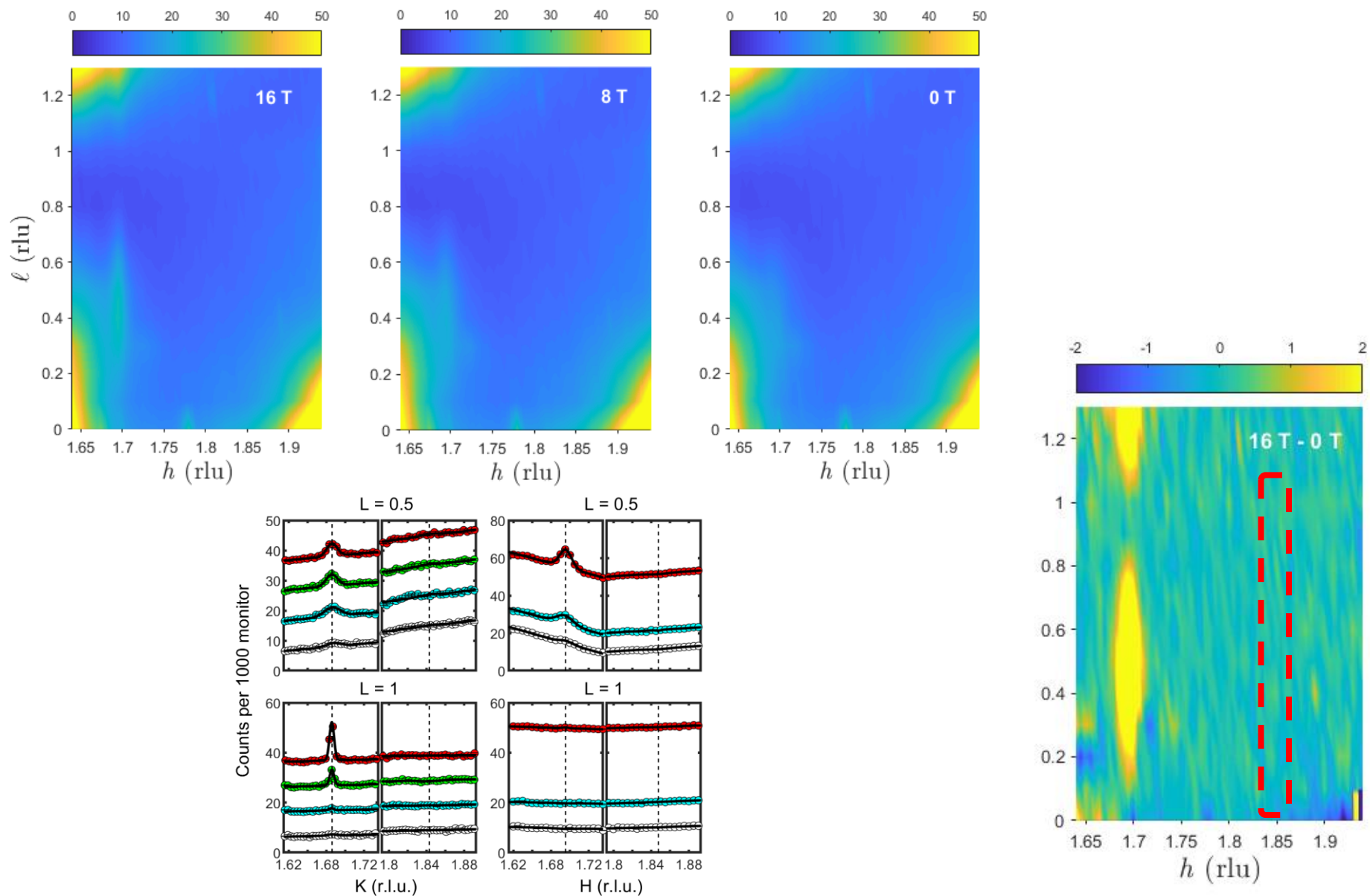


Example data at (0 K 0.5) and (0 K 1) – 3 K

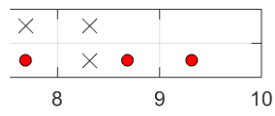
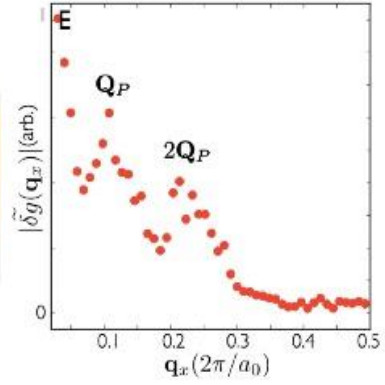
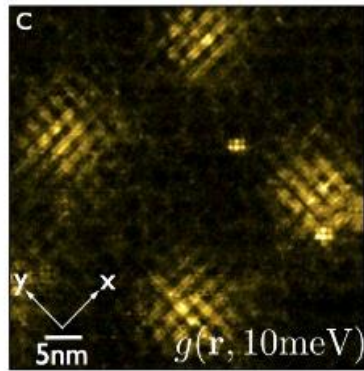
Chang *et al.*, Nature Comms 7, 11494 (2016).



