Quantum Matter Condensed Matter Physics UNIVERSITY OF BIRMINGHAM

Charge Density Waves and Superconductivity in High- T_c materials

Ted Forgan

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Georg Bednorz and Alex Muller's discovery

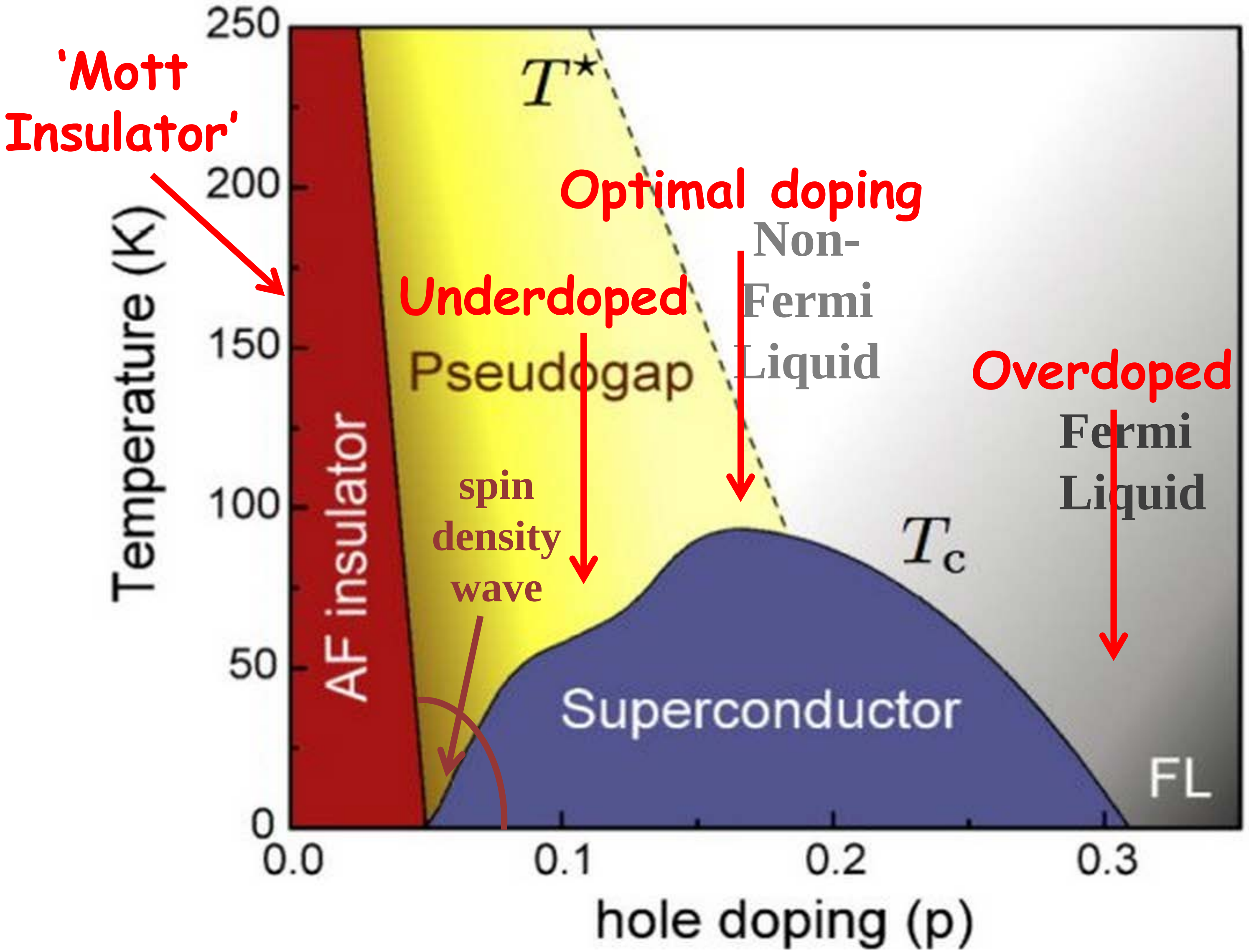
http://www.phys.ntnu.no/brukdef/prosjekter/super/Profiles/bednmull.jpg

received the Nobel Prize 1987 for discovery of the first of the copper-oxide superconductors

> 30 years & ~ 10^5 papers later and we still don't understand these materials!

- applications are nothing like as widespread as hoped in those heady early days…

High- T_c properties versus hole doping



modified from LCMI website

Some simple "chemistry"

La_2CuO_4

Lanthanum: 3+ ; La_2 => 6+

Oxygen: 2- ; O_4 => 8-

∴ Copper: 2+

Cu has $3d^{10}$, $4s^1$

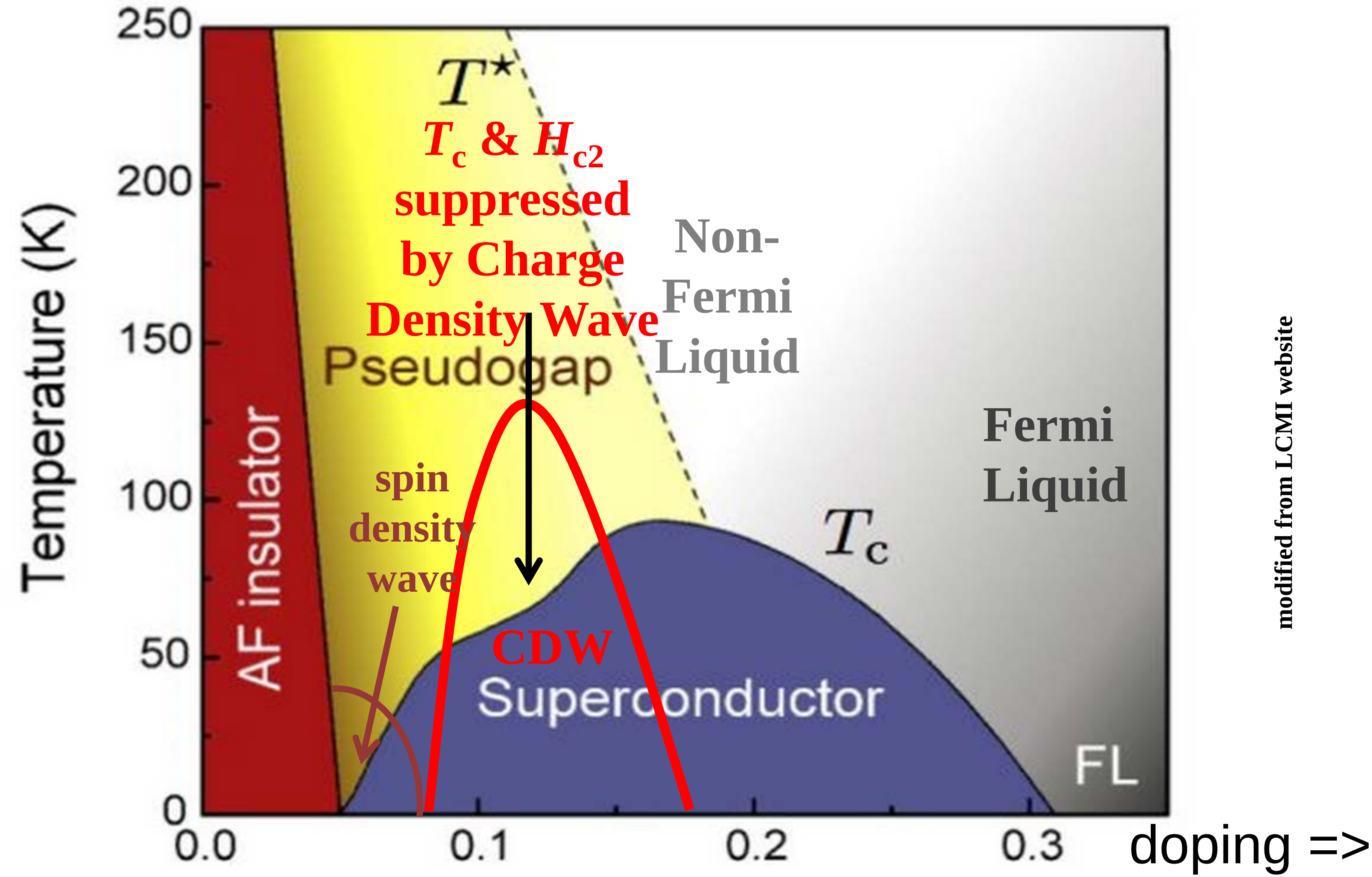
∴ Cu^{++} has $3d^9$, i.e. 1 hole (unpaired electron) in the d-shell..

