Charge density waves in high-T_c superconductors

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ECRYS 2017 – 22 August 2017

Acknowledgements

EPSRC
Engineering and Physical Sciences Research Council

Alex Holmes
Ted Forgan
Amy Briffa
Martin Long

University of BRISTOL
Stephen Hayden

Universität Zürich
Johan Chang

DTU
Niels Christensen
Jacob Larsen

BROOKHAVEN NATIONAL LABORATORY
Markus Hücker

DESY
Anke Watenphul
Martin von Zimmerman
Uta Rütt
Olof Gutowski

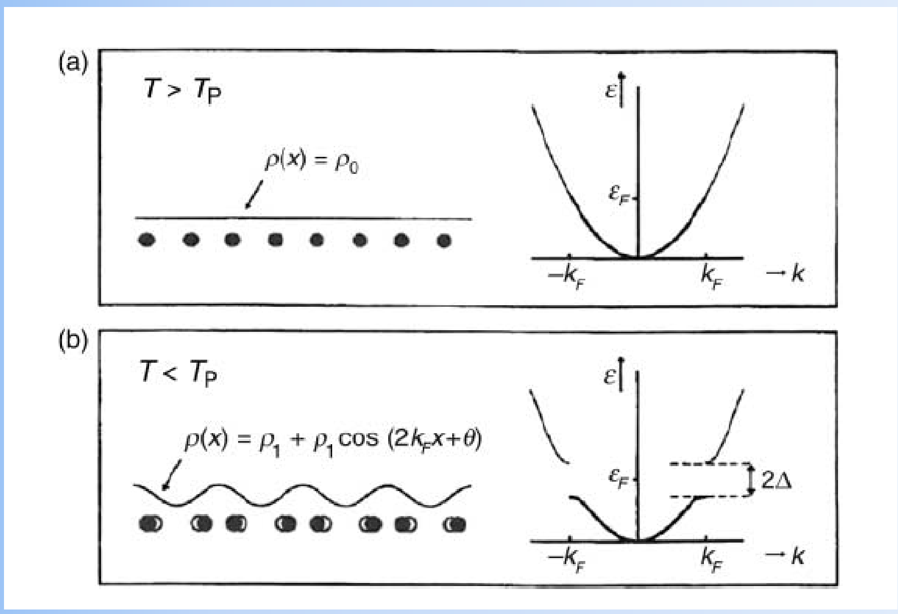
XMaS the UK-CRG
Laurence Bouchenoire
Simon Brown
Paul Thompson

LNCMI
Wojciech Tabis

UBC
Ruixing Liang
Doug Bonn
Walter Hardy

Introducing CDWs and Superconductivity

CDWs

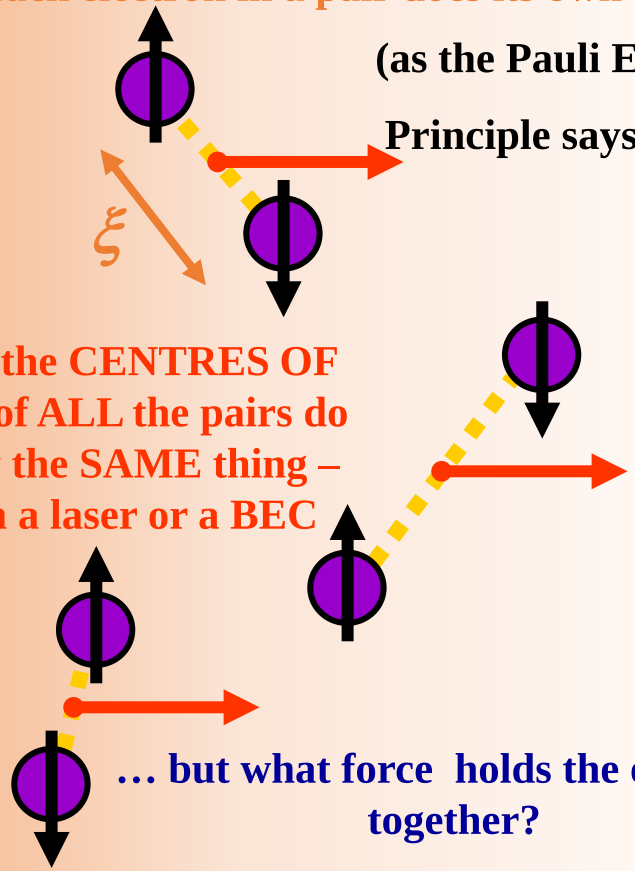


Monceau, Advances in Physics **61**, 325 (2012).

Superconductors

each electron in a pair does its own thing …

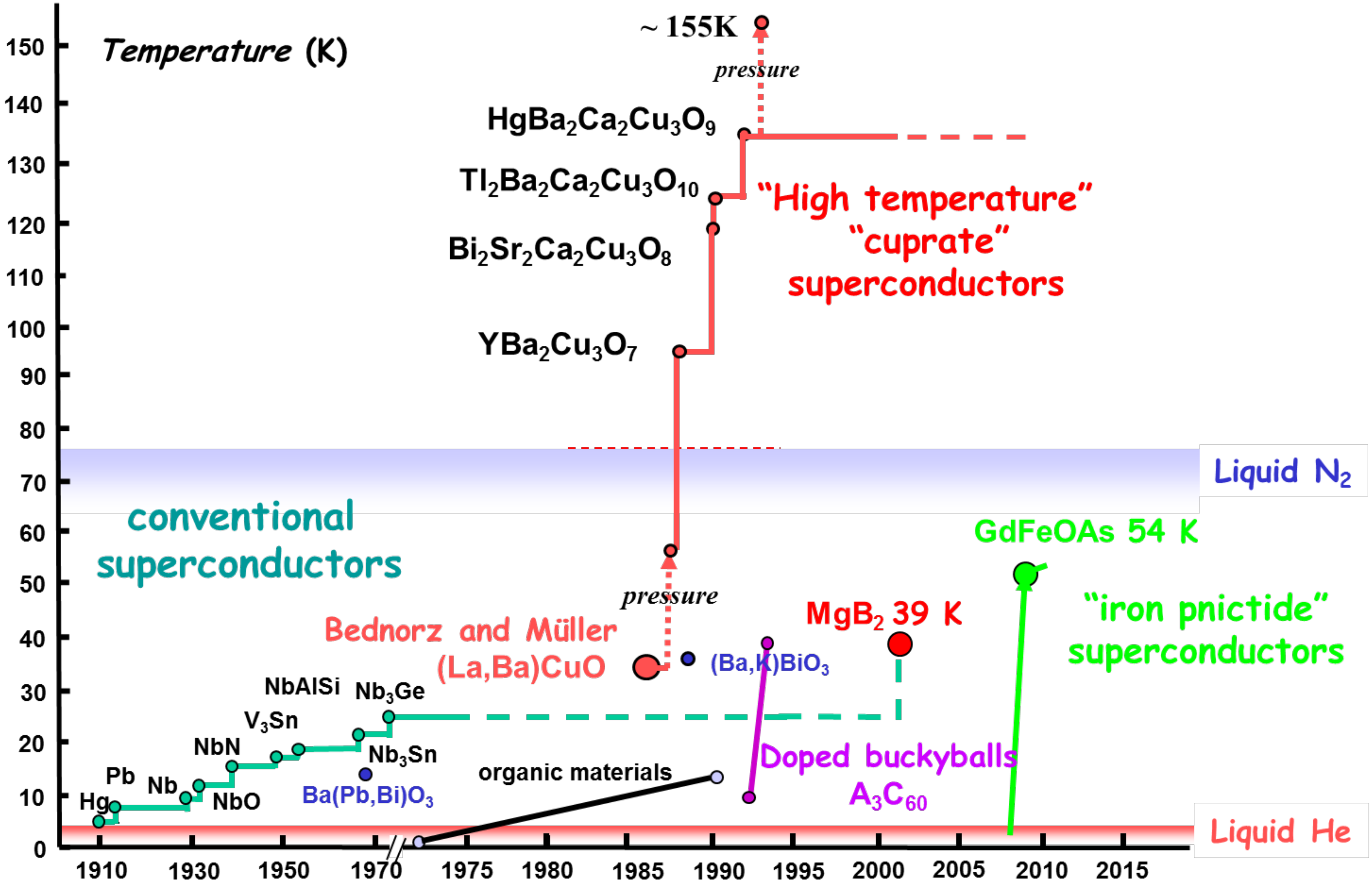
(as the Pauli Exclusion Principle says it must)



… 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” ξ apart)



Temperature (K)
~ 155K
pressure
HgBa2Ca2Cu3O9
Tl2Ba2Ca2Cu3O10
"High temperature"
"cuprate"
superconductors
Bi2Sr2Ca2Cu3O8
YBa2Cu3O7
Liquid N2
conventional
superconductors
GdFeOAs 54 K
pressure
MgB2 39 K
"iron pnictide"
superconductors
Bednorz and Müller
(La,Ba)CuO
(Ba,K)BiO3
NbAlSi
Nb3Ge
V3Sn
NbN
Nb3Sn
Doped buckyballs
A3C60
organic materials
Pb
Nb
Hg
NbO
Ba(Pb,Bi)O3
Liquid He
0
10
20
30
40
50
60
70
80
90
100
110
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2000
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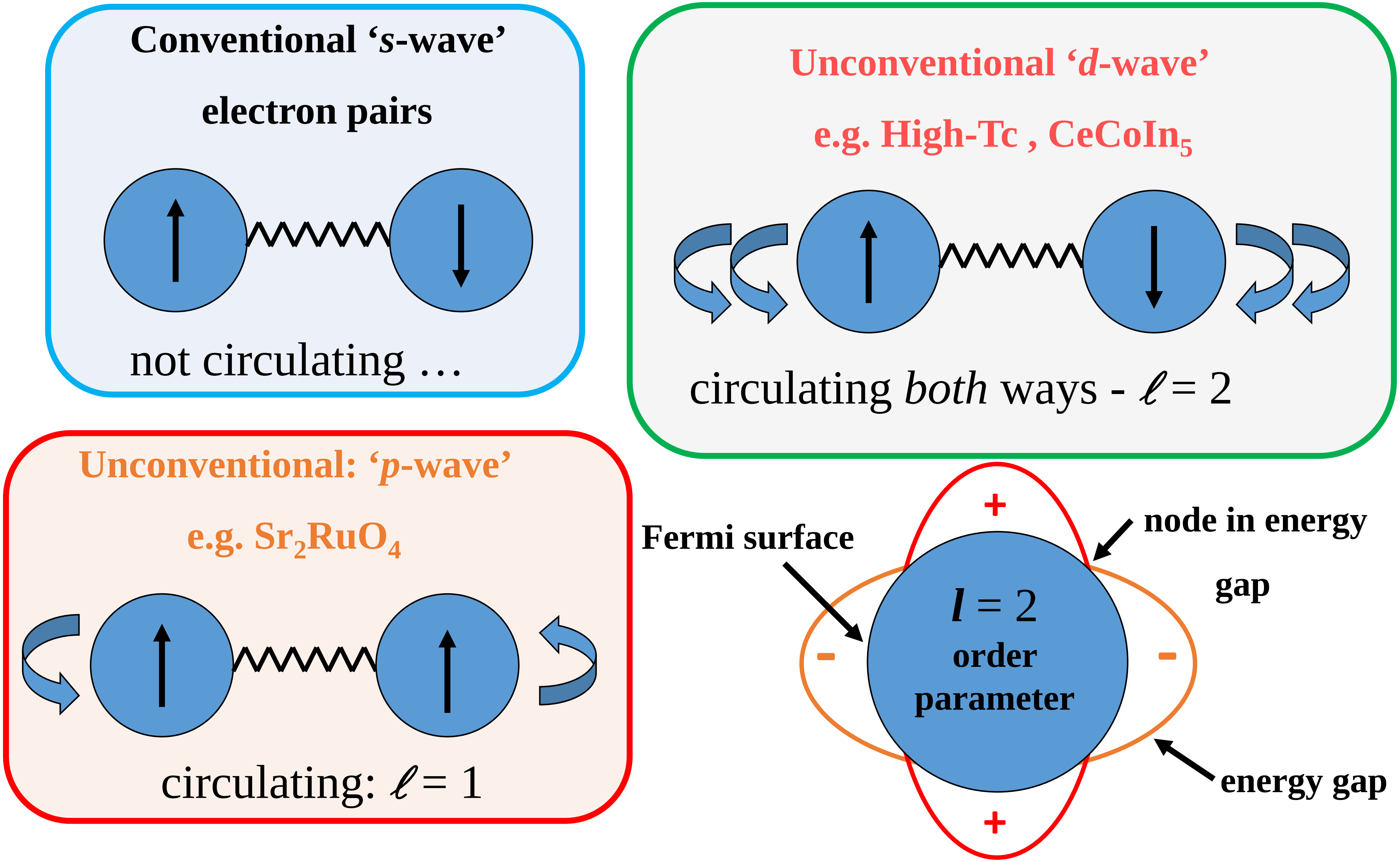
2010
2015

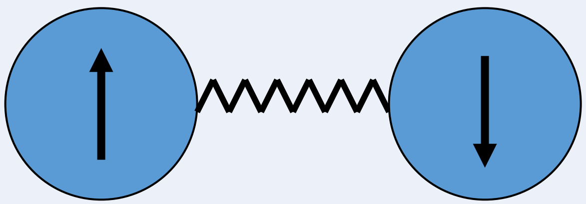
Cooper pairs in superconductors



Cooper pairs in superconductors

Conventional ‘*s*-wave’

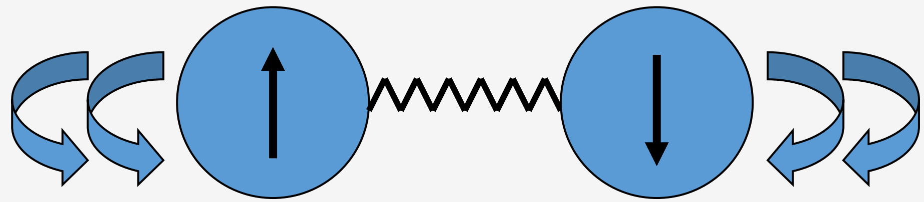
electron pairs



not circulating …

Unconventional ‘*d*-wave’