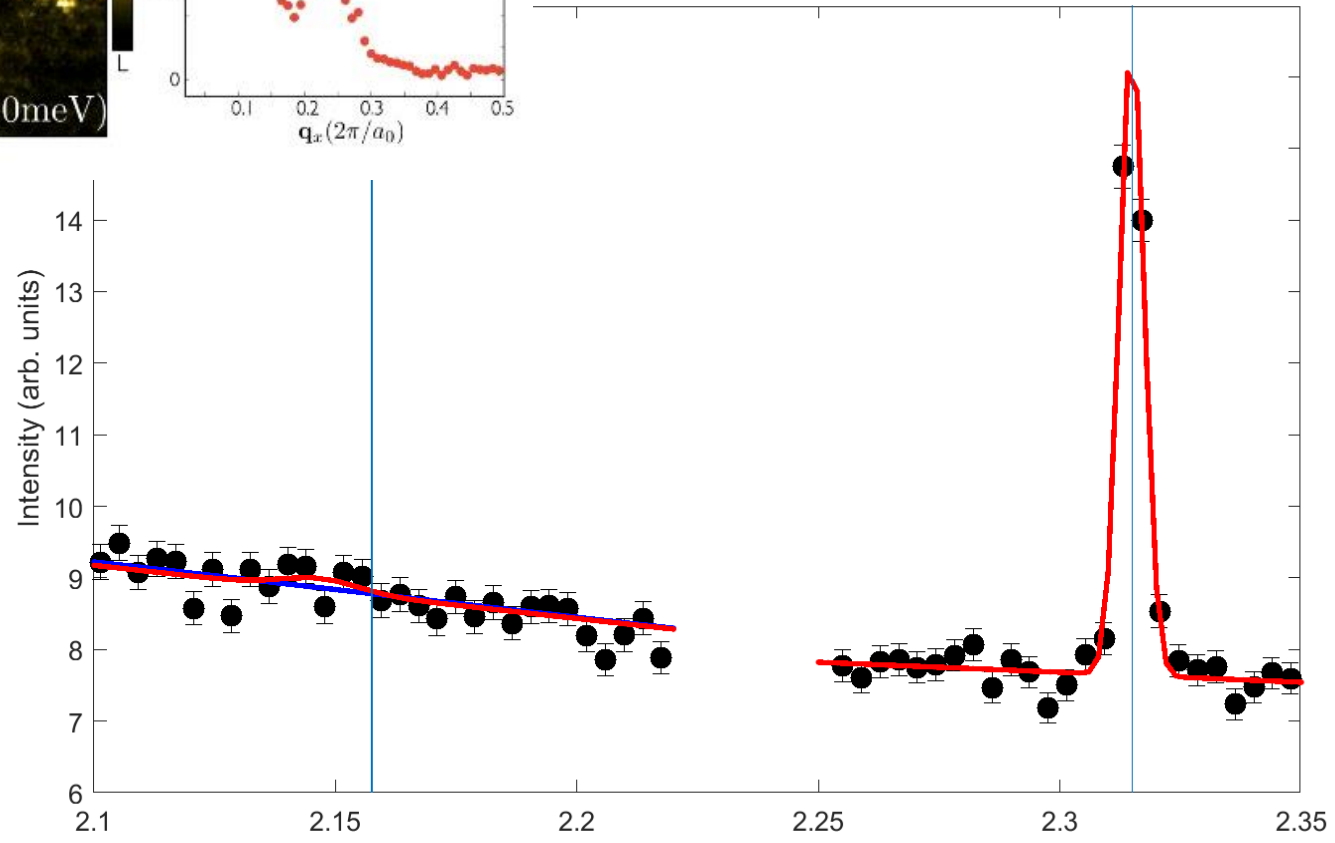
Along the \mathbf{a}^* axis – (H 0 L) - 3 K



(0 K 1) – 16 T, 3 K



- good CDW signal
- weak CDW signal and/or background issues
- × no clear CDW signal

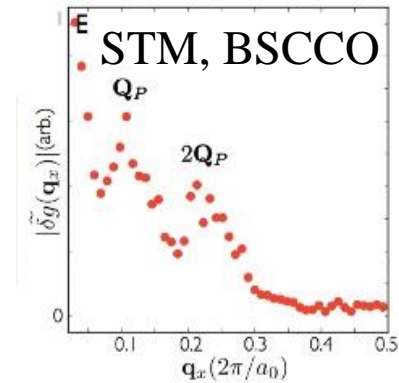


Integrated intensity = 3.3 ± 4.3 arb. units
Width $\sim 3 \times$ the CDW peak

Conclusions

- A diffraction signature from the pair density wave?
 - not seen – Δ_0 at least one order of magnitude smaller than $\Delta_1 = \Delta_{\text{PDW}}$ in YBCO ortho-II

$$\rho_e(r) \propto (\Delta_0^2 + 2\Delta_0\Delta_1 \sin(qr) + \Delta_1^2 \sin^2(qr))$$