But La_2CuO_4 is a "Mott insulator": electron repulsion keeps them localised on Cu++ and their spins line up antiferromagnetically

Consider $YBa_2Cu_3O_7$:
(slightly overdoped superconductor)
Doing the same calculations, we get an average of 1.33 holes per $Cu^{2.33+}$

What happens as we go from an insulator to a metal?

High- T_c properties versus hole doping - current ideas



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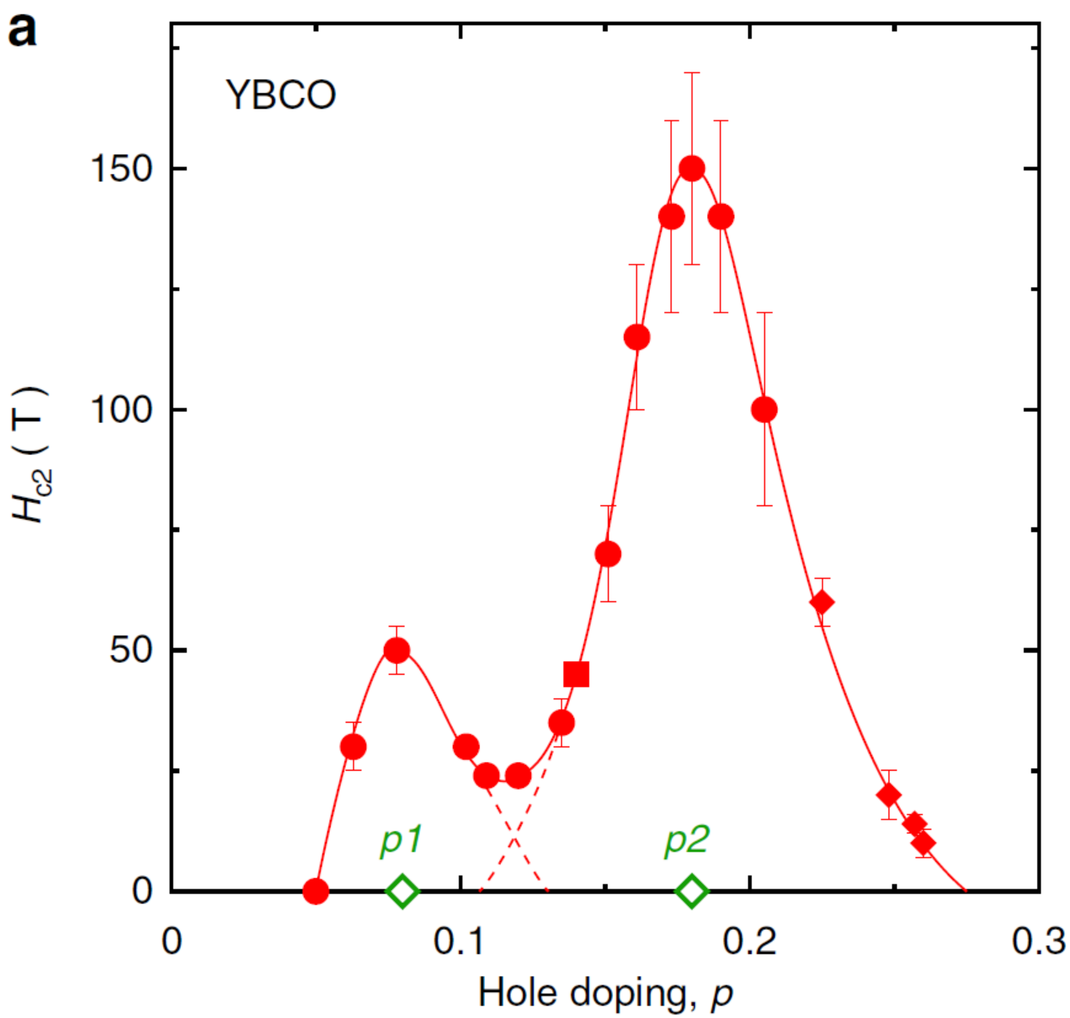
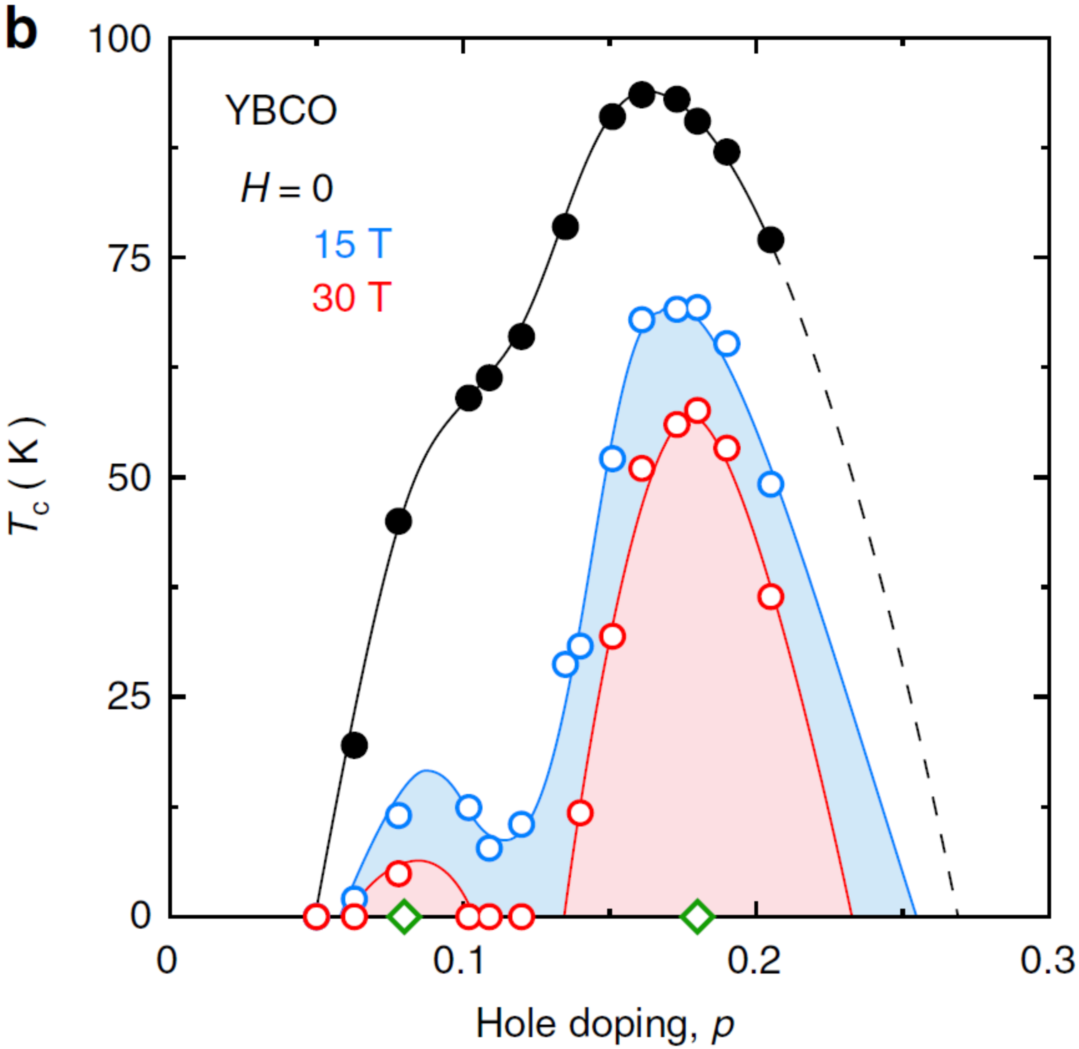
Superconductivity *vs.* doping in YBCO