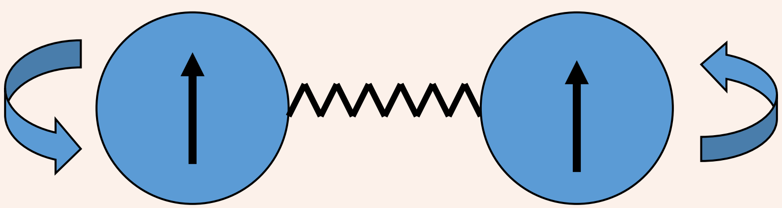
e.g. High-Tc , $CeCoIn_5$



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

Unconventional: ‘*p*-wave’

e.g. Sr_2RuO_4

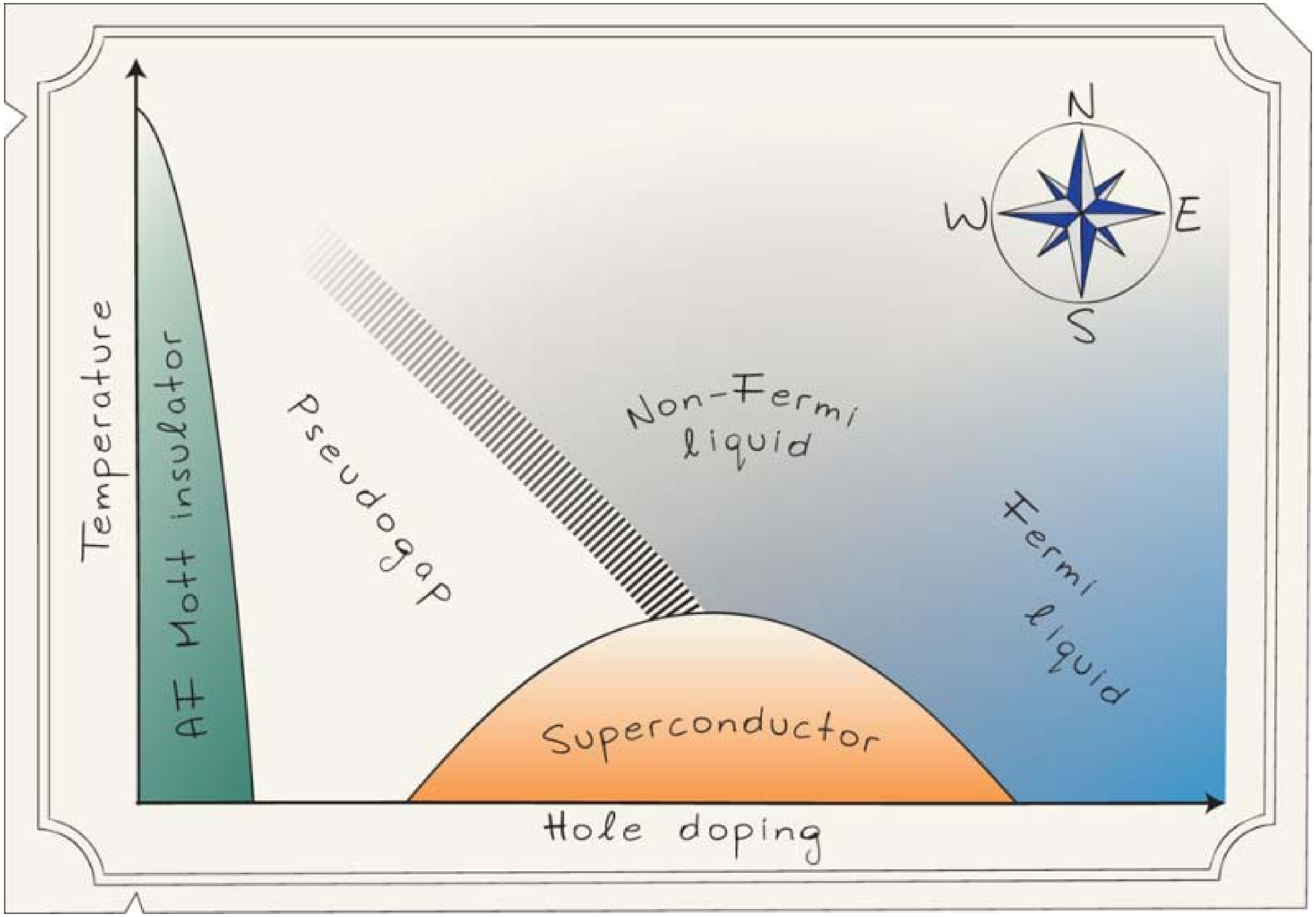


circulating: $\ell = 1$

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

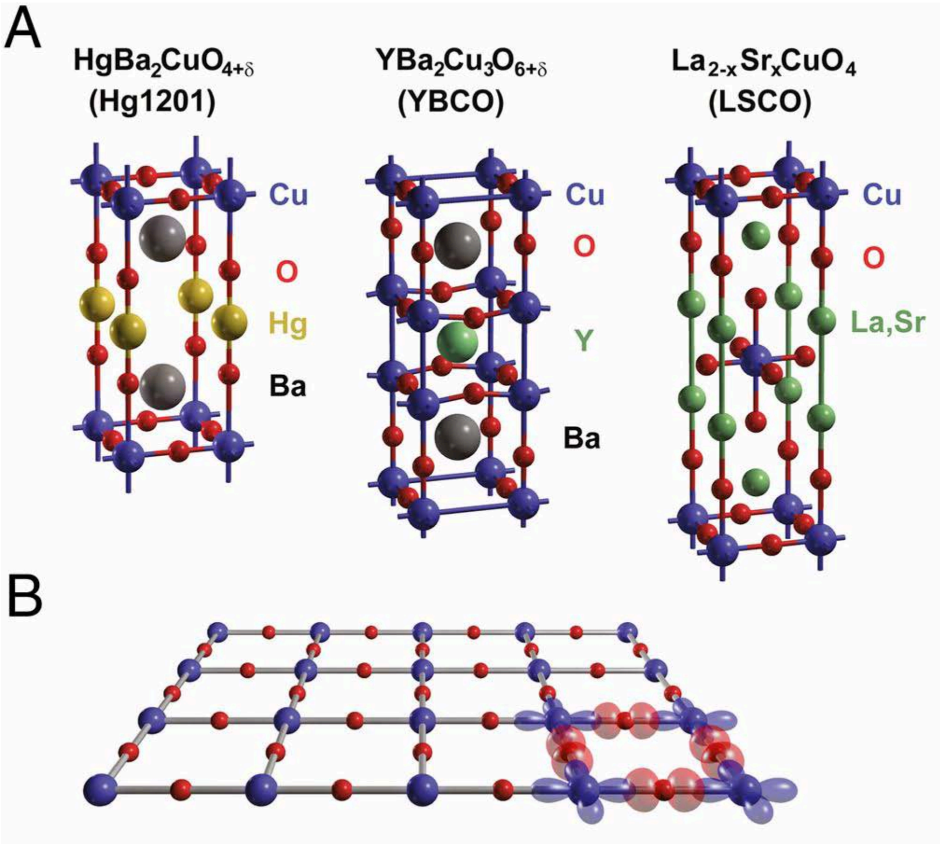
How does the pairing arise??

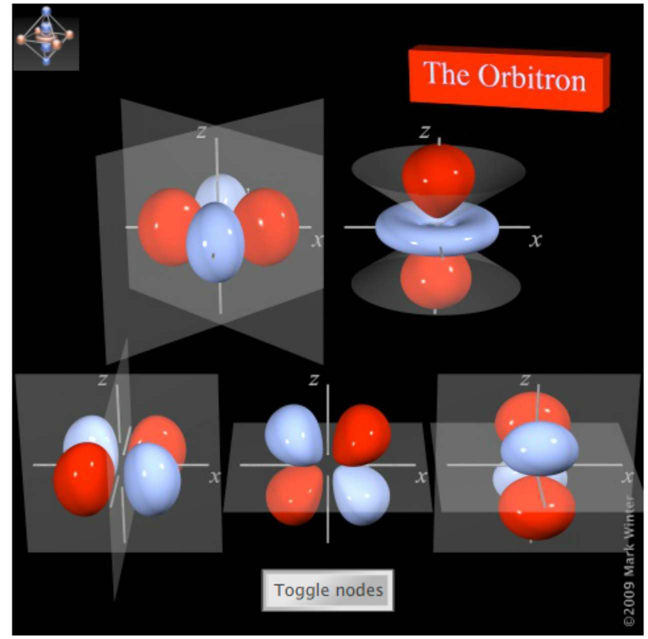
High T_C superconductors – the cuprates



Wahl, Nature Physics (2012)

High T_C superconductors – the Cu-O plane





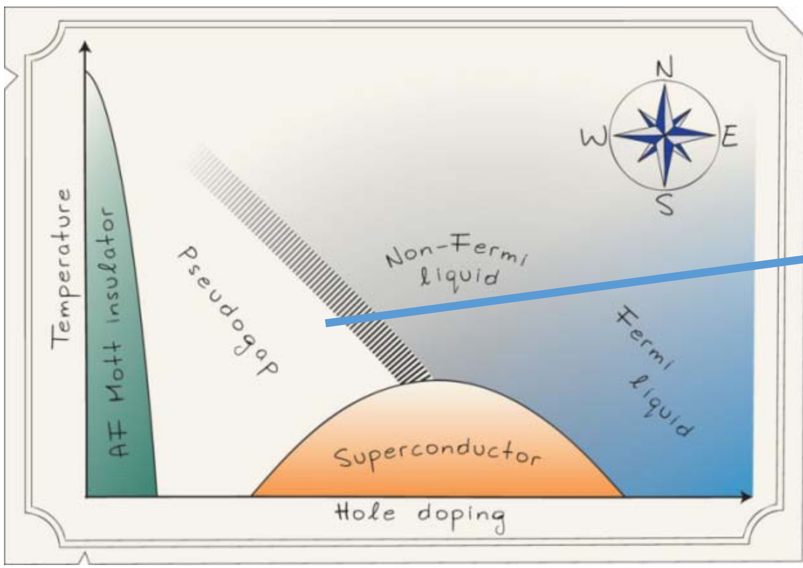
The shape of the five 3d orbitals. *From left to right: (top row) $3d_{x^2-y^2}$ and $3d_{z^2}$ (bottom row) $3d_{xy}$, $3d_{xz}$, and $3d_{yz}$. For each, the yellow zones are where the wave functions have negative values and the blue zones denote positive values.*

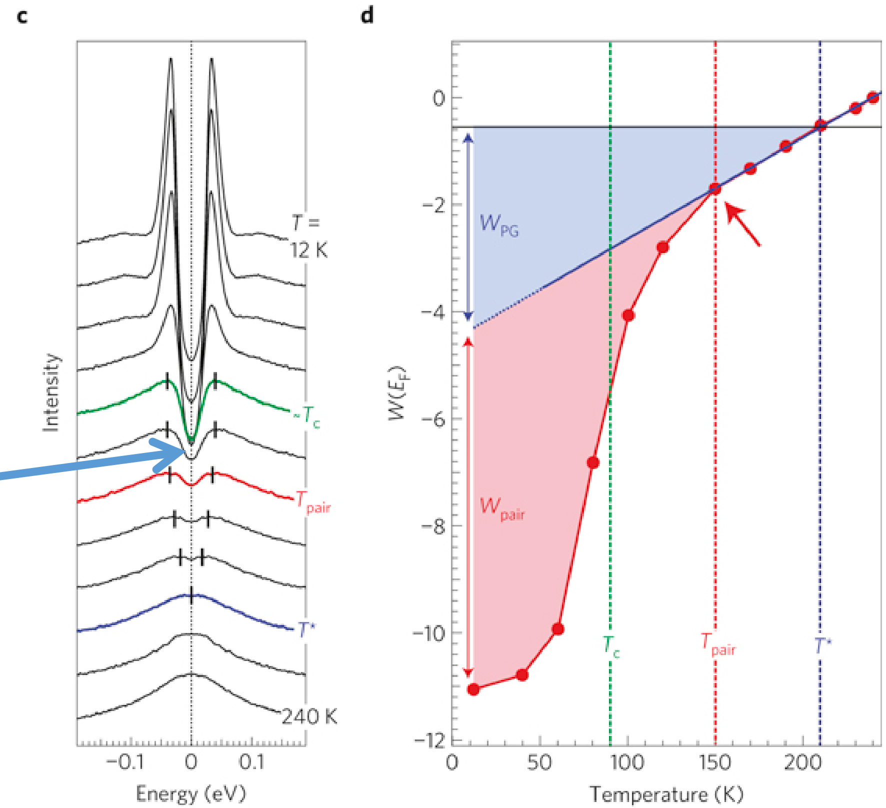
Barisic *et al.*, PNAS **110**, 12235 (2013)

Mark Winter,
http://www.shef.ac.uk/chemistry/orbitron/

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

- Pre-formed pairs?
- Competing order?

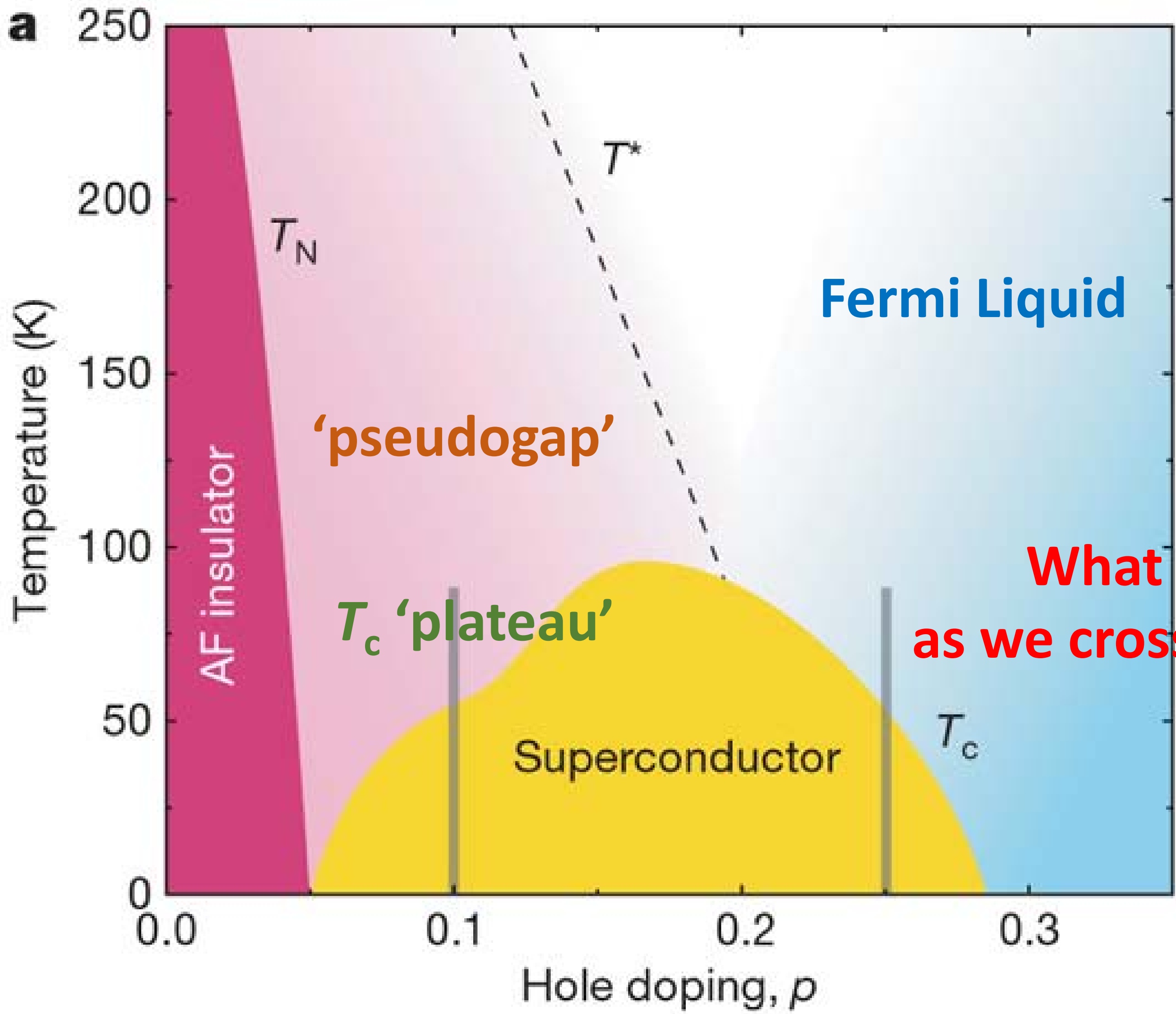




Wahl , Nature Physics (2012)