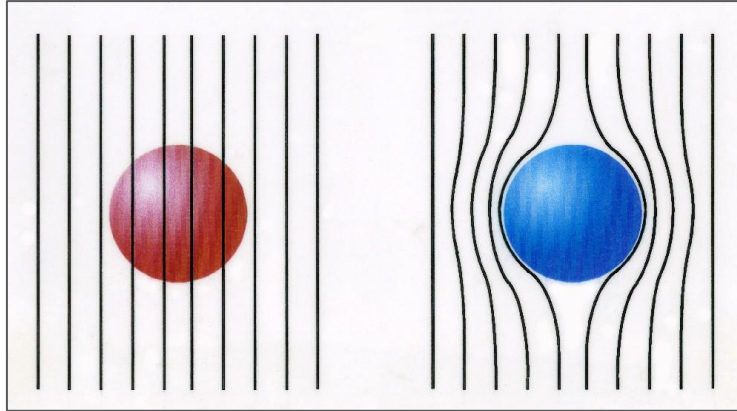


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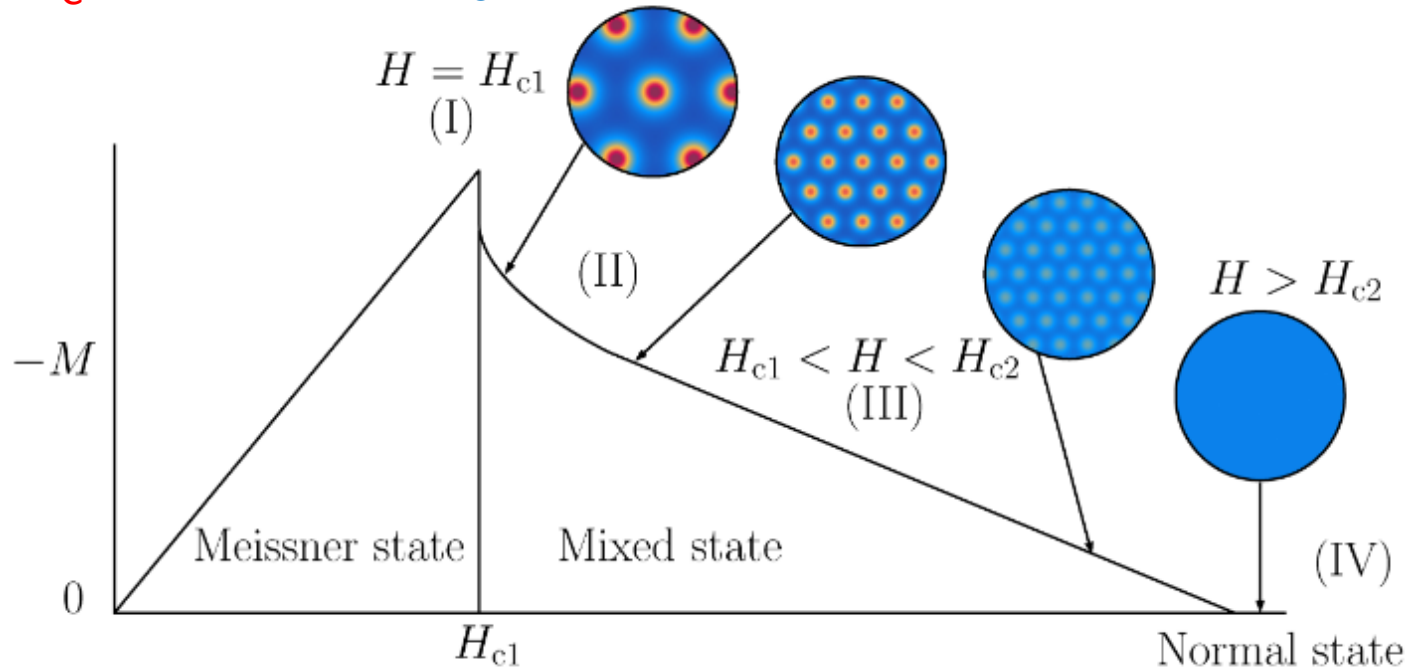
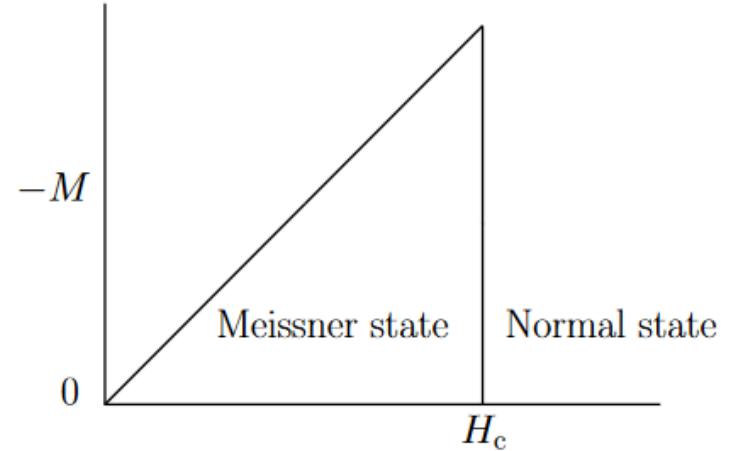
Vortices in Type-II superconductors