B_{c2} drops down to ~22 T at the maximum CDW

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

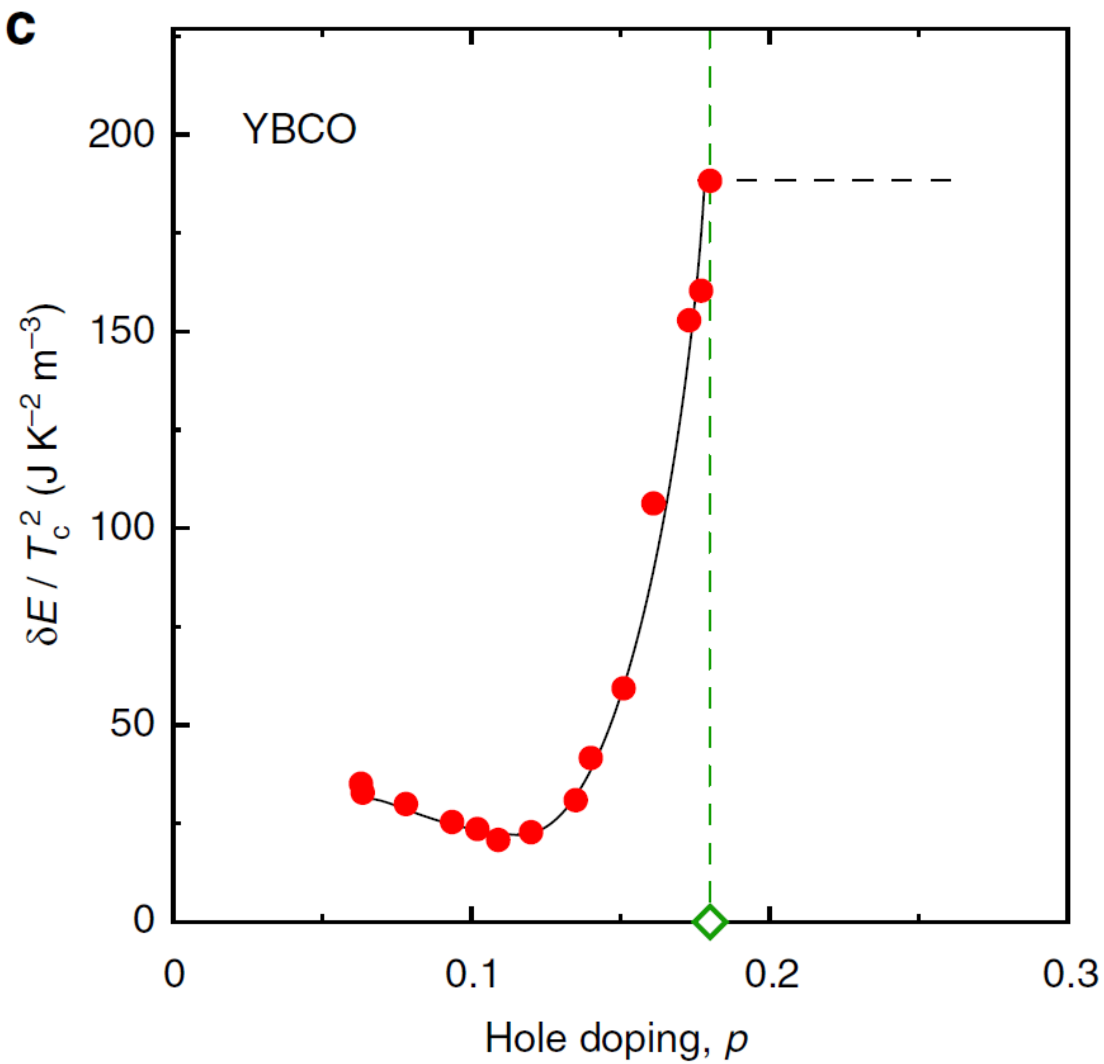
Superconductivity *vs.* doping in YBCO



T for $\rho = 0$ as a function of doping for various fields.

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

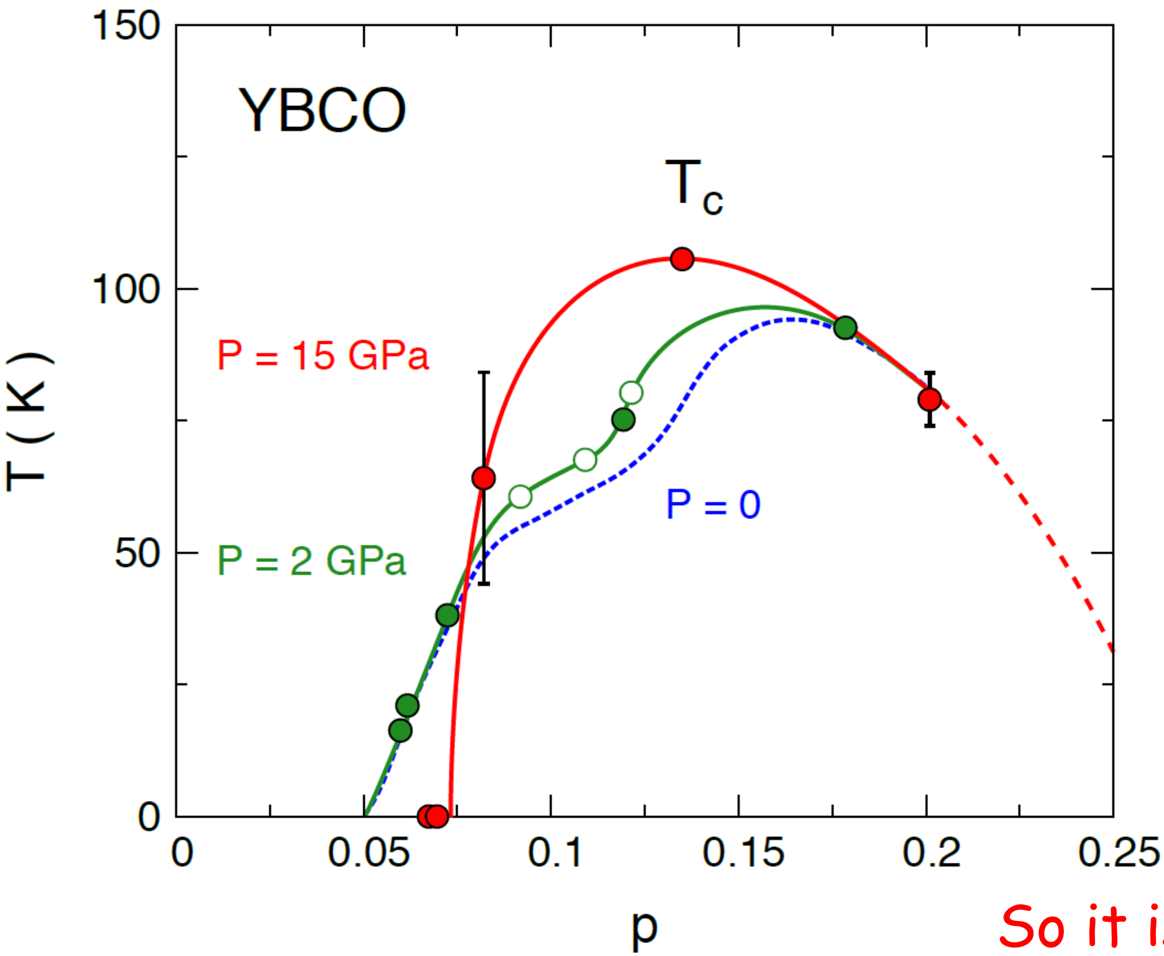
Superconductivity *vs.* doping in YBCO



Superconducting condensation energy versus doping.