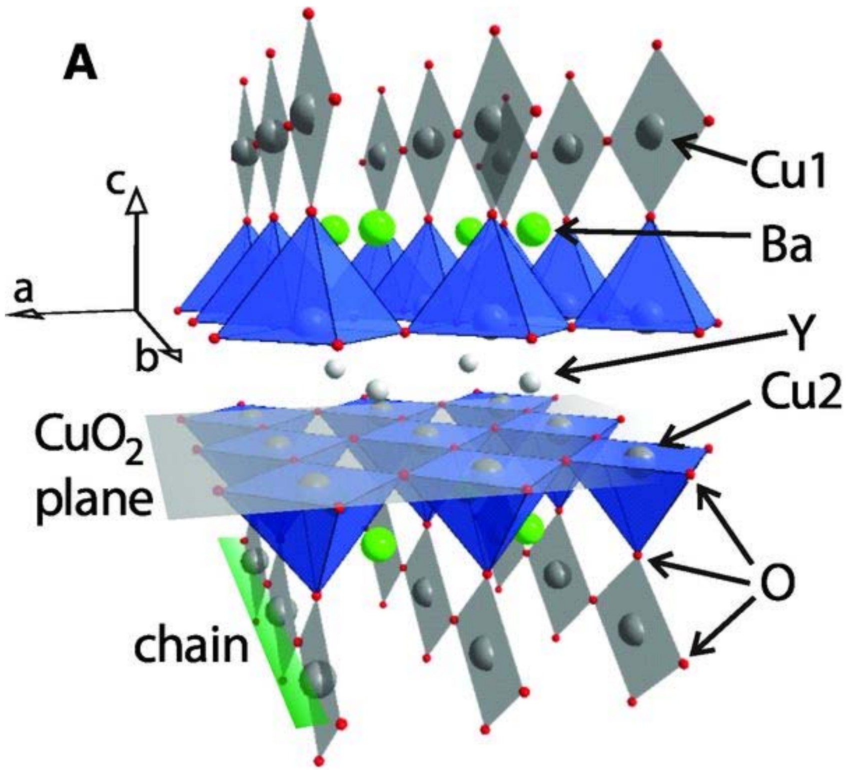
Kondo *et al.*, Nature Physics (2011)

Phase diagram of $YBa_2Cu_3O_{7-x}$ versus doping



What changes
as we cross the 'dome'?

Superconductivity in YBCO$_{6+x}$

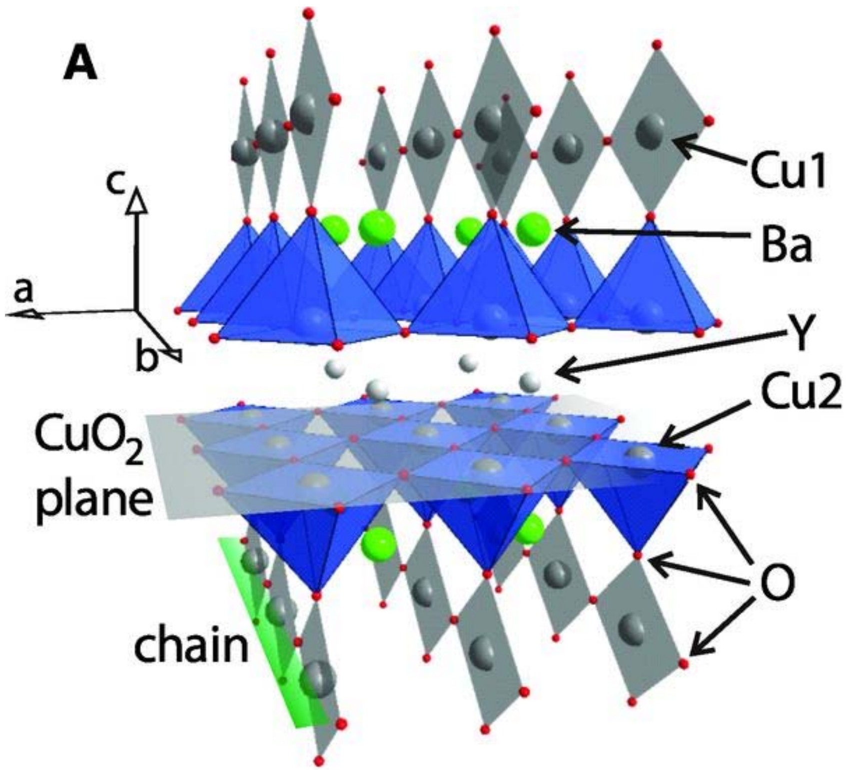


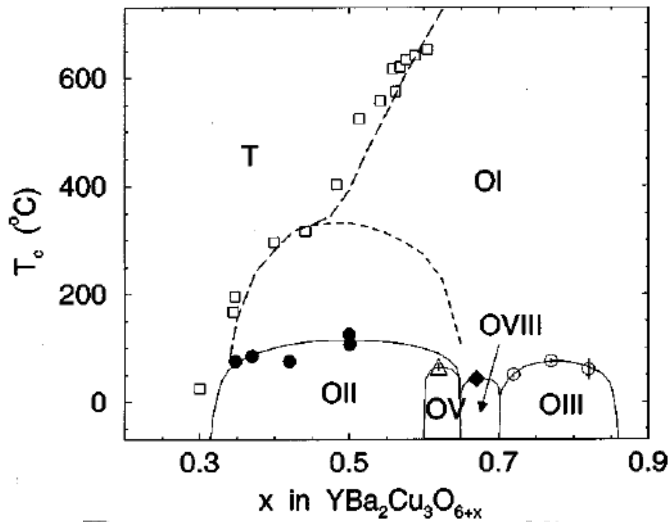
Ghiringhelli *et al.*, Science (2012)
Andersen *et al.*, Physica C (1999)
v. Zimmerman *et al.*, Phys.Rev.B (2003)

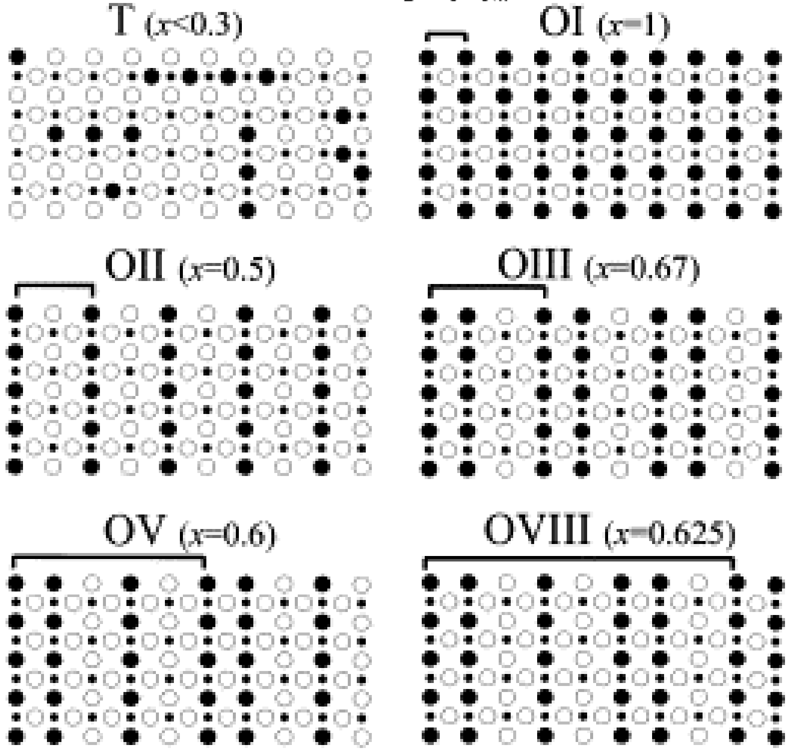
Superconductivity mainly resides in the CuO_2 bi-layered planes

Oxygen content is varied from O_7 to O_6 by removing O from the chains running along ***b***

Superconductivity in YBCO$_{6+x}$







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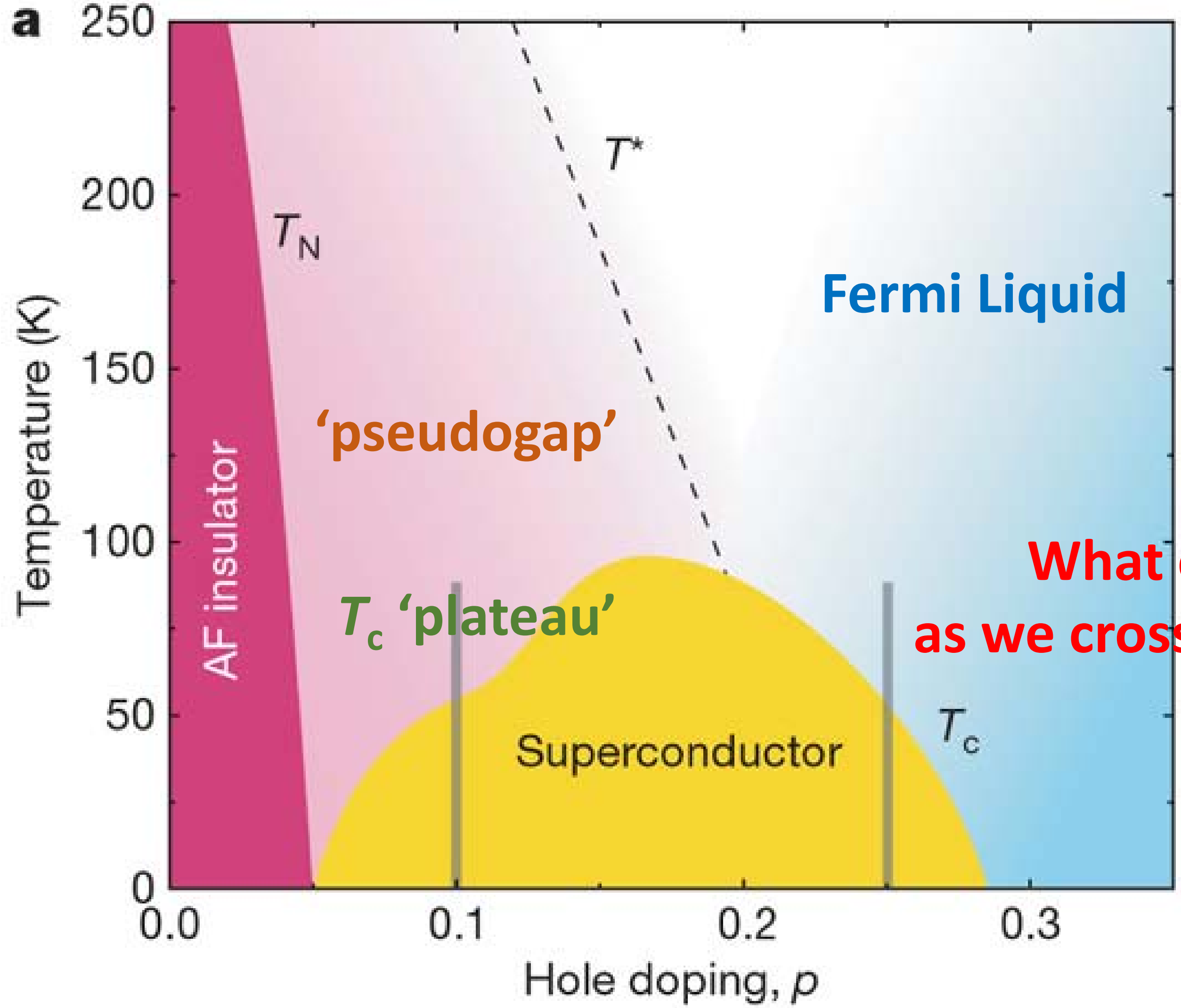
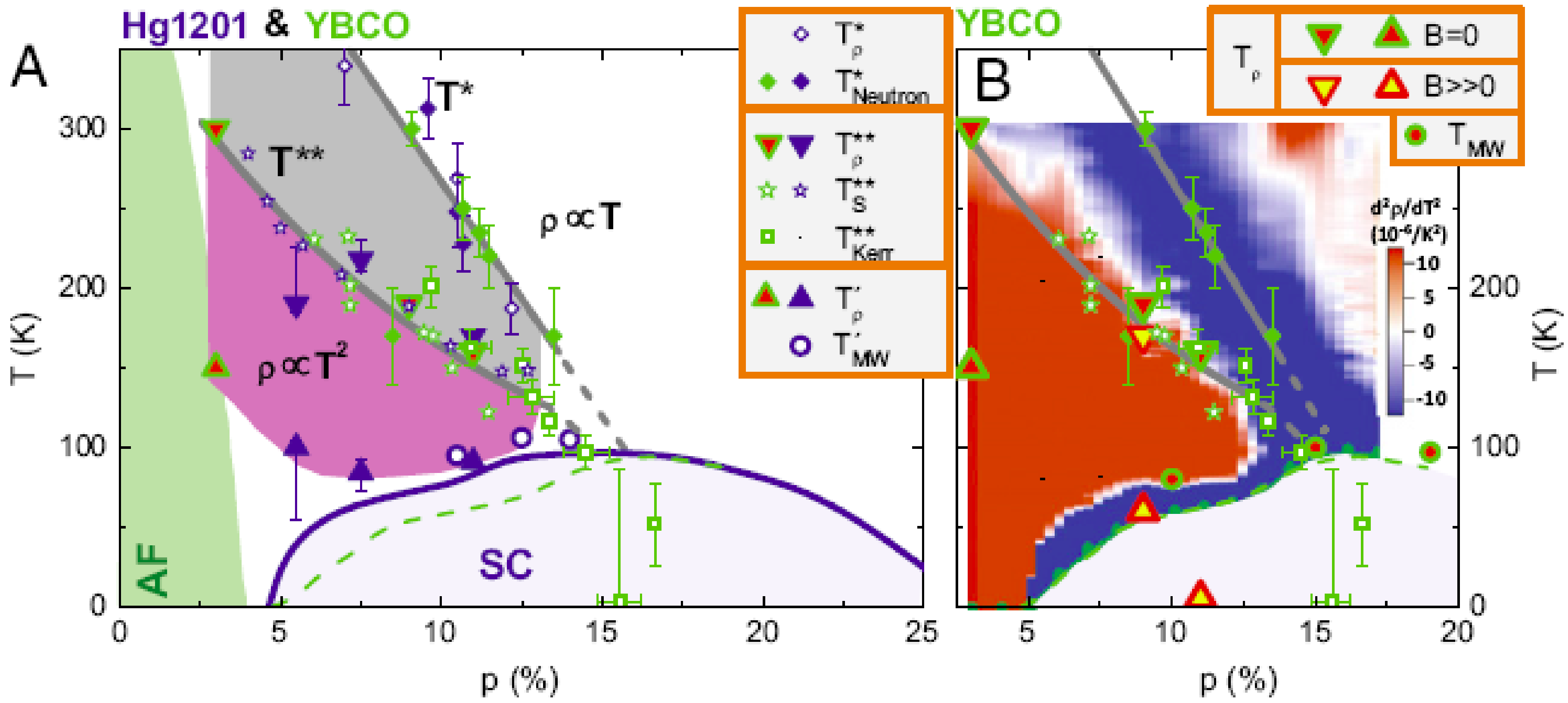


What changes
as we cross the 'dome'?