Meissner-Ochsenfeld effect



$T > T_c$

$T < T_c$

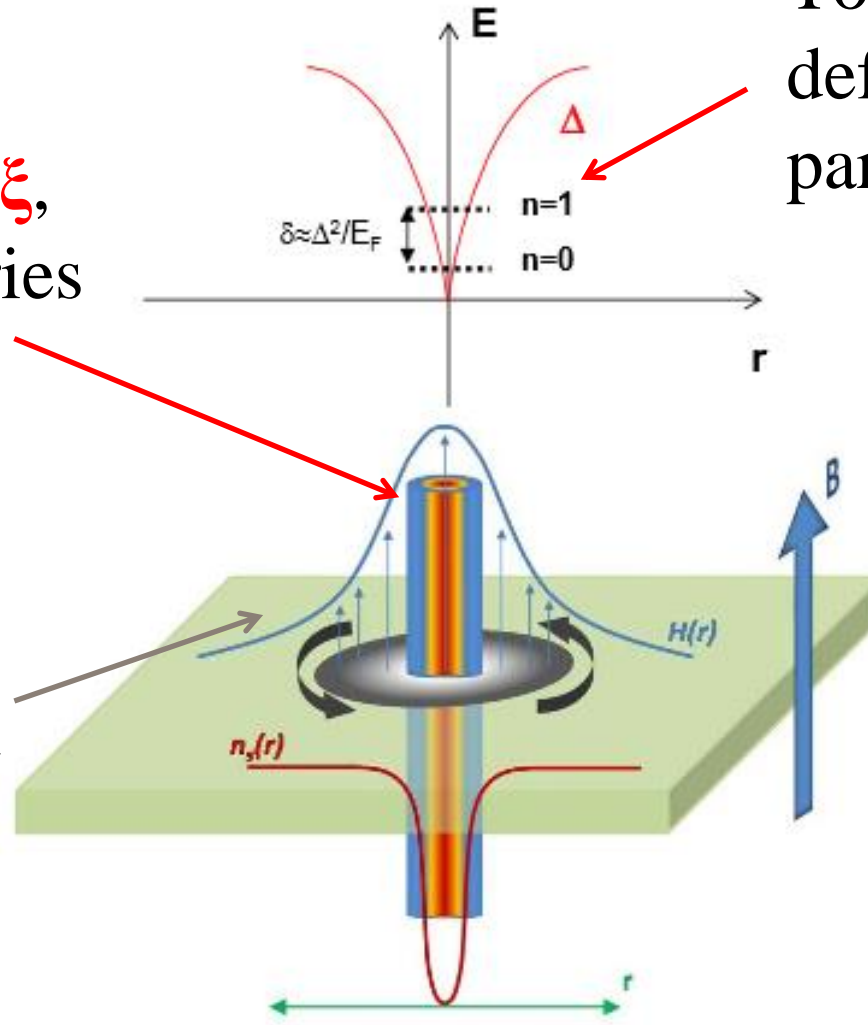


Vortices in superconductors

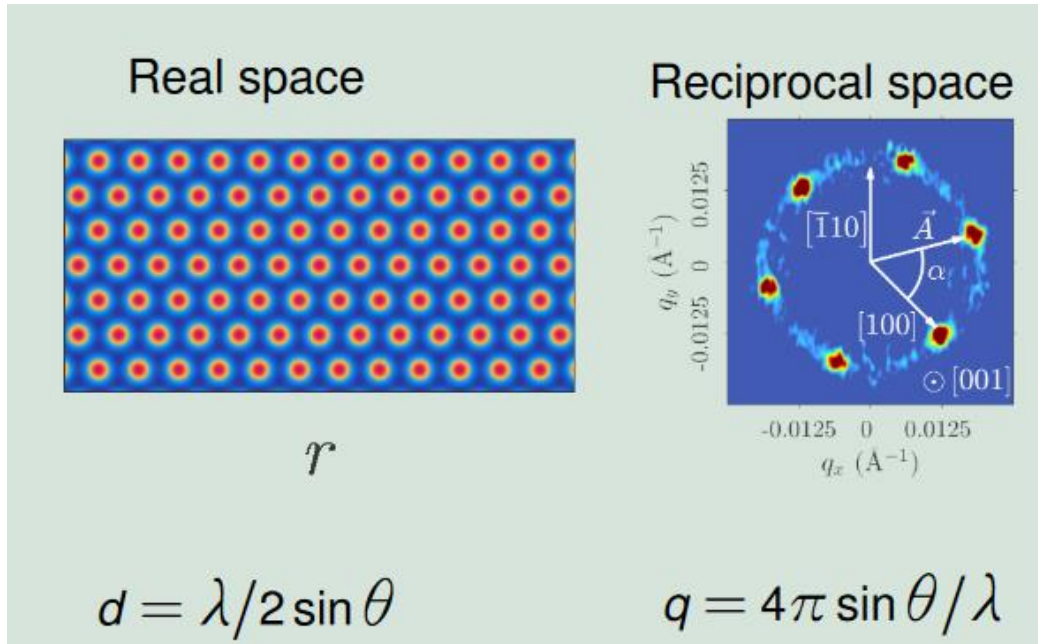
Topological defects in the order parameter

Vortex core, size ξ , over which OP varies rapidly

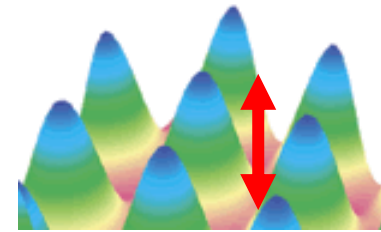
Field drops off to zero over distance λ_L



Diffraction from the vortex lattice



$$a \cong \sqrt{\frac{\Phi_0}{B}} \approx 950 \text{ \AA} \text{ at } B = 0.2 \text{ T}$$



few $\times F_{10}$

$$B(\mathbf{r}) = \sum_{hk} F(\mathbf{q}_{hk}) e^{i\mathbf{q}_{hk} \cdot \mathbf{r}}$$

F_{hk} , “form factor” = Fourier component at q_{hk} of spatial variation of field inside FLL

We can measure this using small angle neutron diffraction.

The form factor as a function of field

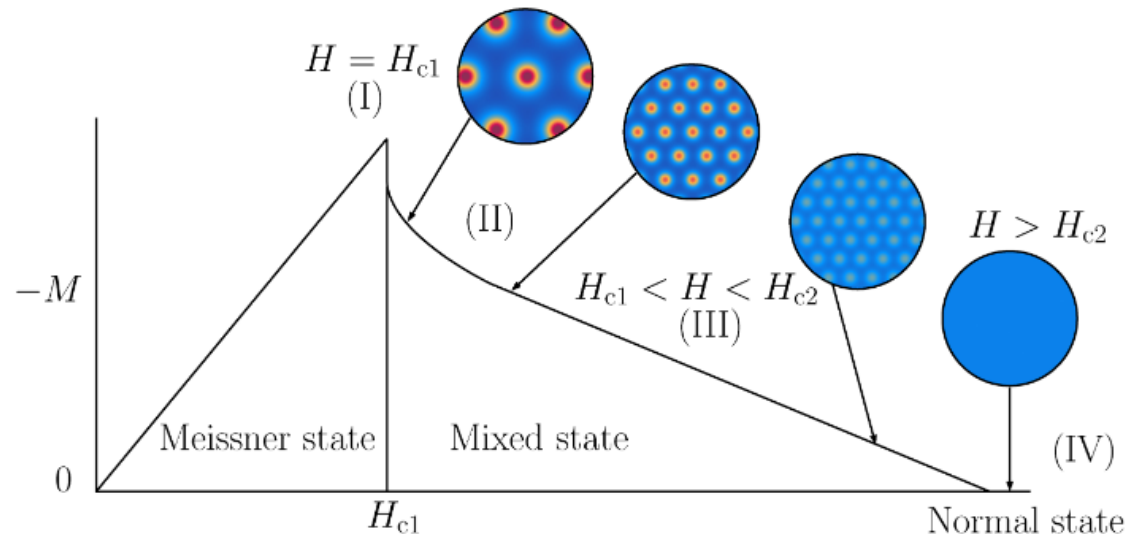
London Model

$$F(q)_{\text{London}} = \frac{B}{1 + (\lambda q)^2}.$$

For $B_{c1} < B \ll B_{c2}$, the London model gives:

$$F_{10} = \left(\frac{\sqrt{3}}{8\pi^2} \right) \times \frac{\Phi_0}{\lambda_L^2}$$