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

Can the Charge Density Wave be avoided?



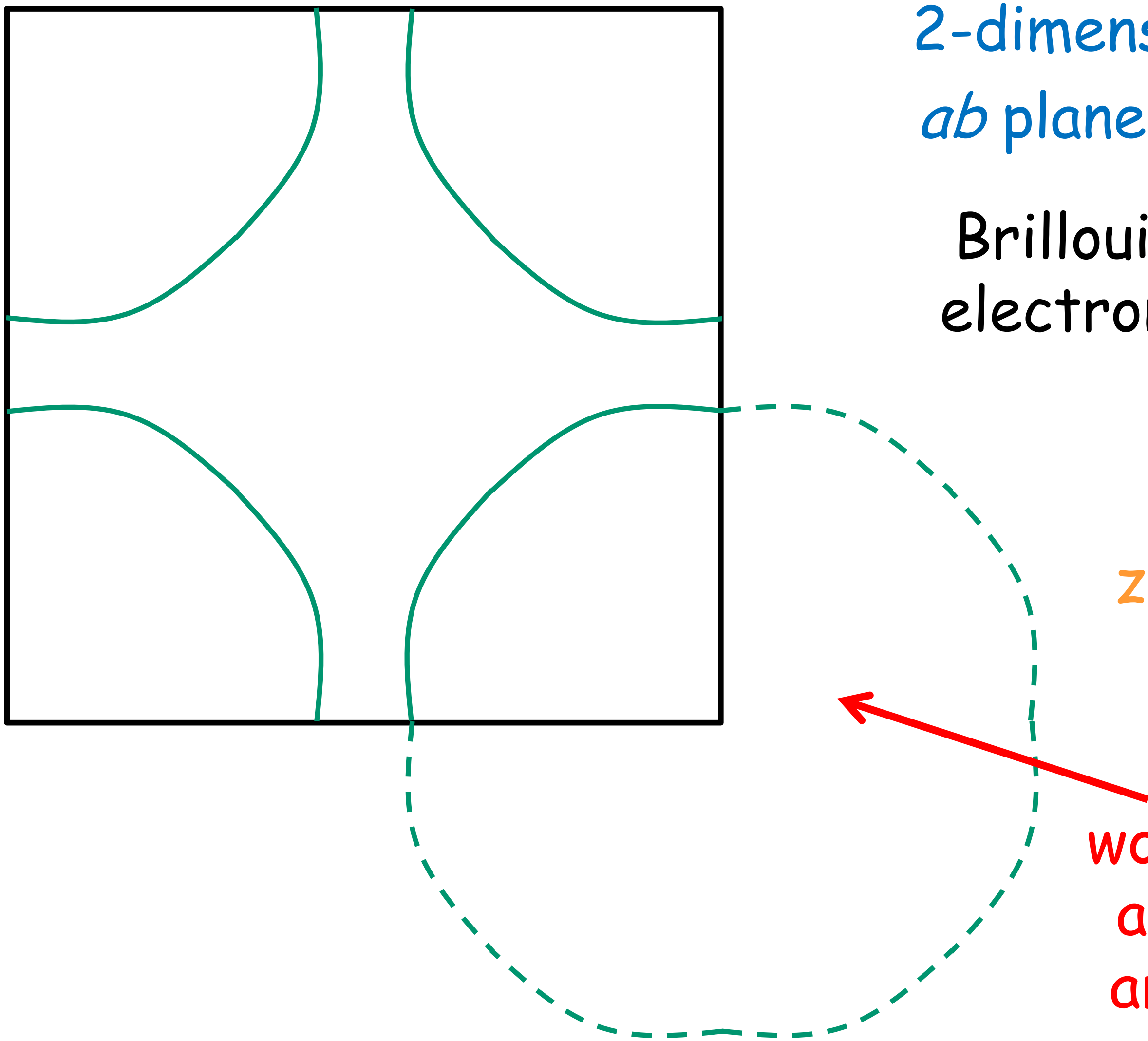
Not very good error bars, but it appears that pressure suppresses the CDW

The max. value of T_c rises and moves closer to the AFM region

So it is important to understand the CDW

Cyr-Choiniere *et al.* arXiv:1503.02033 (2015)

What "should" a High- T_c Fermi Surface look like?



2-dimensional: -look at *ab* plane cross-section

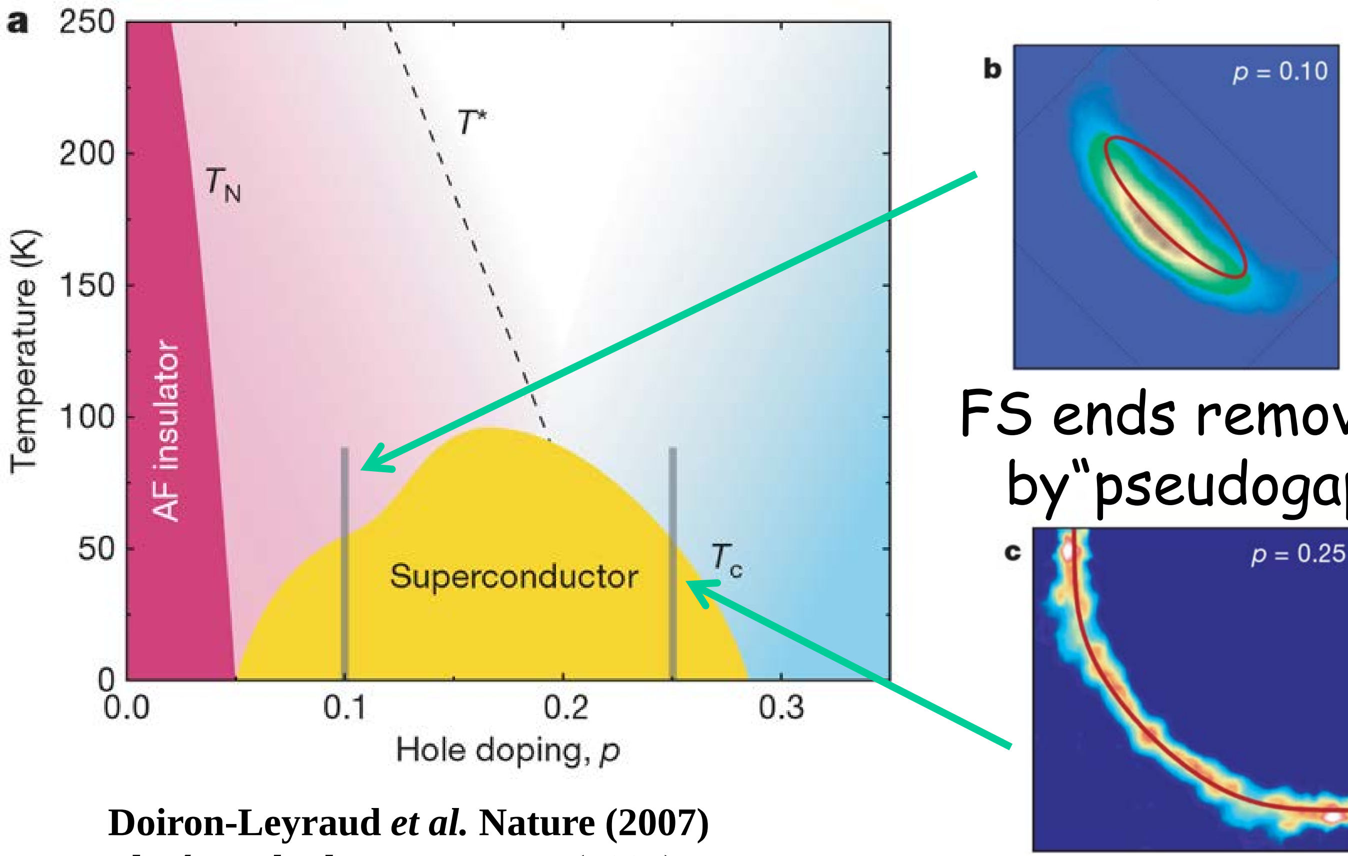
Brillouin Zone holds 2 electrons or holes/cell