Signs of something changing inside the PG region

- Transport measurements

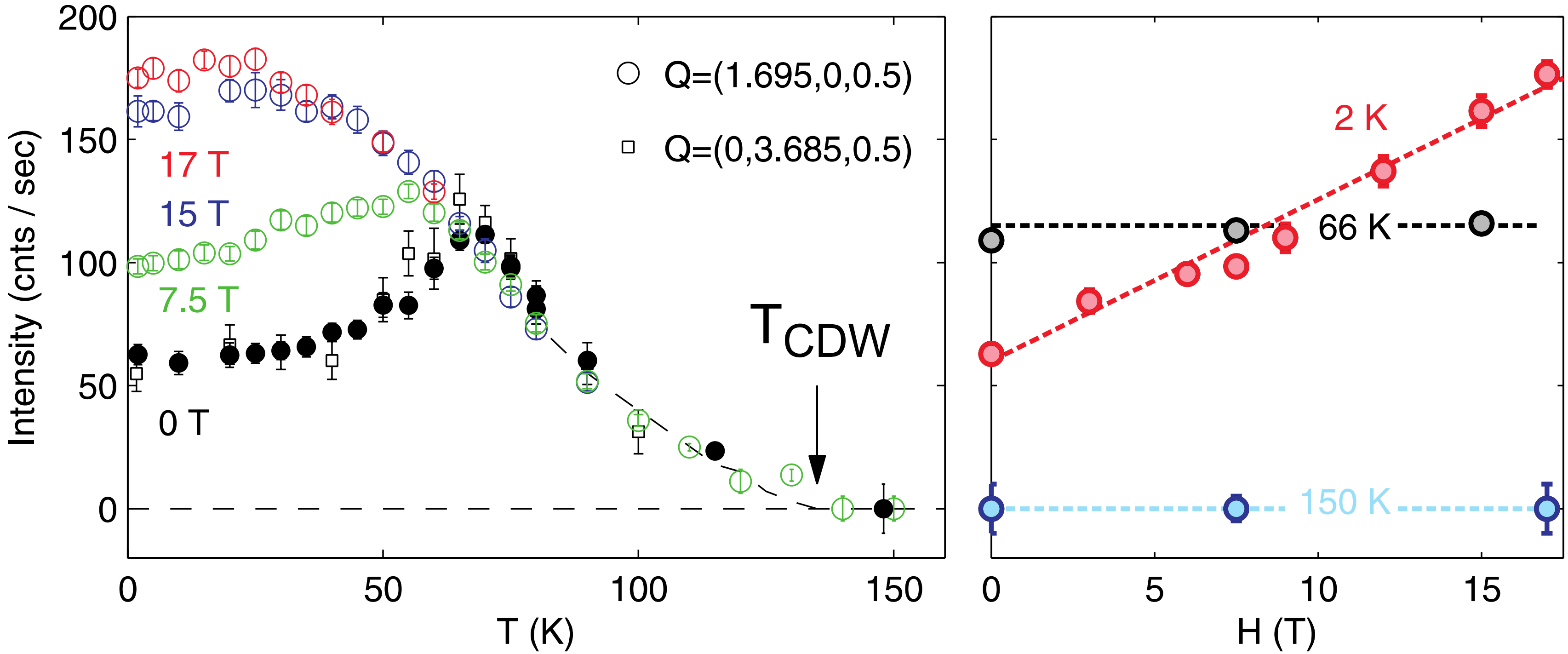
Sheet resistance



Barisic *et al.*, PNAS **110**, 12235 (2013)

What is changing?

The $YBa_2Cu_3O_y$ family shows charge density wave order which competes with superconductivity

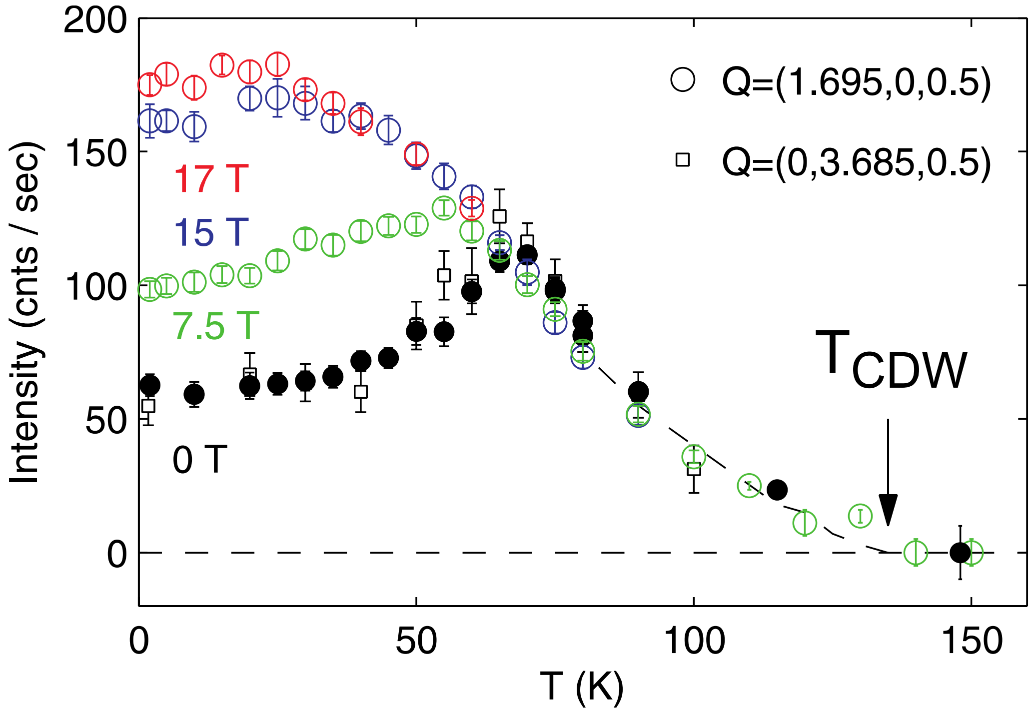


Ortho-VIII

Chang, EB *et al.*, Nature Physics (2012)

What is changing?

The $YBa_2Cu_3O_y$ family shows charge density wave order which competes with superconductivity



Correlation lengths:

$\xi_a = 95 \pm 5$ Å

$\xi_c \approx 0.6$ c

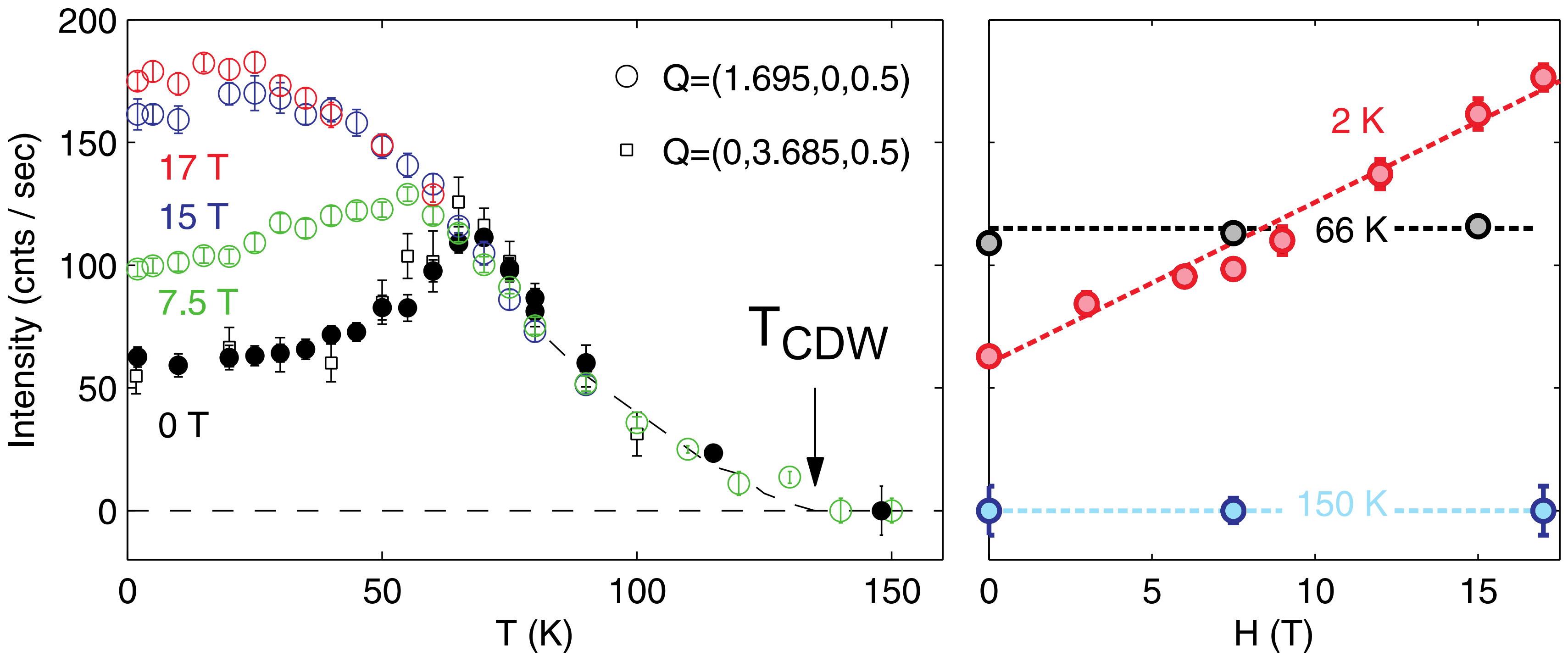
(Gaussian sigmas)

Ortho-VIII

Chang, EB *et al.*, Nature Physics (2012)

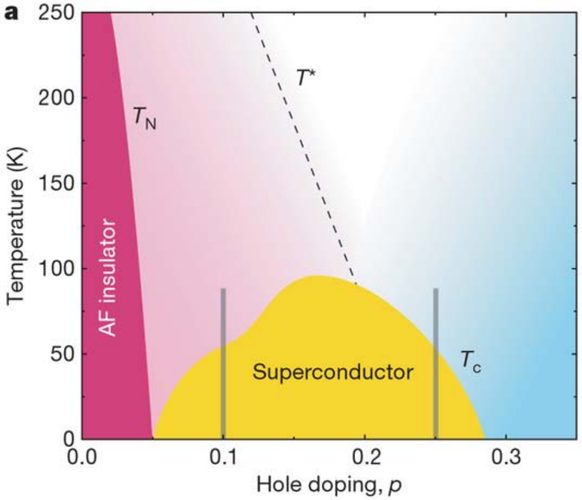
What is changing?

… also seen in a large range of cuprates; this appears to be an almost universal instability of the Cu-O plane

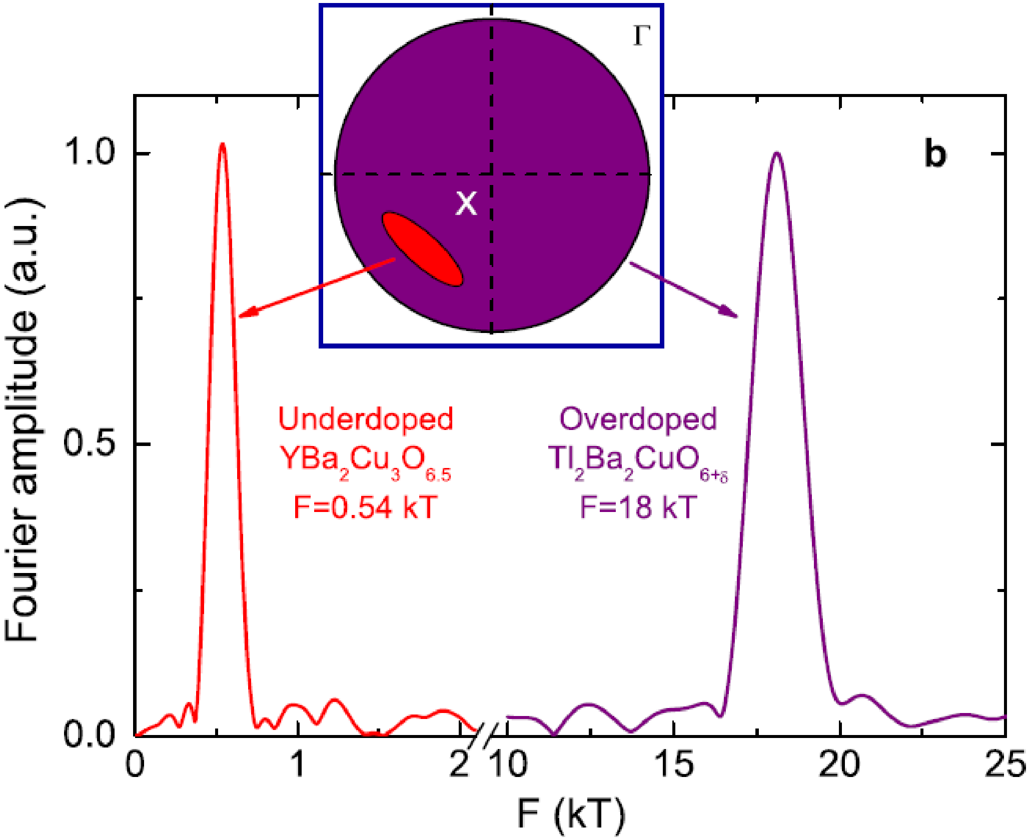


Chang, EB *et al.*, Nature Physics (2012)

This CDW affects the Fermi surface



Overdoped – all holes visible - obeys Luttinger theorem

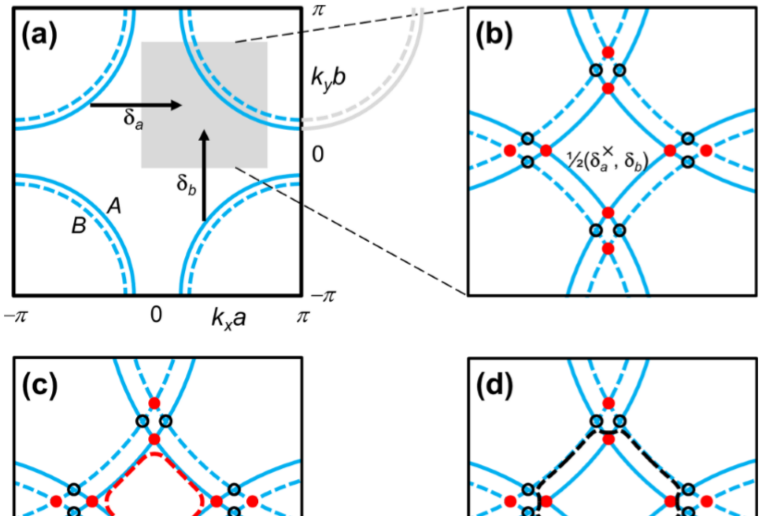


Underdoped – tiny number of *electrons* not holes

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

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

We can chop up the Fermi surface with our CDW wavevectors.