... where λ_L is the magnetic penetration depth, and $\lambda_L = 2500 \text{ \AA}$
 $\Leftrightarrow F_{10} \sim 0.7 \text{ mT}$



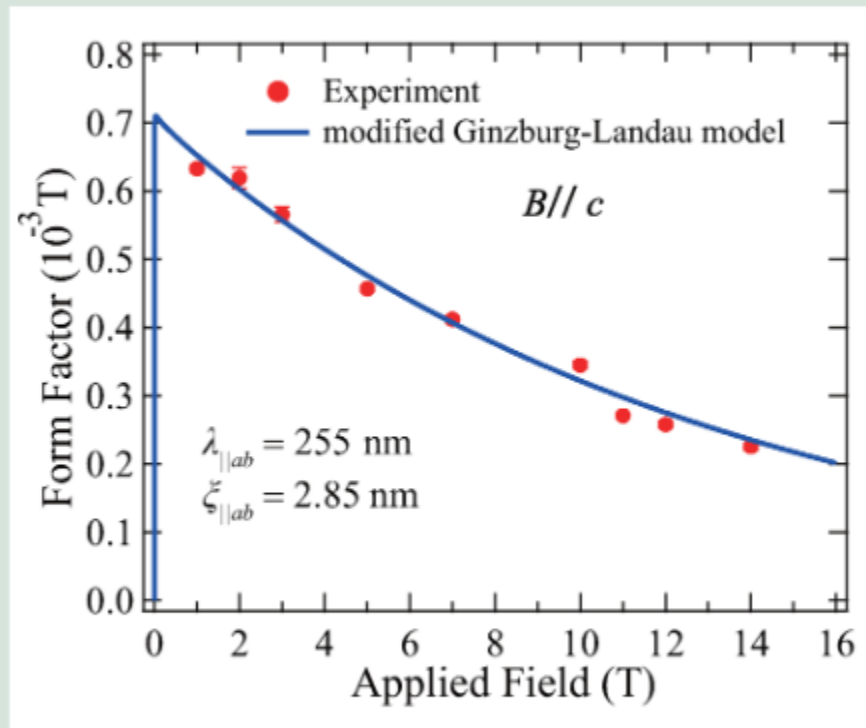
The form factor as a function of field

Brandt Model

$$F(q)_{\text{Brandt}} = \frac{B}{1 + (\lambda q)^2} e^{-c(\xi q)^2}.$$

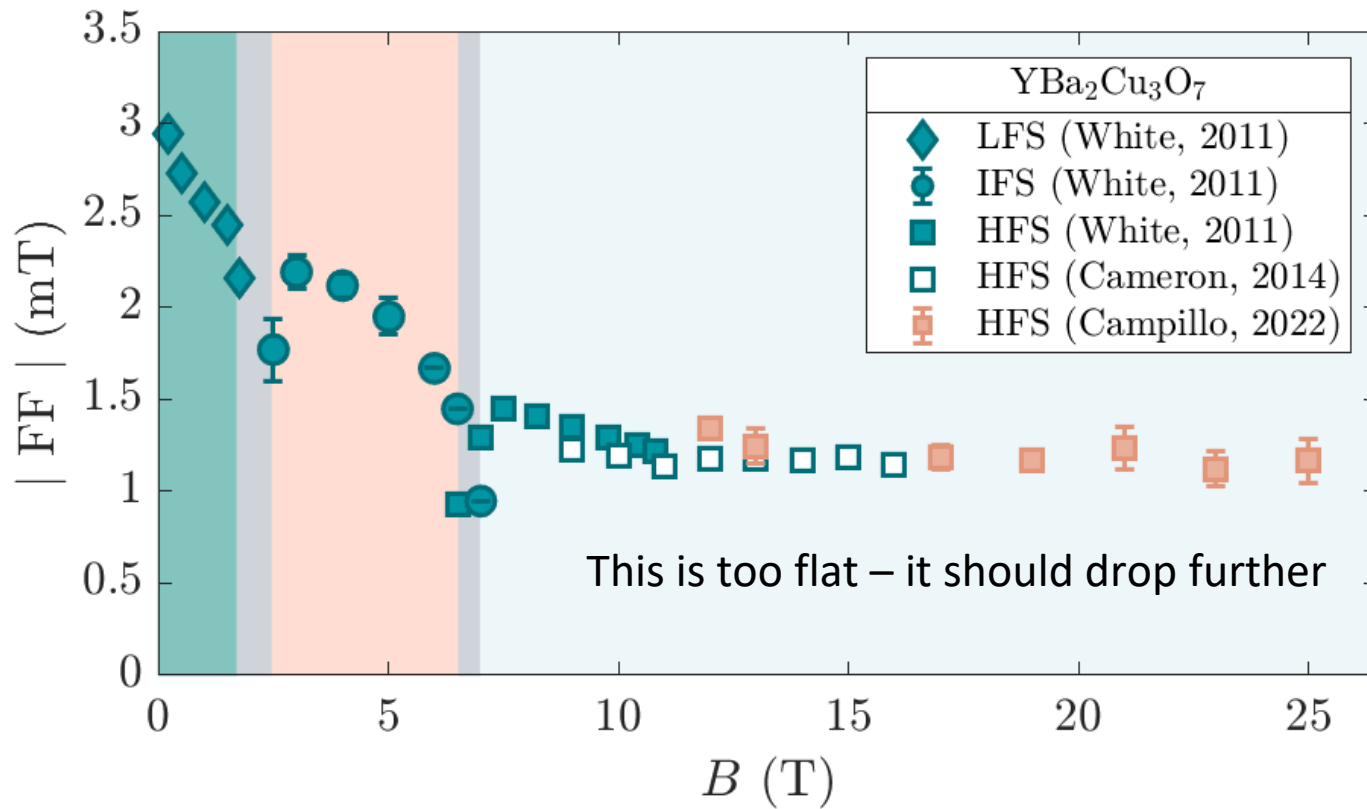
Brandt, Rep. Prog. Phys. **58**, 1465 (1995)