1 hole/Cu at zero doping: $p = 0$

This area would be ∝ (1+p) if all the electrons are free to move

ARPES (photo-electron spectroscopy) shows changes in Fermi Surface with doping

"Fermi arc"



FS ends removed by"pseudogap"

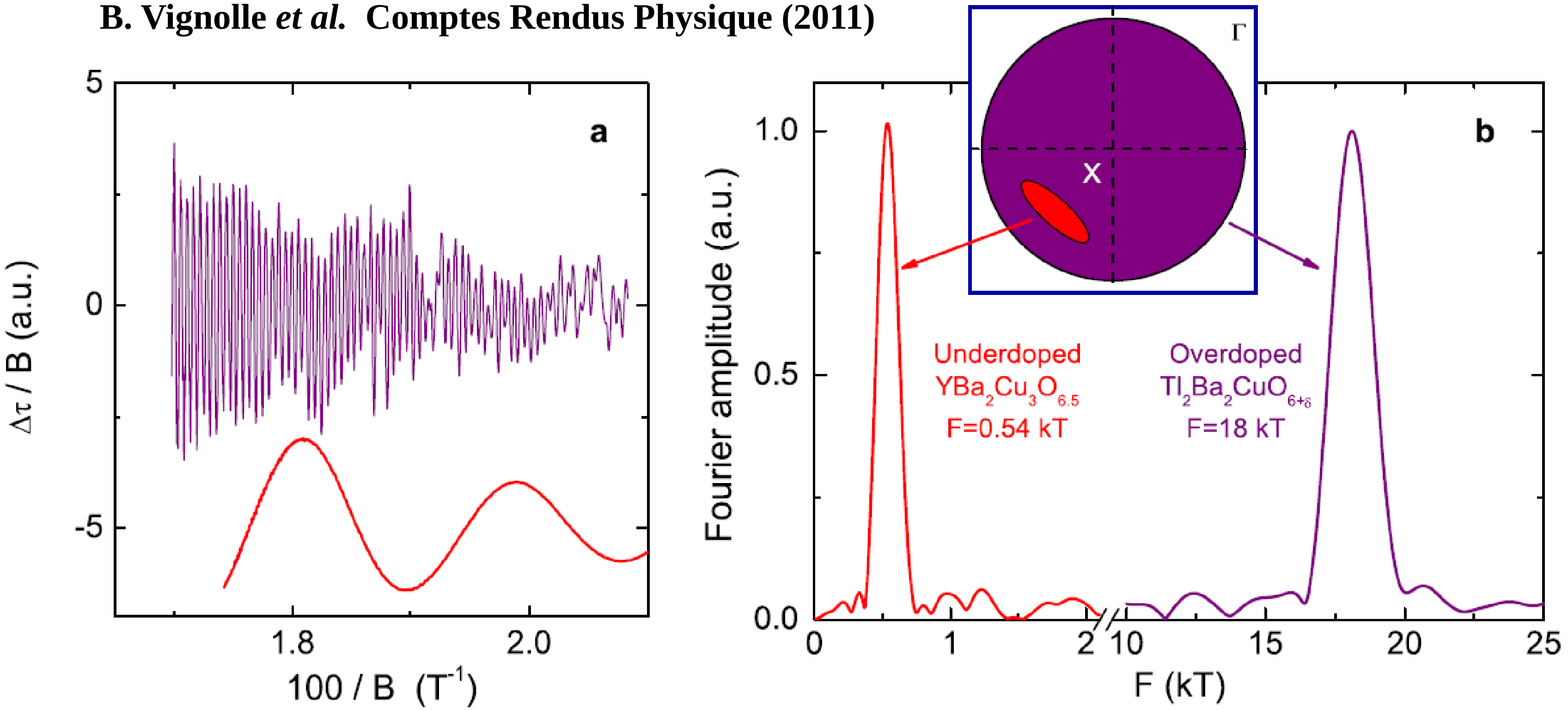
Full Fermi surface

Doiron-Leyraud *et al.* Nature (2007)
Platé, *et al.* Phys. Rev. Lett. (2005)
Shen, *et al.* Science (2005)