[redacted]

A = antibonding
B = bonding
= A-B degenerate -> hybridization possible
= A-A or B-B degeneracy -> weaker hybridization

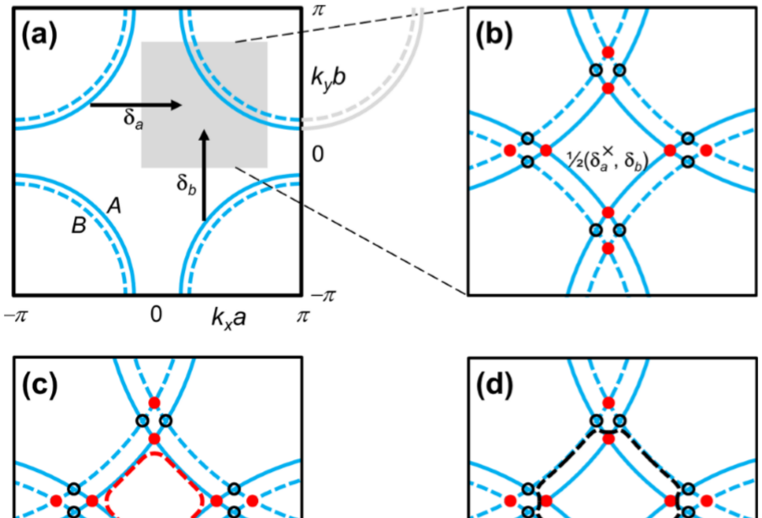
Electron-like Fermi surfaces

Possible magnetic breakdown routes

This is schematic; one should also consider e.g. effect of pseudogap on FS, spin-orbit coupling, *c*-axis effect, etc.

Briffa, EB, *et al.*, *Phys. Rev. B* **93**, 094502 (2016)

We can chop up the Fermi surface with our CDW wavevectors.



[redacted]

A = antibonding

B = bonding

= A-B degenerate -> hybridization possible

= A-A or B-B degeneracy -> weaker hybridization

Electron-like Fermi surfaces

Possible magnetic breakdown routes

There is a lot of ongoing quantum oscillation work investigating the exact nature of these pockets.

Briffa, EB, *et al.*, *Phys. Rev. B* **93**, 094502 (2016)

What is the actual CDW distortion?

To find this we had to measure a sufficient number (>200) of different X-ray diffraction satellites due to the CDWs in an o-II sample to derive the ionic displacements that fit the data.

It should then be possible to deduce something about the physics of the CDW from these ionic displacements

This was successful, and from the results it may be argued that the result is not a ‘standard’ CDW.

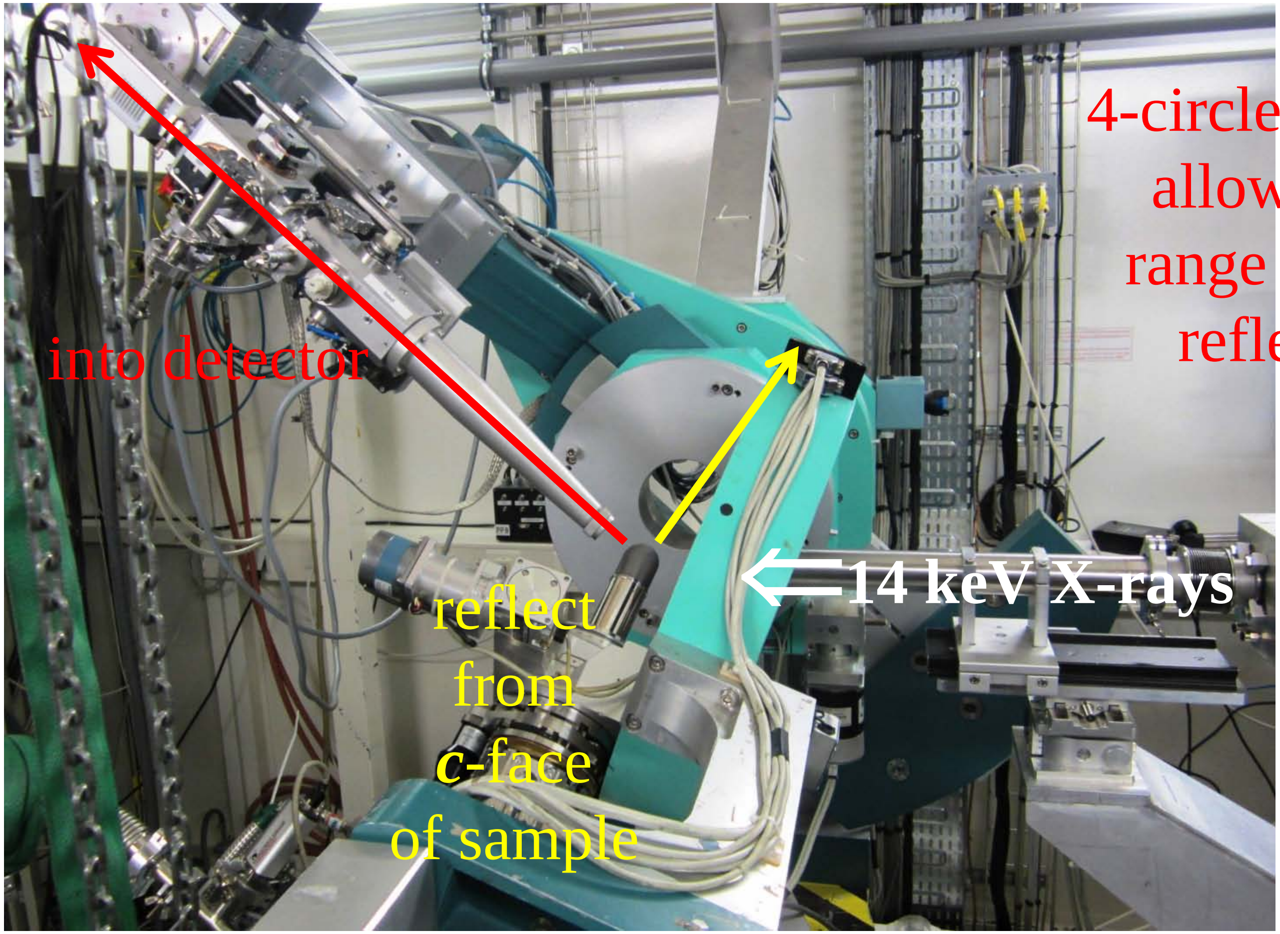
Measurements at the Cu-L-resonant X-ray wavelength are not suitable: you only see one atom and a very restricted range of reciprocal space due to the long wavelength

But non-resonant X-rays see ALL the 13 atoms in the YBCO unit cell, so the results are difficult to analyse!

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

What is the actual CDW distortion?

Measurements done at XMaS Facility, ESRF



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

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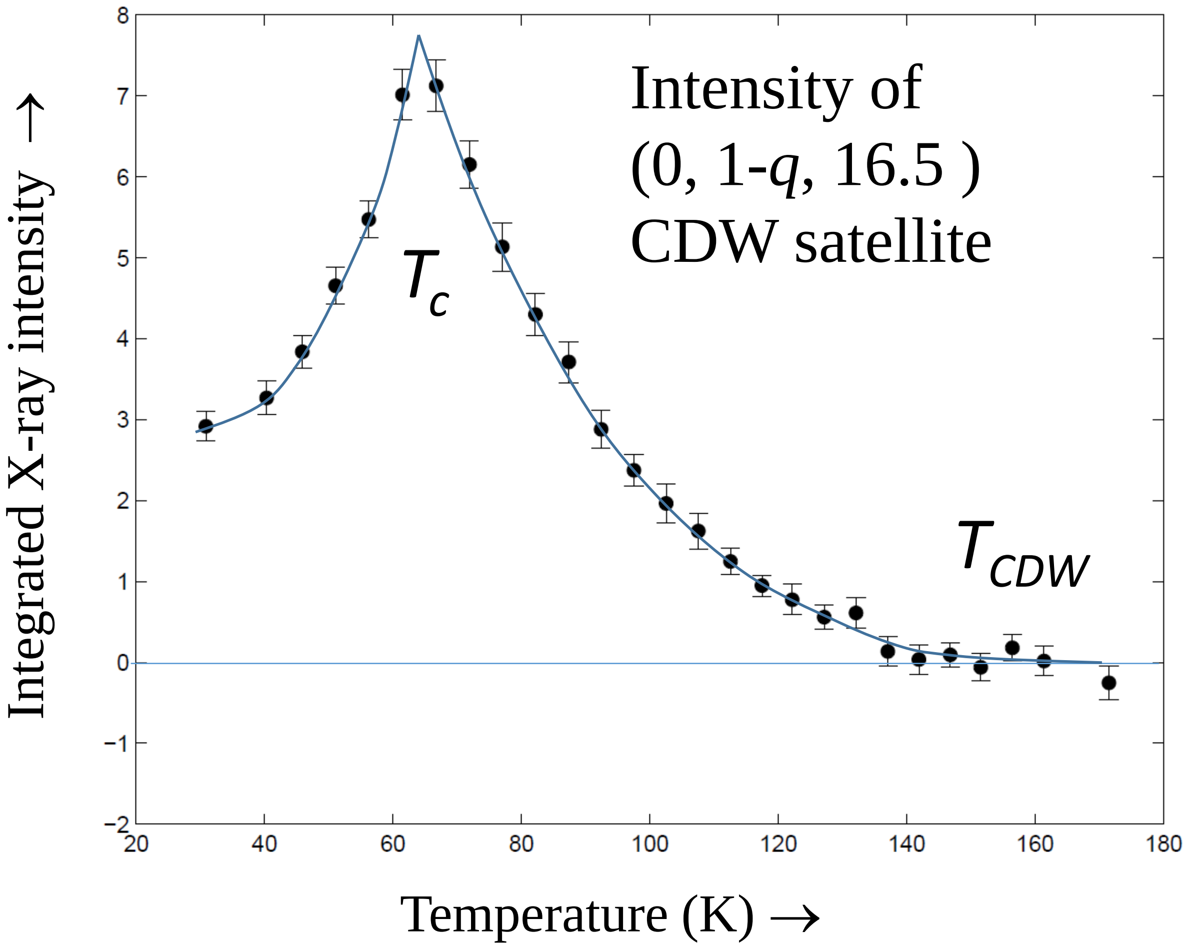


Make all observations of CDW intensities at T_c (superconductivity) = 60 K

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

Assumptions made in analysing the data

Non-resonant X-rays are insensitive to small charge density changes.
Instead they respond to the associated/resultant ionic *displacements* from their usual positions.
(Because ALL the electrons in a displaced ion scatter X-rays)

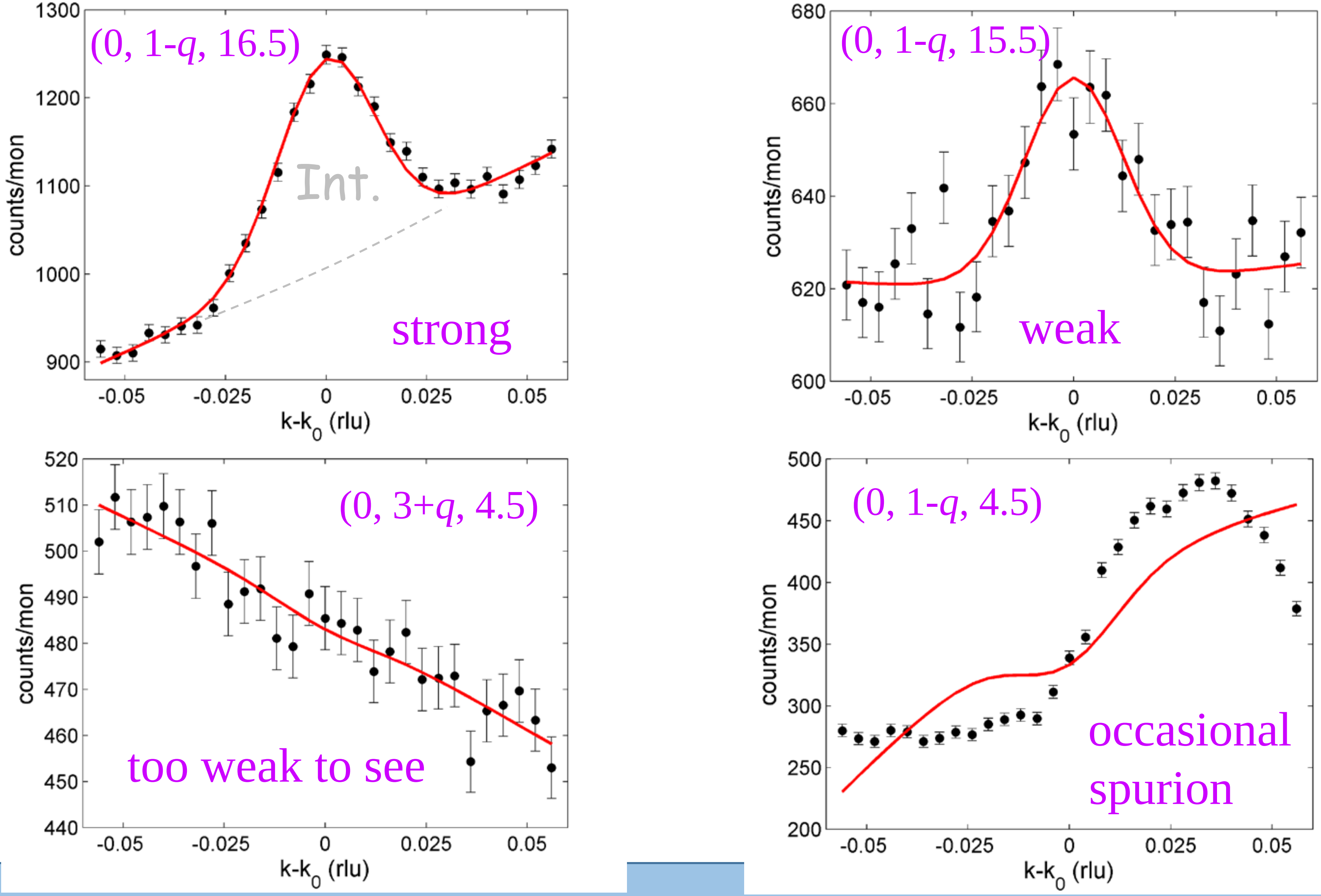
A single CDW can be described by an incommensurate ***q***-vector along either the ***x*** or ***y*** (***a*** or ***b***) crystal directions.

Adjacent unit cells in the ***c***-direction are in antiphase
(Doubled cell indicated by CDW satellites at half-integral ℓ)

CDWs are longitudinal, with atomic displacements (e.g. for ***q*** // ***y***) along *both* ***y*** & ***z*** directions.