Brandt, Phys. Rev. Lett. **78**, 2208 (1997)

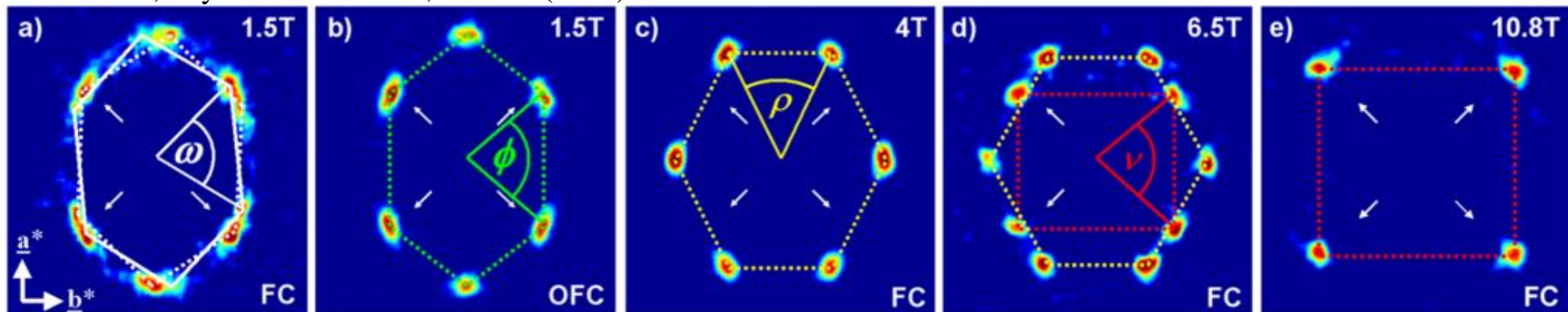


R. Morisaki-Ishii, et al., Phys. Rev. B, **90**, 125116 (2014).

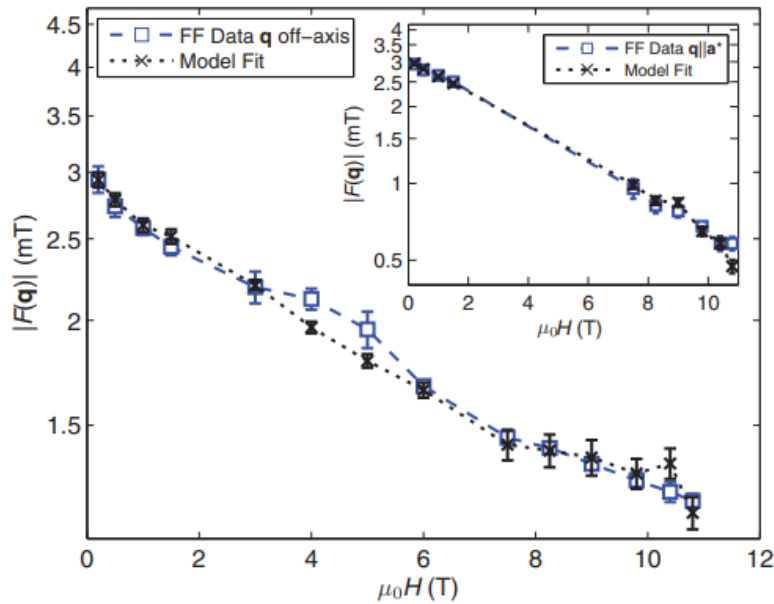
YBCO7 – fully occupied chains



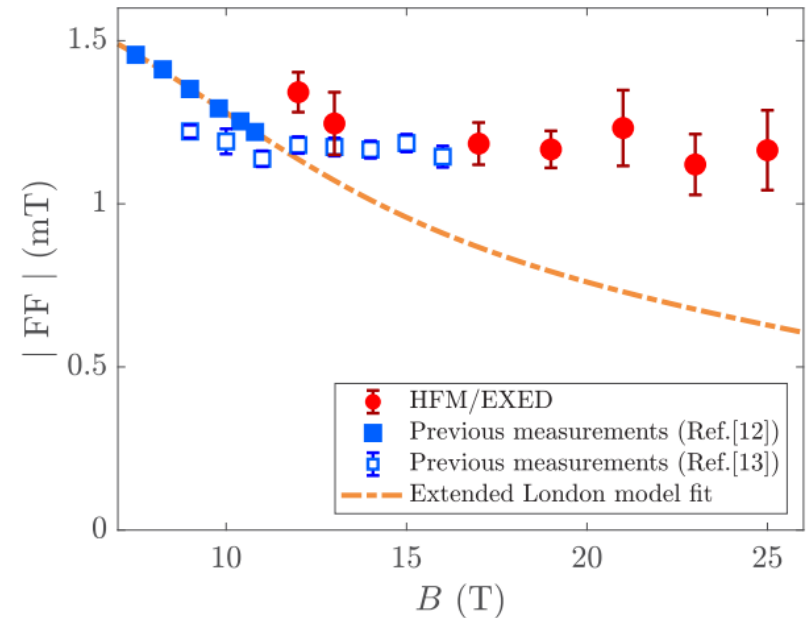
White *et al.*, Phys. Rev. Lett. **102**, 097001 (2009)



The form factor of the VL in YBCO



$$F(q)_{\text{Brandt}} = \frac{B}{1 + (\lambda q)^2} e^{-c(\xi q)^2}.$$



λ_a (nm)

λ_b (nm)

138(2)

107(1)

ξ_a (nm)

ξ_b (nm)

3.04(4)