Some Quantum Oscillation Data

Overdoped – all holes visible - obeys Luttinger theorem

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

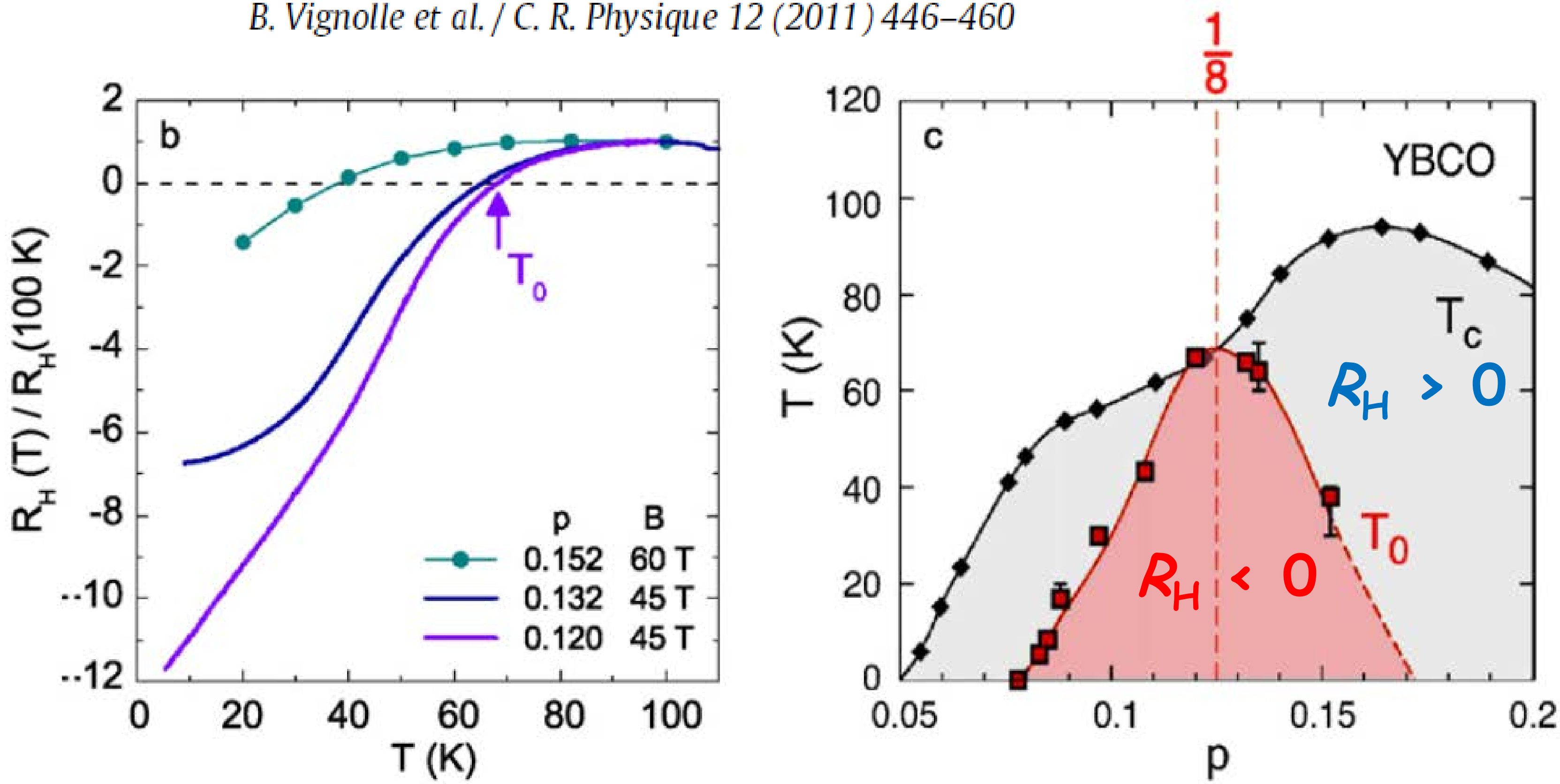


Underdoped – tiny number of *electrons* not holes

N.B. QOs give the *area* of the electron pocket, not shape

At low T, the Hall effect changes sign in underdoped $YBCO_y$

B. Vignolle et al. / C. R. Physique 12 (2011) 446–460

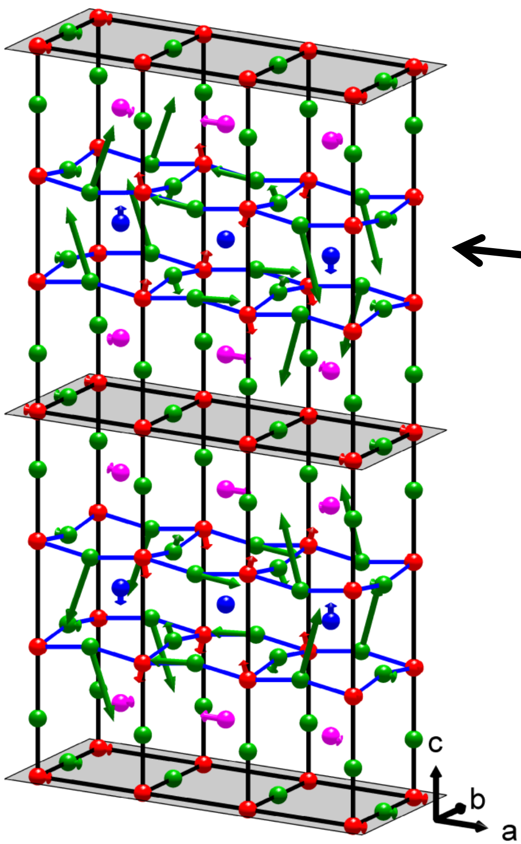


This suggests that for doping levels around $p \sim 1/8$ the Fermi surface changes topology below >~ T_0 …

… from big hole FS (R_H small, +ve) to tiny electron FS (R_H large, -ve)

What do we think is causing this?

Charge Density Wave (CDW) order - a tiny modulated charge density – and associated lattice distortion, - which forms in a *wide range* of slightly under-doped cuprate high-T_c materials.



It is centred on the CuO_2 layers and *competes* with superconductivity

Exaggerated view of CuO_2 plane displacements (oxygen, copper)

This CDW order has an *incommensurate* period ~3 unit cells along *both* ***a*** and ***b***. (***a*** shown)

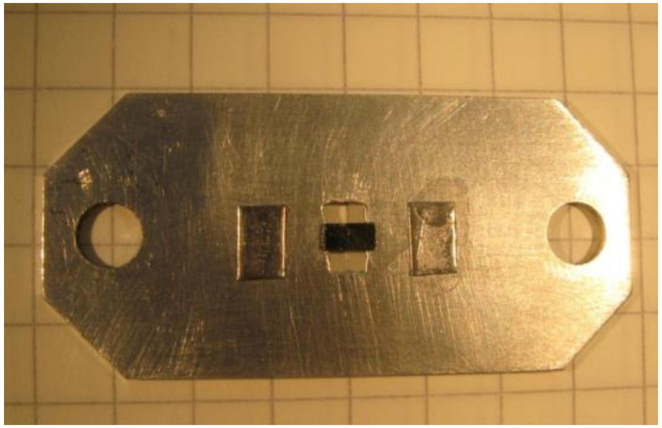
It disappears as doping is increased to about optimum for superconductivity

Observing the CDW by diffraction - 100 keV X-rays, 17 T

Our first experiment:
was on $YBCO_{6.67}$
3.1 x 1.7 x 0.6 mm^3
99% detwinned
T_c = 67 K

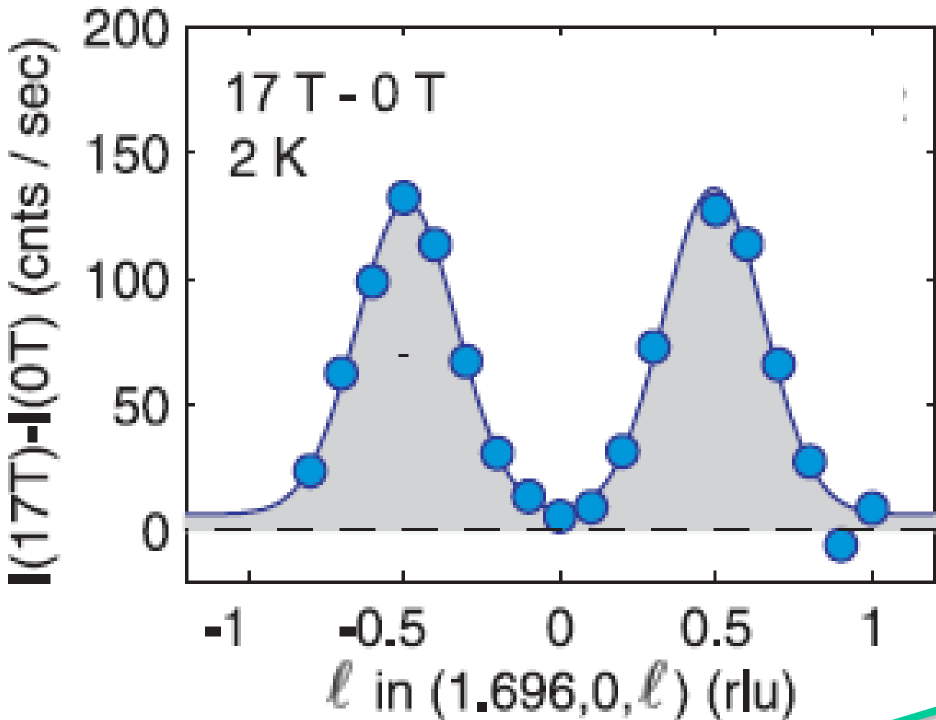
Others measured at zero field using Cu-L-edge resonant X-rays*

BW5 – on DORIS (RIP),
HASYLAB, DESY, Hamburg
- using the Birmingham beamline cryomagnet –taken there by truck



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

Our results: a Field- & Temperature-dependent diffracted peak



Intensity: few x 10^{-6} of the (200) (strongest charge peak)