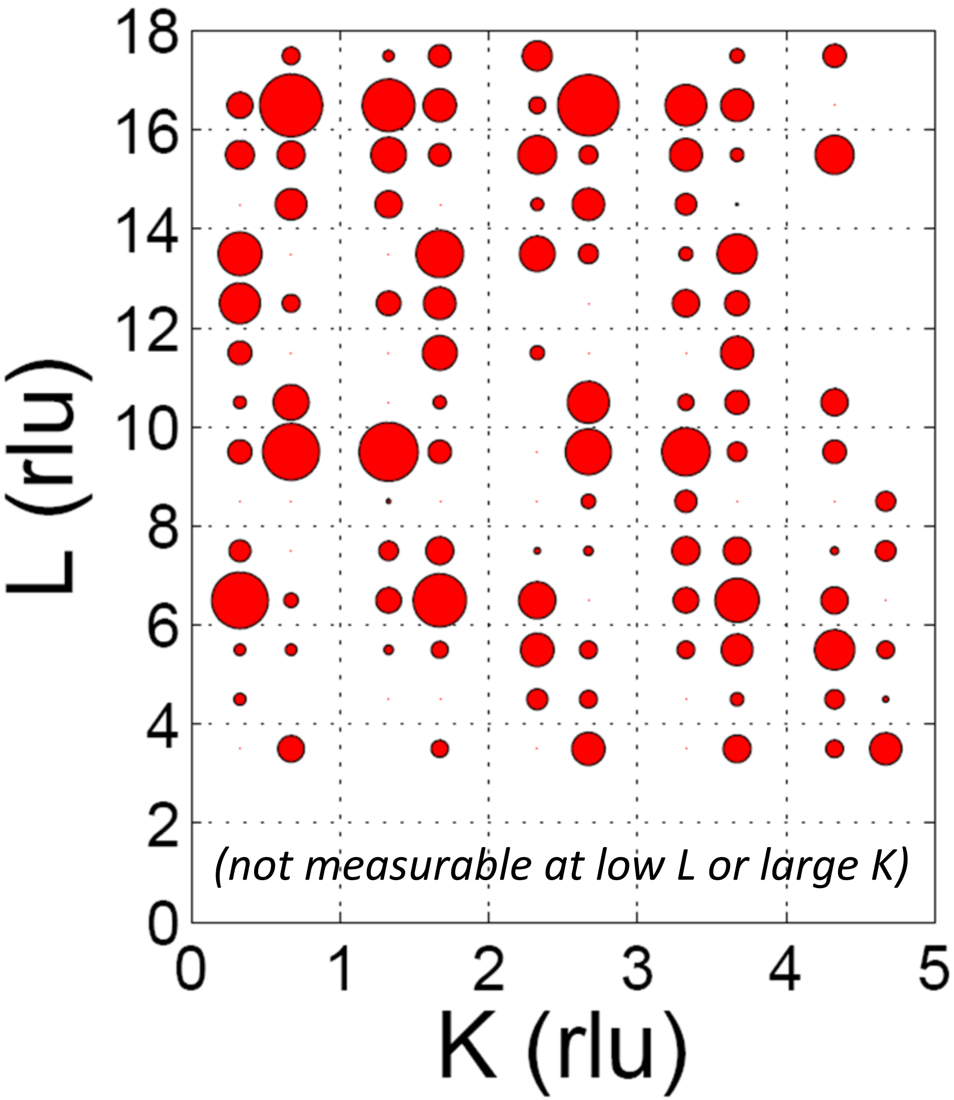
Forgan, EB *et al.*, *Nature Comms* **6**, 10064 (2015).

Example CDW satellites at 60 K



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

The CDW intensity pattern in the K-L plane



A total of 269 satellite positions were observed for $\boldsymbol{q}_b$ and 193 for $\boldsymbol{q}_a$

Area of circle $\propto$ Intensity

blank = not observed

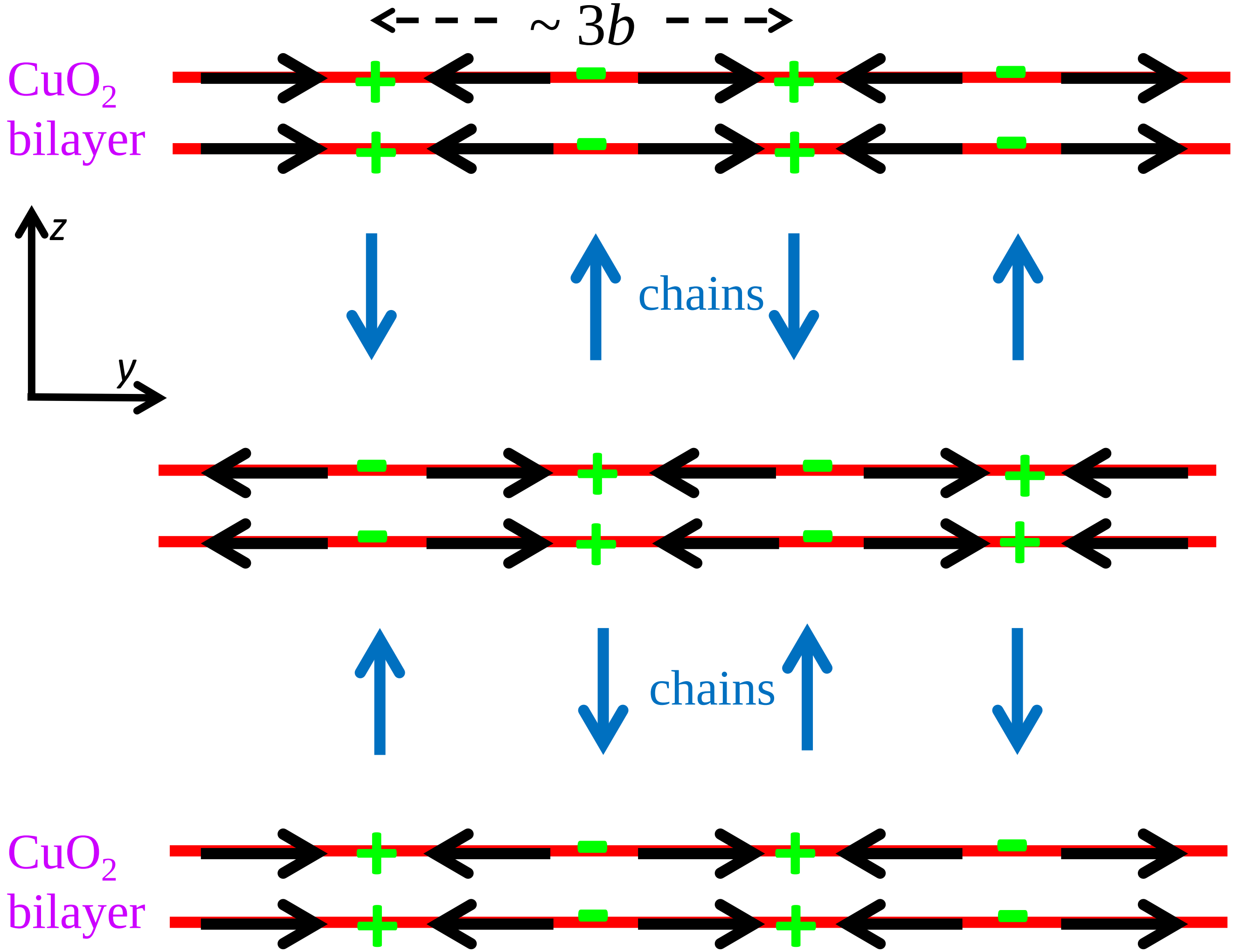
Not a simple pattern so the displacements do not involve just one or two ions

You can always get from a model to the diffraction pattern - but not vice versa

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

What did we expect? ionic displacements with this *symmetry*

$\leftrightarrow$ motion is even in z about bilayer, note: $\uparrow\downarrow$ is odd in z



CDW $\Leftrightarrow$ ionic displacements

Next unit cell in antiphase ($\equiv \ell = 0.5$)

also $\exists$ ***c***-axis displacements

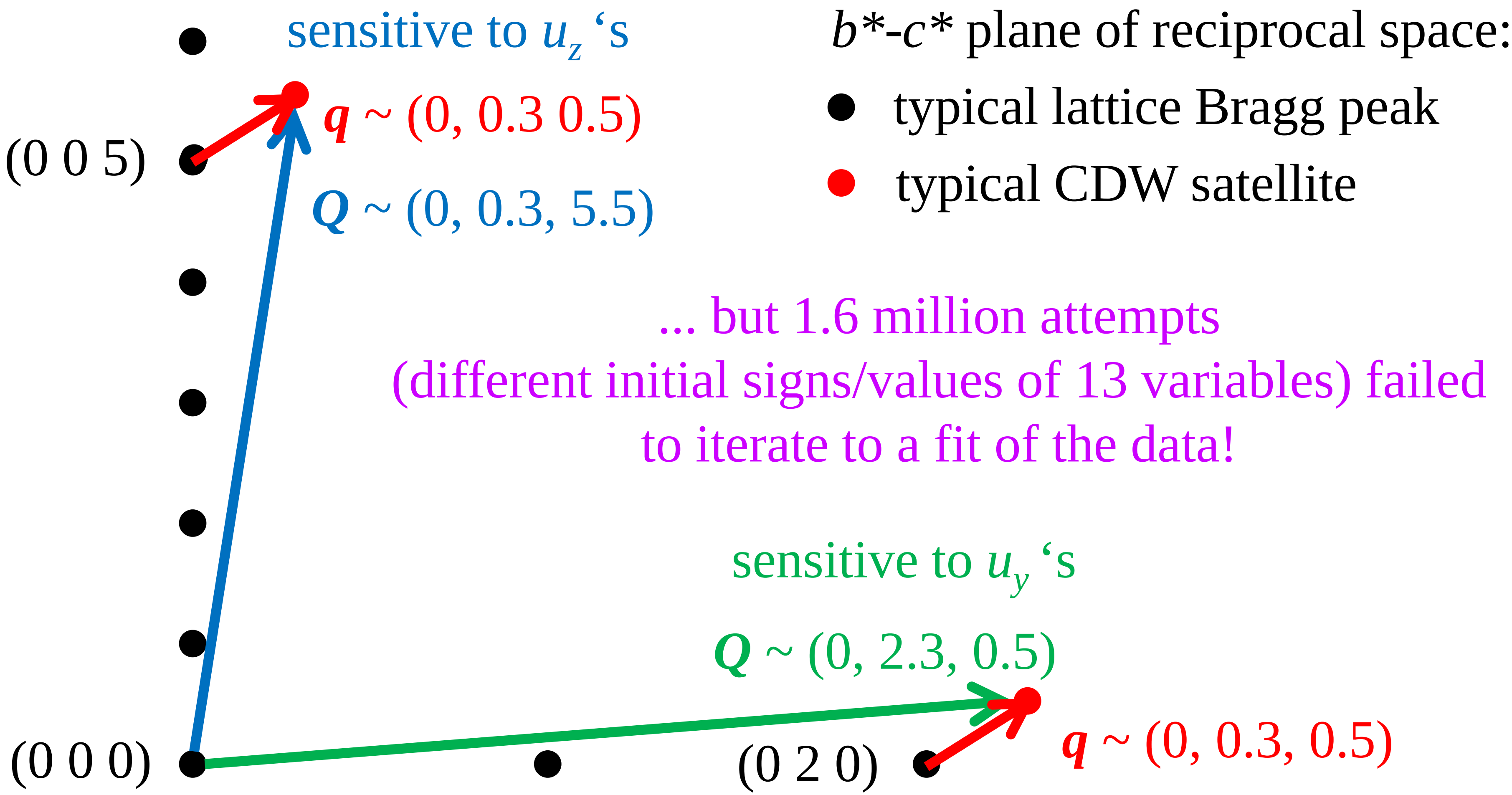
$\Rightarrow$ total of 13 ionic motion variables to fit the data

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

How do we make deductions from the data?

CDW satellite intensities are proportional to $(\boldsymbol{Q}.\boldsymbol{u})^2$

So we can detect basal and ***c***-axis displacements u_y u_z.

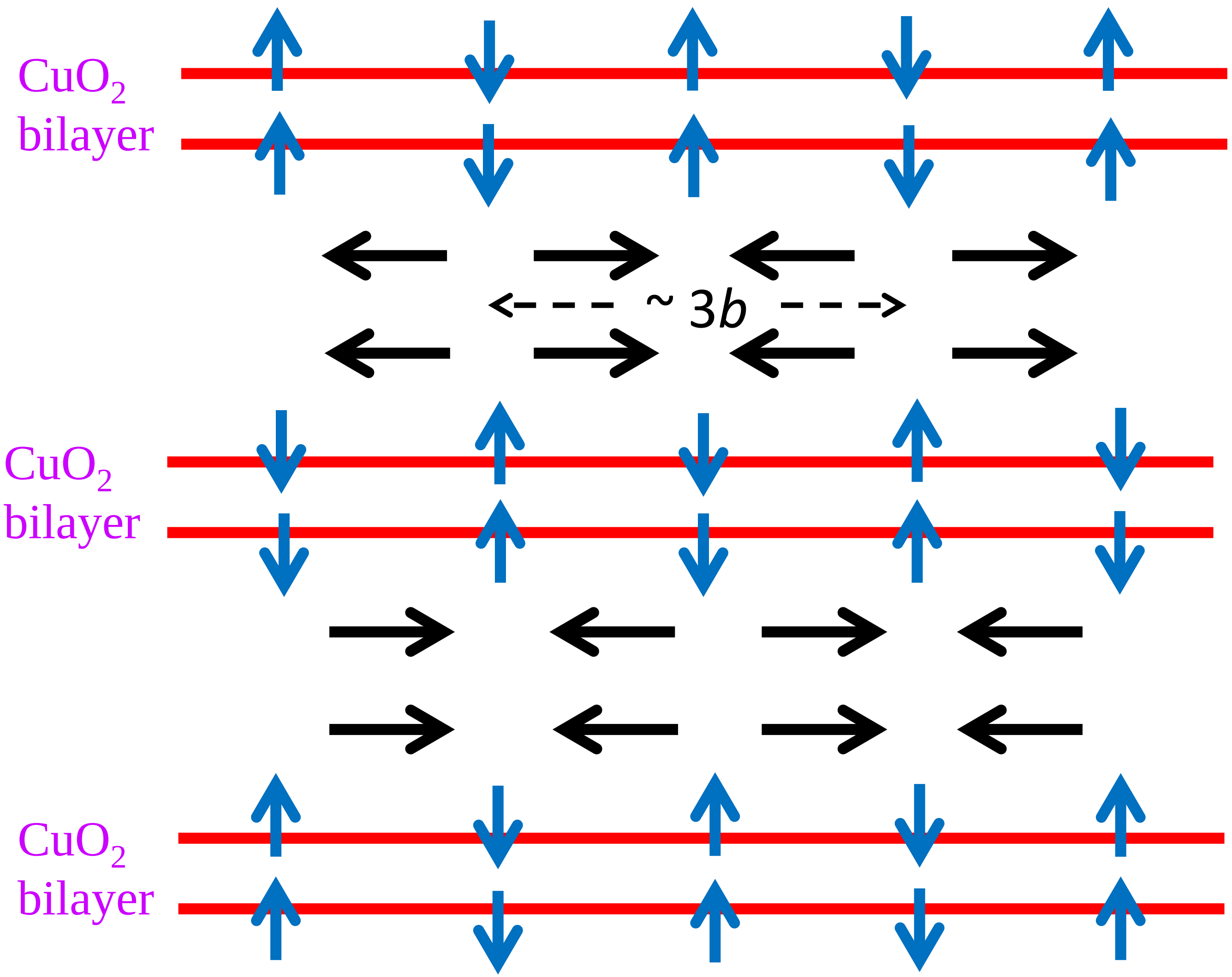


… but 1.6 million attempts
(different initial signs/values of 13 variables) failed
to iterate to a fit of the data!