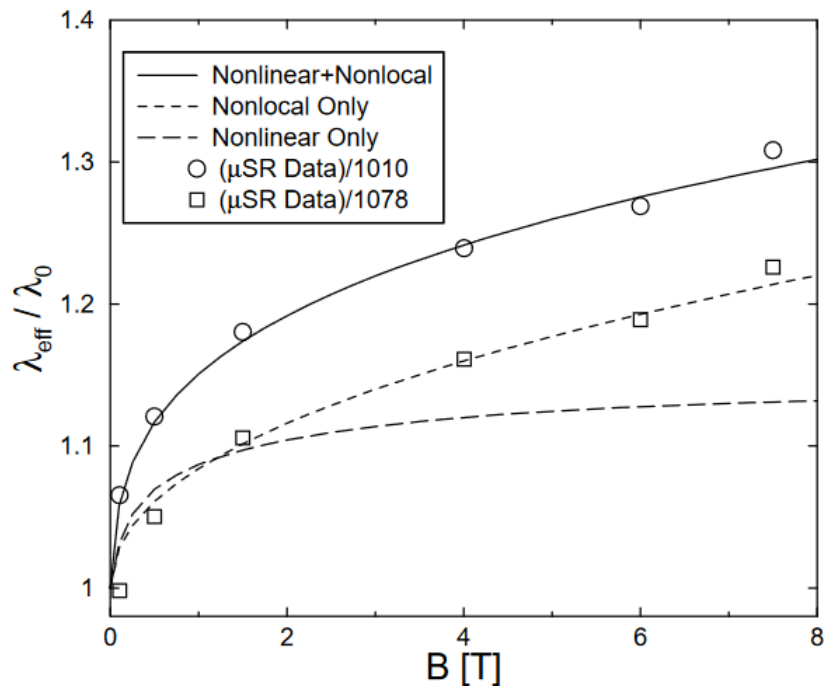
3.54(11)

$\lambda_a = 172(1)$ nm

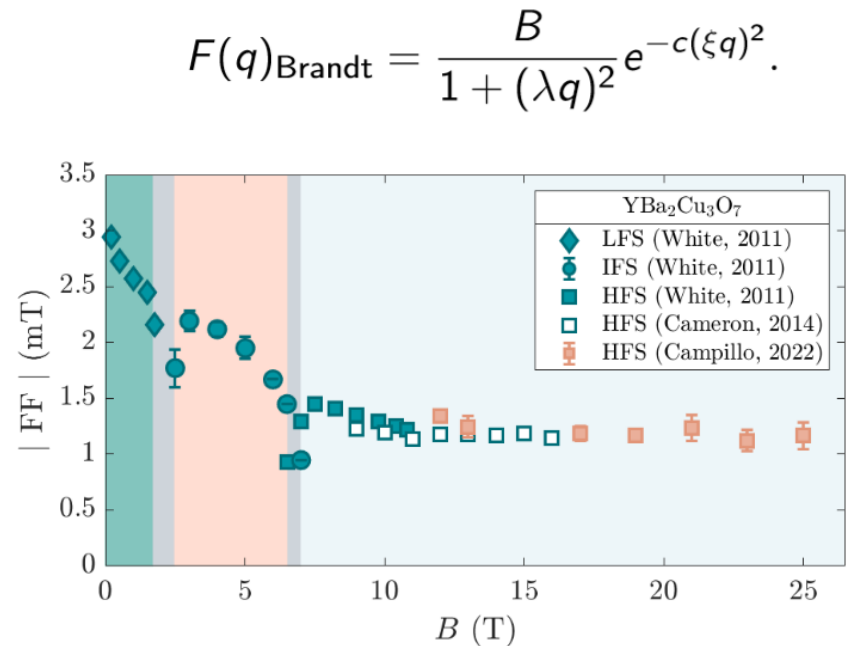
$\xi = 1.9(1)$ nm

Explanations?

- The superconducting characteristic lengths are changing.
The penetration depth changes with field.

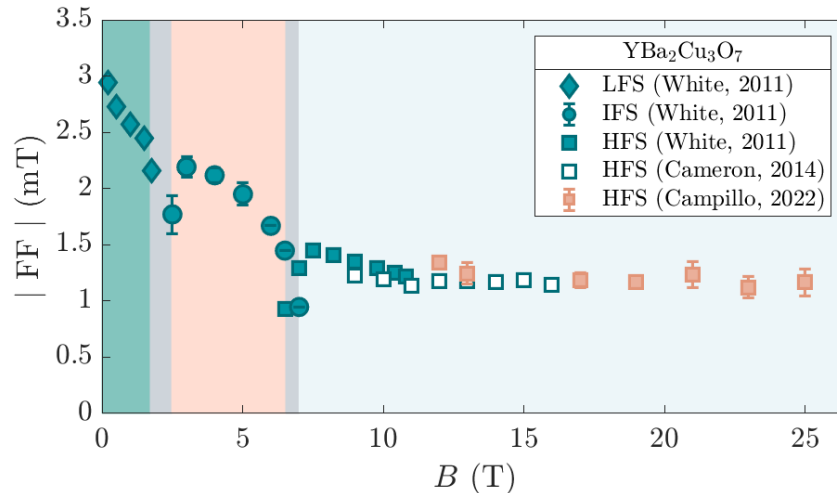


Amin *et al.*, Phys. Rev. Lett. **84**, 5864 (2000)



Explanations?

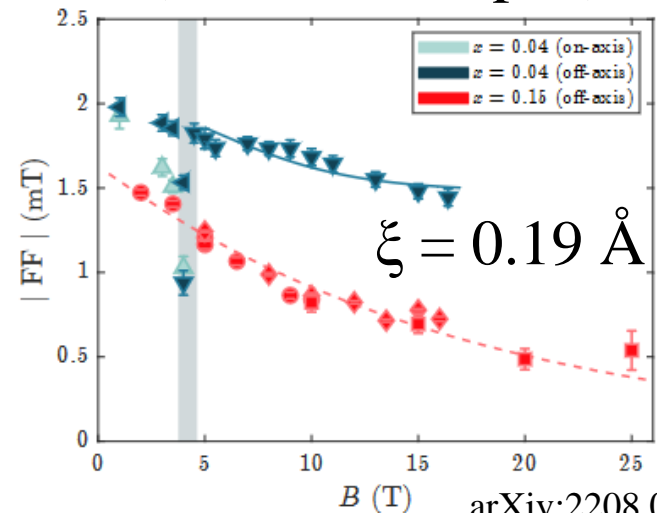
- The superconducting characteristic lengths are changing. The coherence length should also change with field.