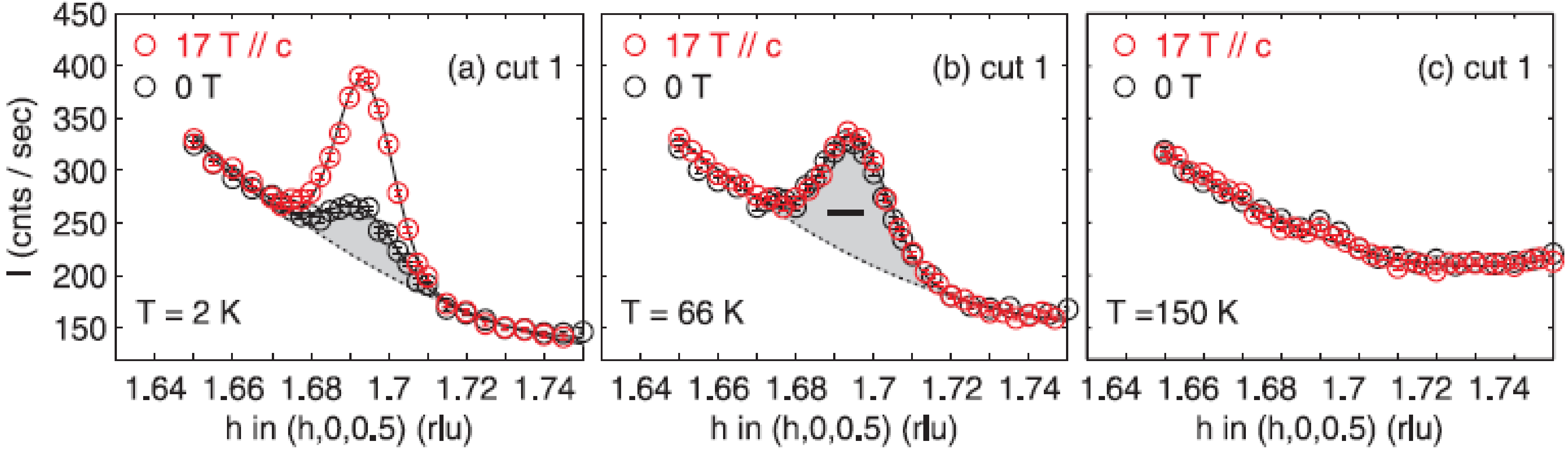
Incommensurate

$q_1 = (0.305, 0, 0.5)$

At zero field, adjacent cells along the *c*-direction in antiphase

Accompanied by a similar modulation along *b*

What happens as we change temperature?



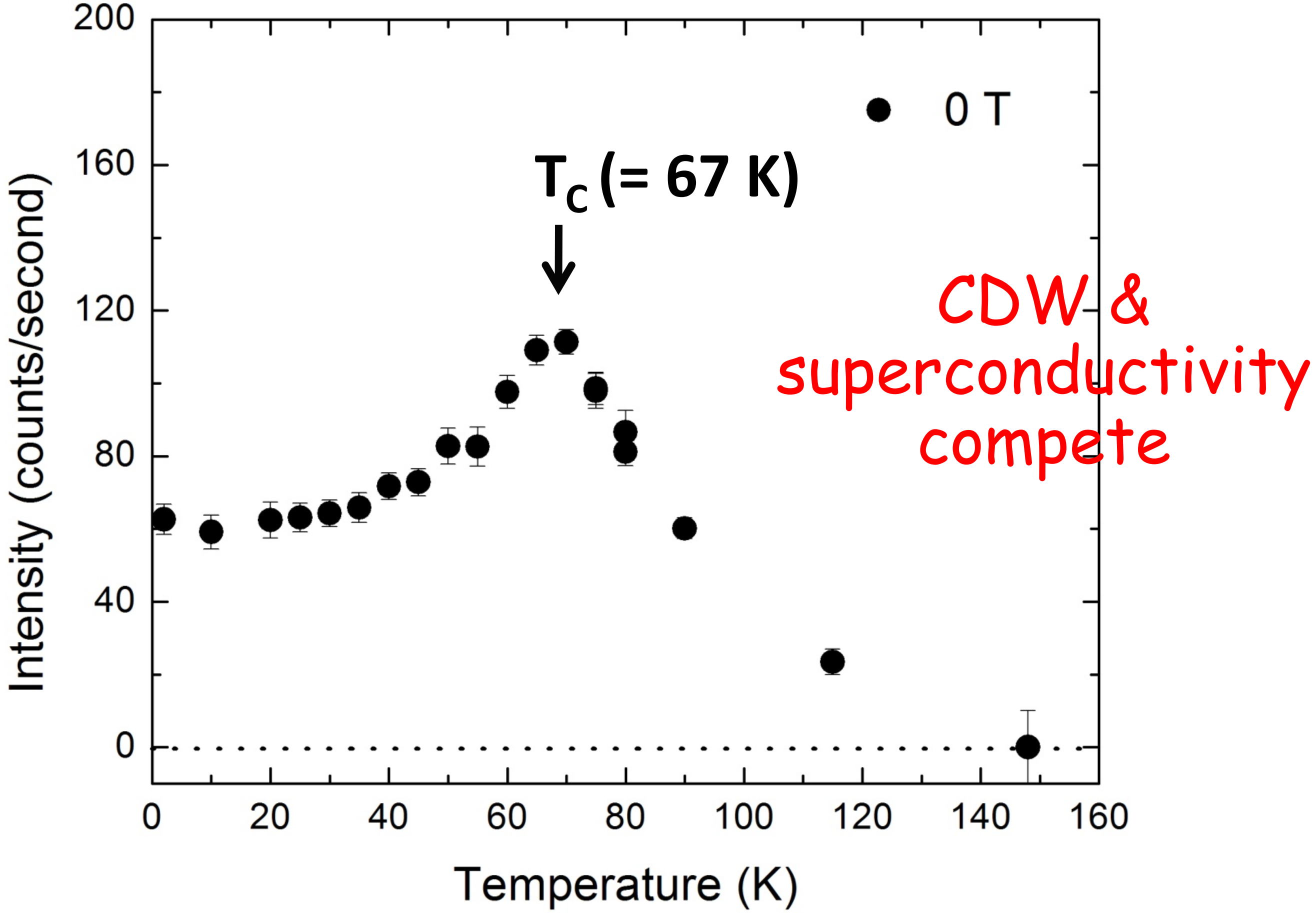
CDW Peak is always finite width – order is finite range

CDW Peak disappears at high *T*

No field-dependence above superconducting T_c

However, at low *T*, superconductivity is suppressed by the *B*-field, and the CDW intensity increases

What happens as we change temperature?



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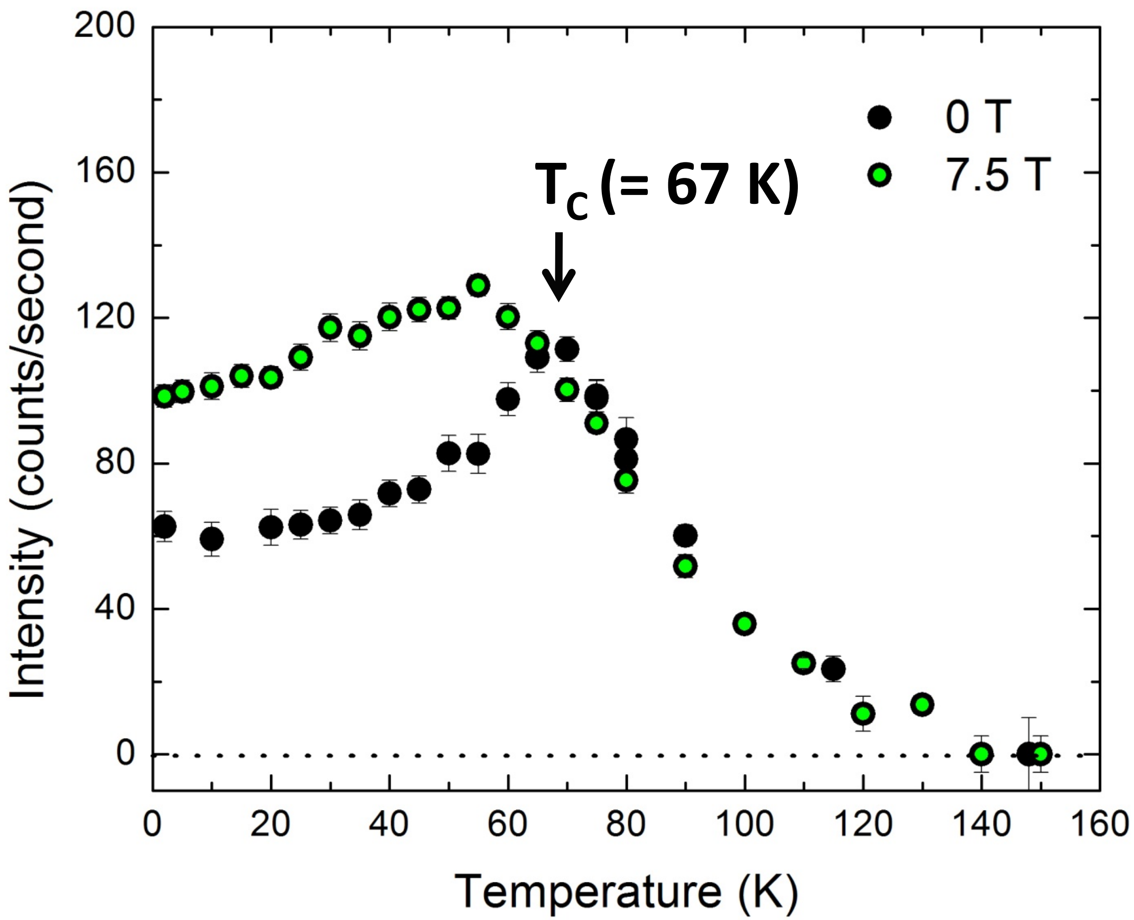