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

We are forced to consider displacements of this symmetry:

↑↓ motion even in z about bilayer, and ↔ odd in z



CuO_2 bilayers sheared

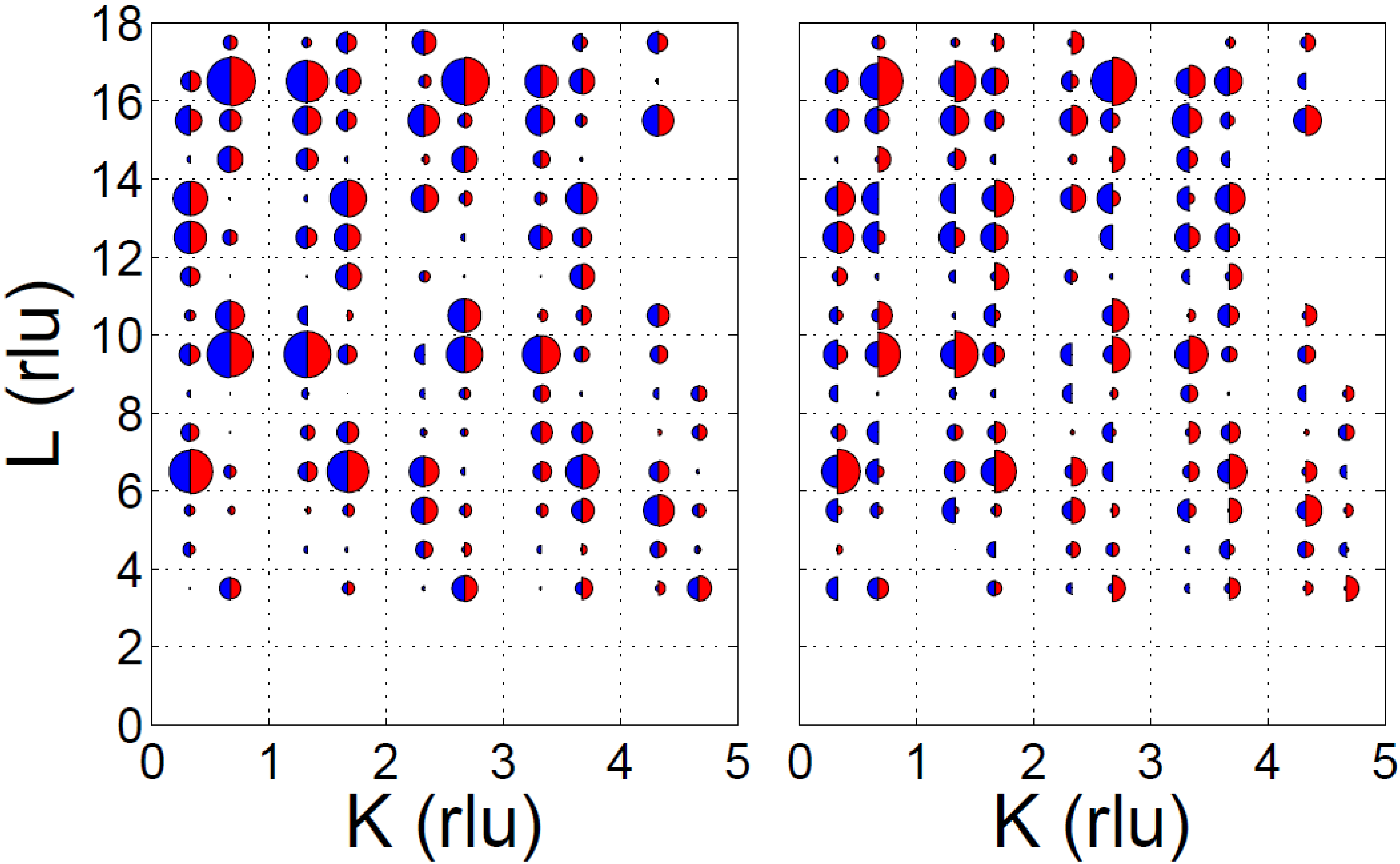
Next unit cell in antiphase ($\equiv \ell = 0.5$)

y & ***z*** ionic displacements => total of 13 variables

fits the data!

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

Good fit ….. Bad fit



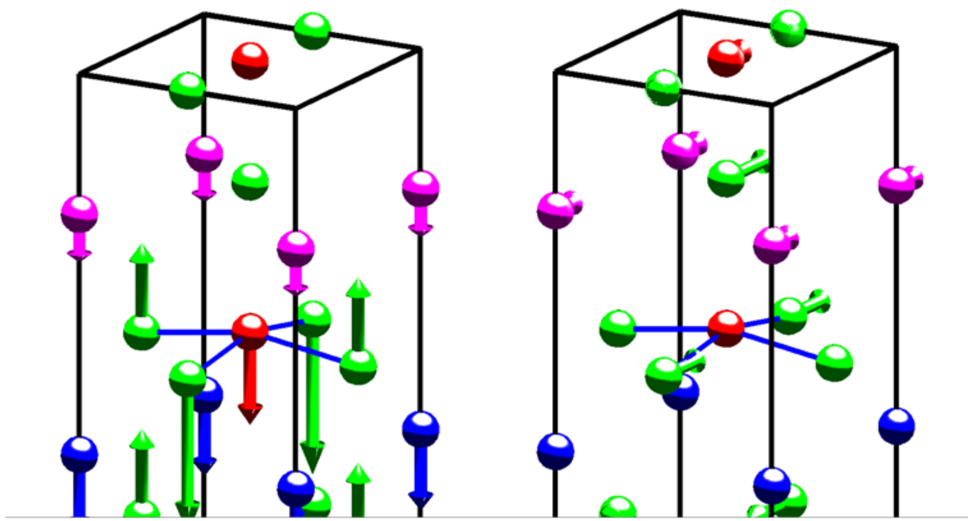
CuO_2 bilayers sheared

CuO_2 bilayers compressed

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

The motif which is modulated to form the CDW

- from the results of the good fit to the $\boldsymbol{q}_b$ mode



CuO chains

BaO layer

CuO_2 plane

Y layer

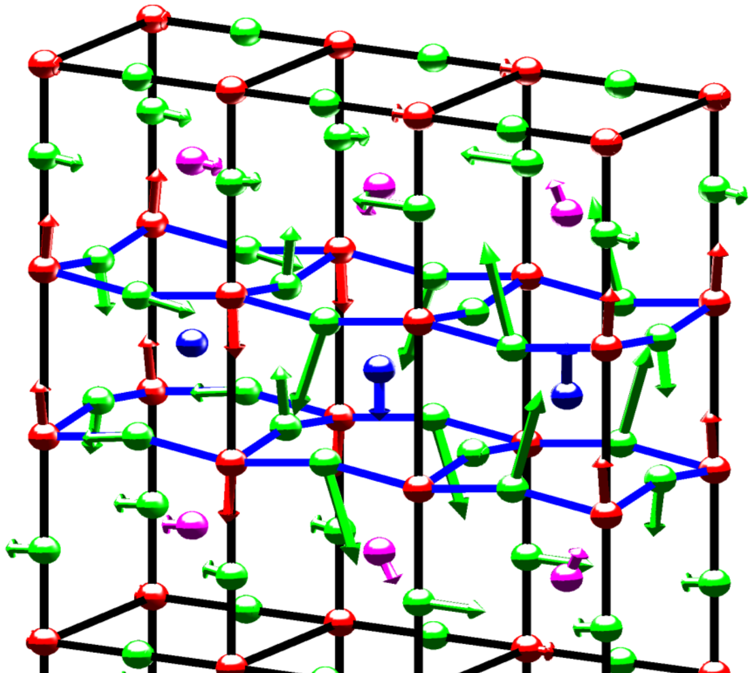
CuO_2 plane

for each ion, $\boldsymbol{r}_0 \Rightarrow \boldsymbol{r}_0 + \boldsymbol{u}(\boldsymbol{r}_0)$

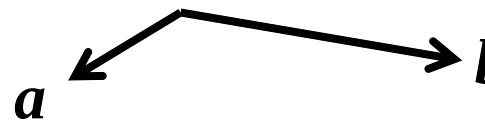
$\boldsymbol{u}_c$ $\boldsymbol{u}_b$

Next unit cell along $\boldsymbol{c}$ is in antiphase

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



Resulting modulated ionic displacements



period only ~ 3 unit cells

so $\boldsymbol{\pi}$ phase change in only 1½ cells

not tilted CuO_5 half-octahedra

Plus a similar modulation in the perpendicular direction

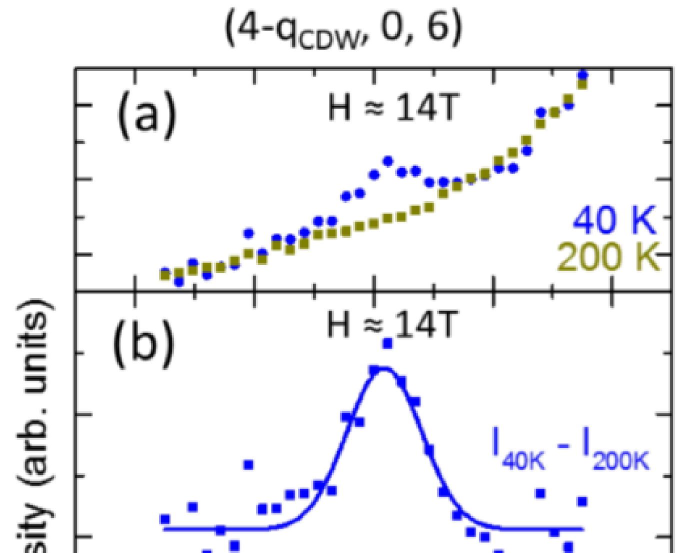
Almost certainly in the same region of space

[redacted]

“double-***q***” or “biaxial” order

=> Fermi surface reconstruction

HgBCO – no bilayer to worry about…

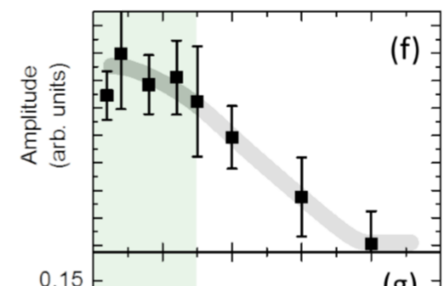


[redacted]

Initially seen using resonant X-ray diffraction at Cu L-edge.

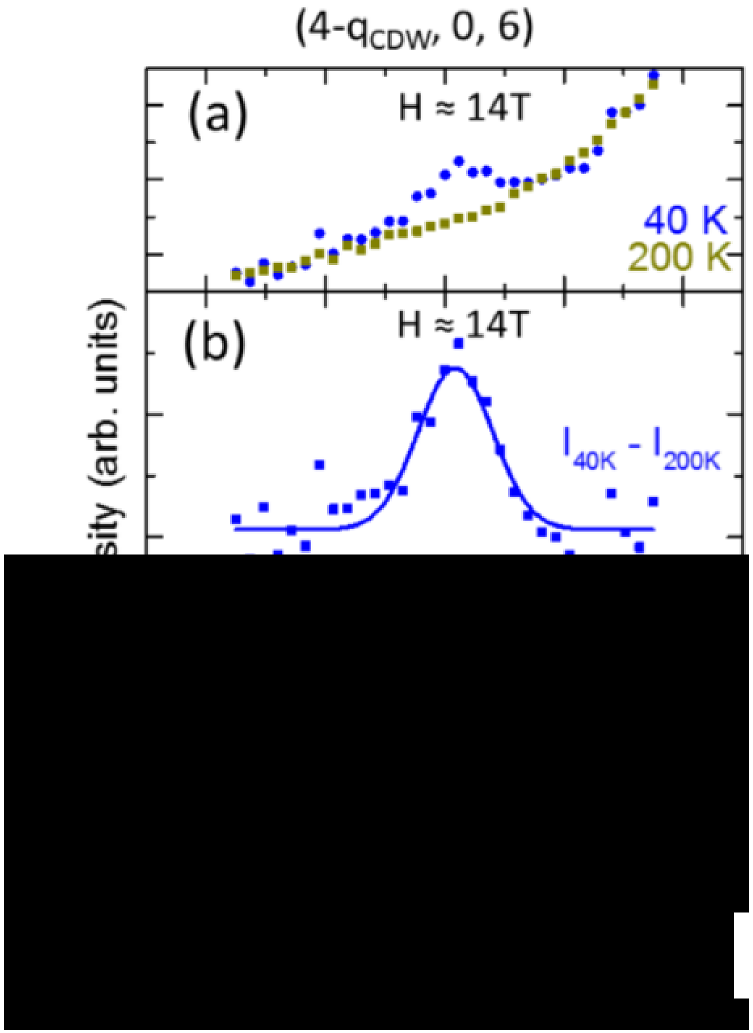
Tabis *et al.*, Nat. Comms. **5**, 5875 (2014).

Needed high field to see clear signal with 80 keV X-rays.



[redacted]

HgBCO – inferences from limited observations



CDWs in adjacent Cu-O planes are in phase.

The Cu-O plane is a mirror plane.

Small shear *c*-axis displacements (as in YBCO) will only affect carrier energies ot 2nd order, whereas 1st order in YBCO.

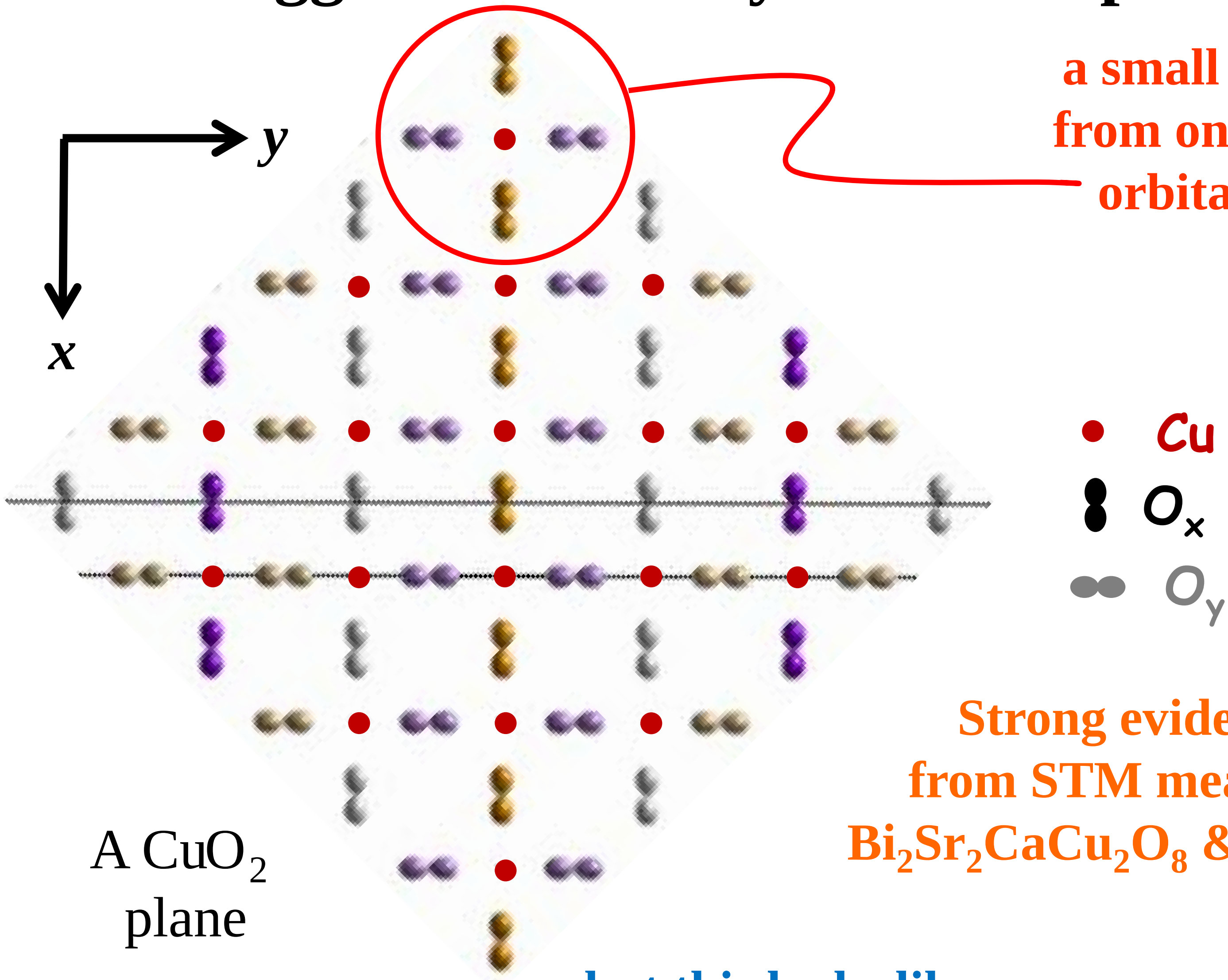
=> Negligible coupling to FS reconstruction

Similarly for transverse basal plane displacements.