It has to decrease a lot (e.g. to a few Angstroms).

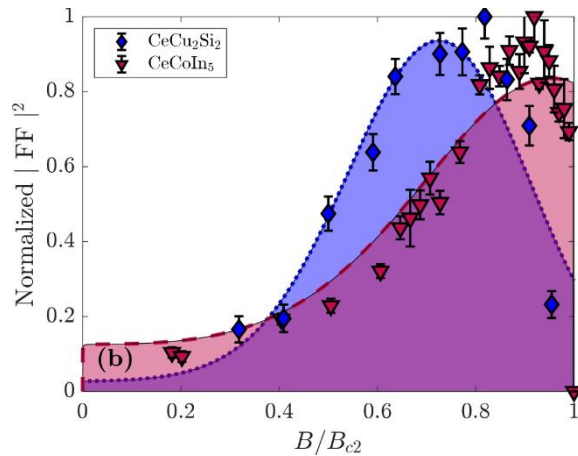
$$B_{c2} = \frac{\Phi_0}{2\pi\xi^2}$$

Ca-doped YBCO (more overdoped)

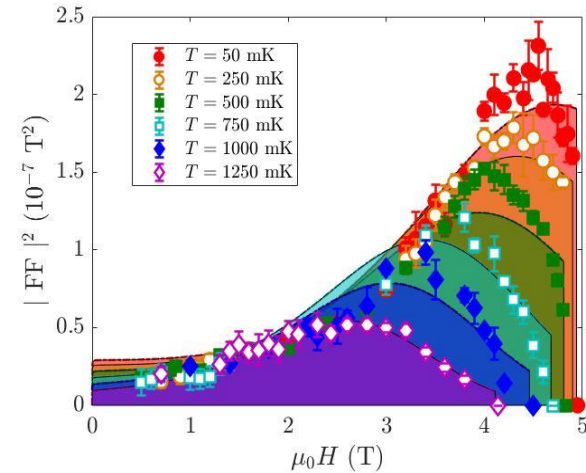


Explanations?

- Additional magnetization in the core (e.g. Pauli paramagnetic effects)

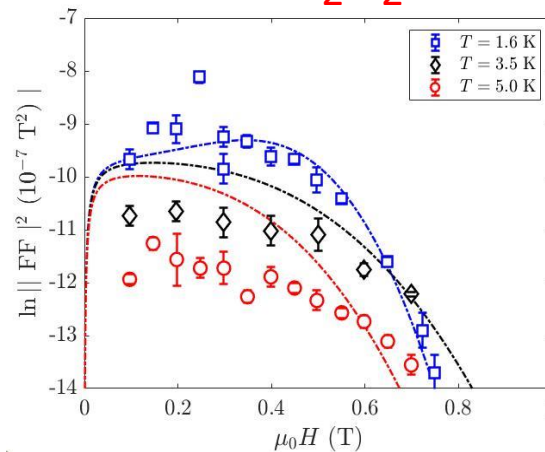


$CeCoIn_5$



$CeCu_2Si_2$

Model used described in Campillo *et al.*, Phys. Rev. B. **104**, 184508 (2021)

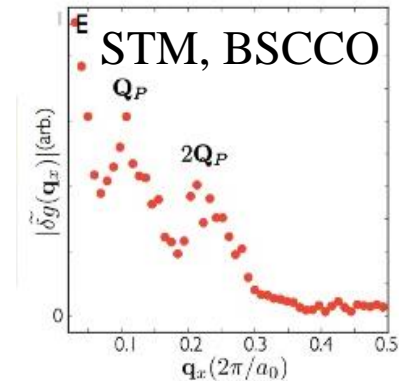


Data from DeBeer-Schmitt *et al.*, PRL **99**, 167001 (2007).

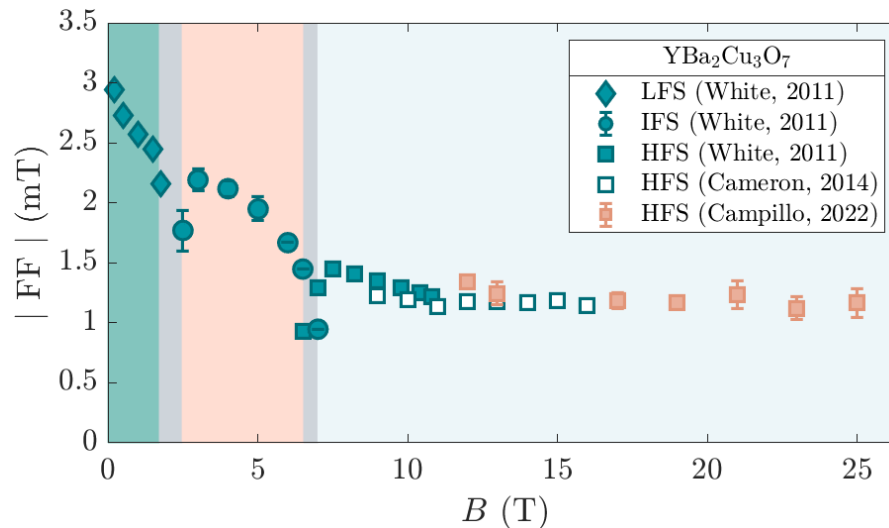
Conclusions

- A diffraction signature from the pair density wave?
 - not seen – Δ_0 at least one order of magnitude smaller than $\Delta_1 = \Delta_{\text{PDW}}$ in YBCO ortho-II

$$\rho_e(r) \propto (\Delta_0^2 + 2\Delta_0\Delta_1 \sin(qr) + \Delta_1^2 \sin^2(qr))$$



- The vortex lattice at high magnetic fields



This is too flat – it should drop further