We therefore deduce that the CDW is longitudinally polarised (and we assume that it is biaxial).

Tabis, EB *et al.*, *submitted PRB.*

STM suggests "*d*-density wave" on planar oxygens



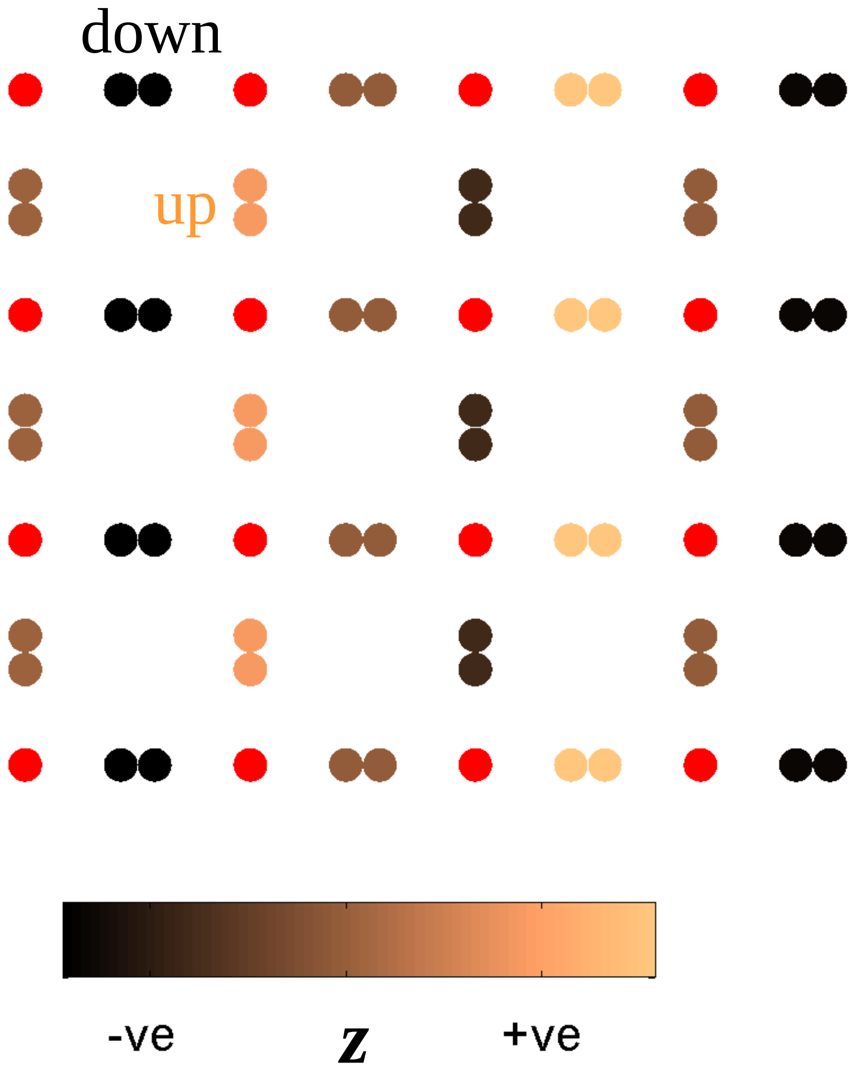
Spatially modulated along y

Strong evidence for this from STM measurements in $Bi_2Sr_2CaCu_2O_8$ & $Ca/NaCuO_2Cl_2$

... but this looks like our *unsuccessful* model !

S. Sachdev & J.C. Seamus Davis *group*, PNAS July 2014

A plot of the modulated oxygen *z*-displacements



for a single CDW mode

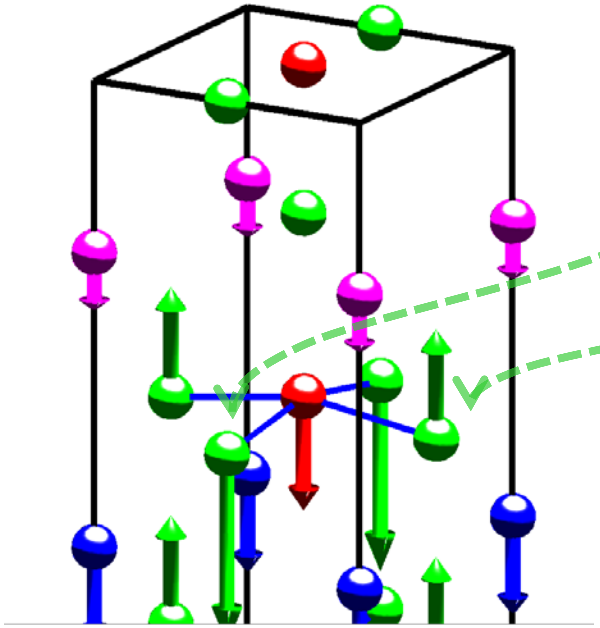
modulation direction ➔

You have seen this pattern before...

An ion closer to an STM tip would appear to have a larger charge

So our CDW shear ***simulates*** a "bond *d*-density wave"

Or is it the other way round? The chicken or the egg…



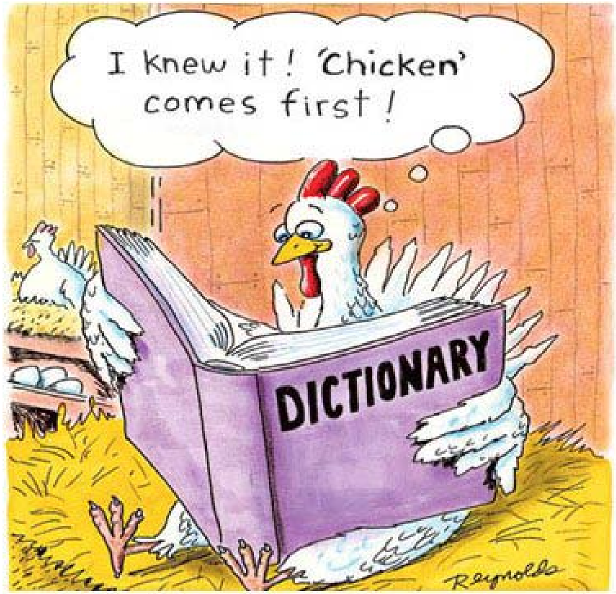
- If these O_y develop a –ve charge, they are attracted to Y^{3+}

- and these O_x with a +ve charge are repelled by the Y^{3+}

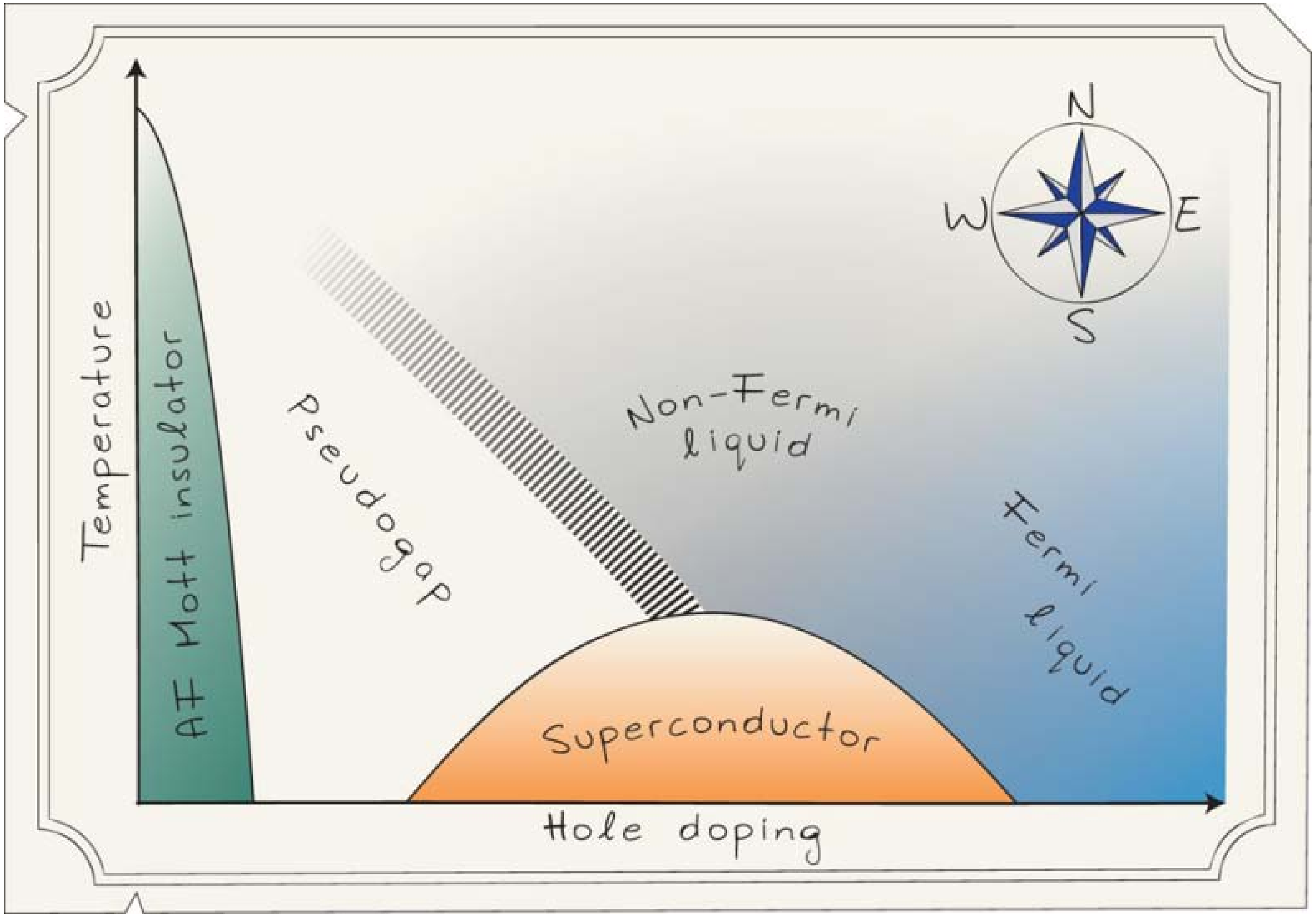
- conversely if O_x & O_y move relative to Y^{3+}, they will develop induced charges!

- but Cu's in the bilayers move <u>*with*</u> the Y's

- at least in YBCO, it's Chicken!



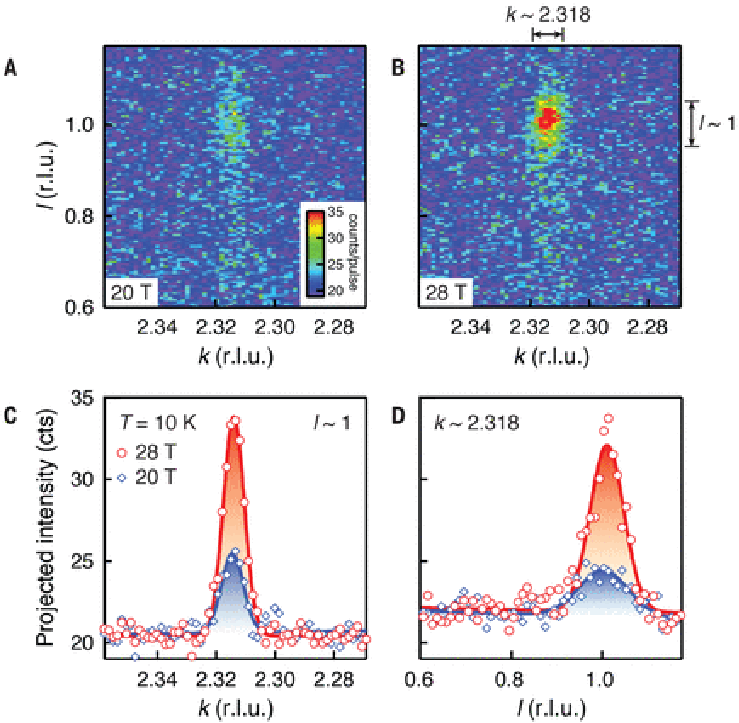
Reassessing the phase diagram



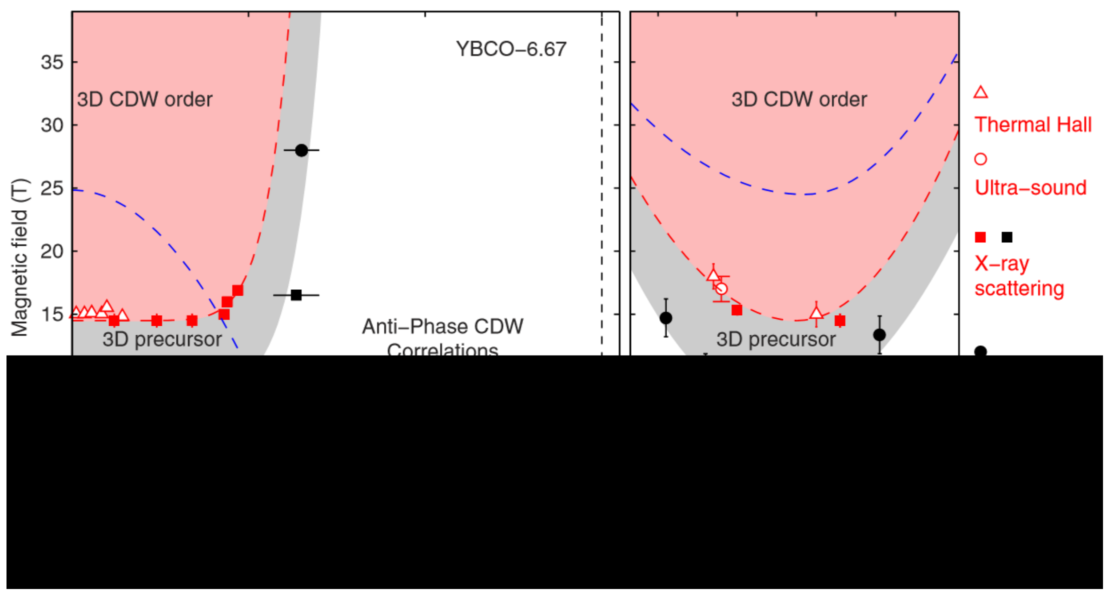
Wahl, Nature Physics (2012)

Final words

In high fields, one of the CDWs in YBCO (along *b*) becomes 3D



Gerber *et al.*, Science **350**, 949 (2015)



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