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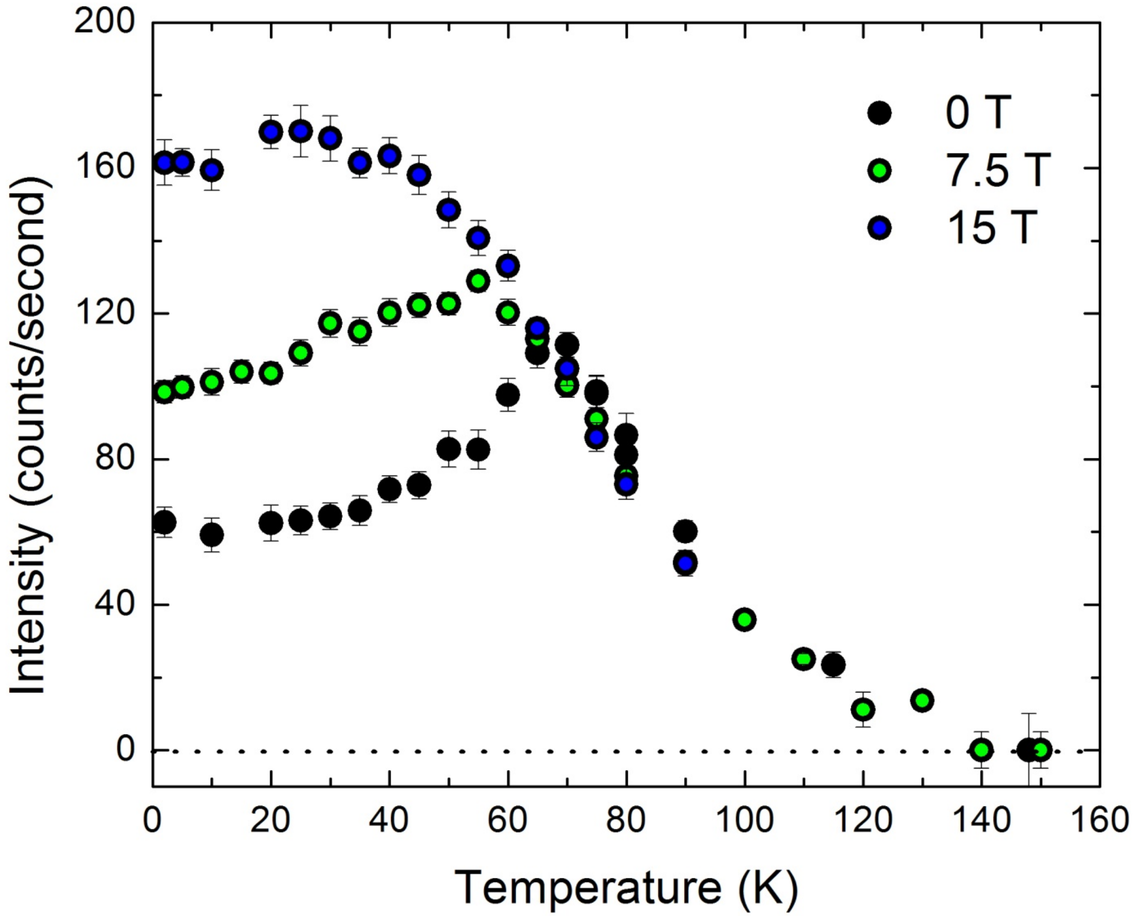

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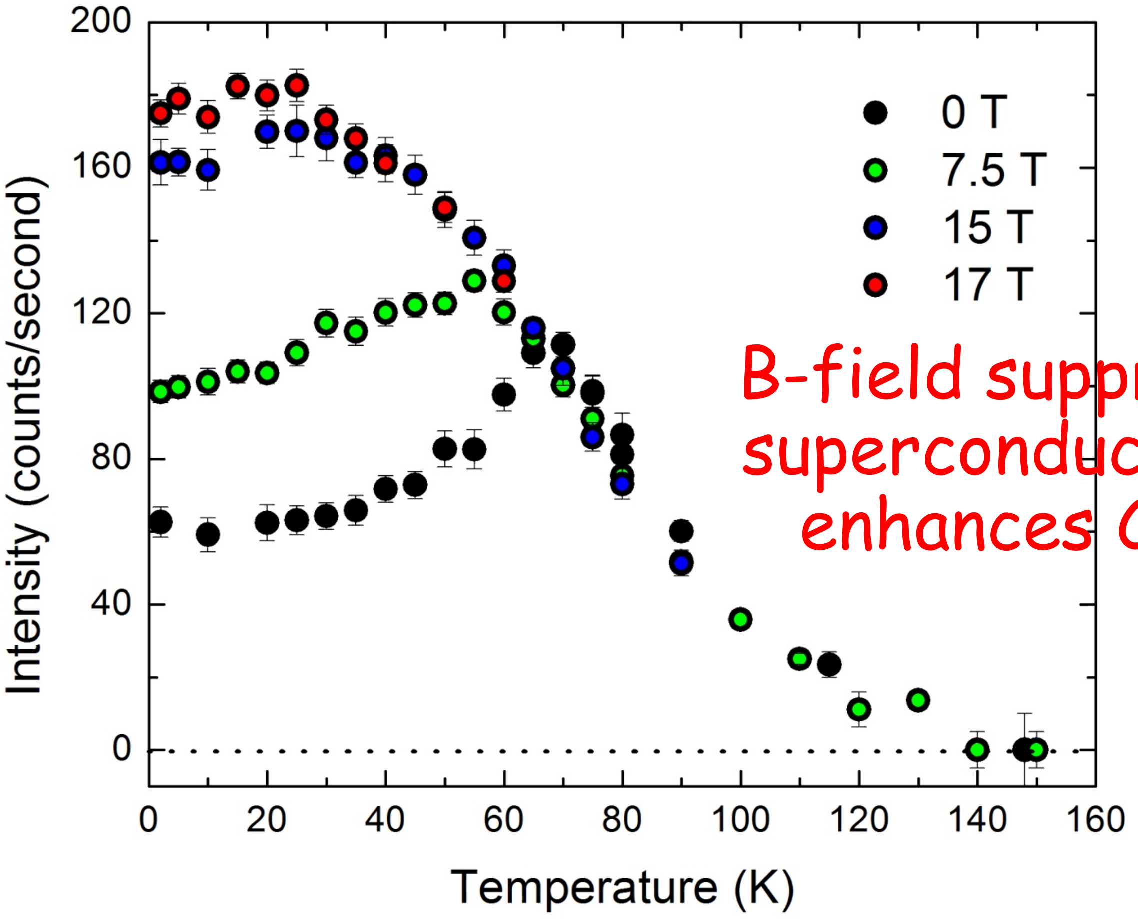
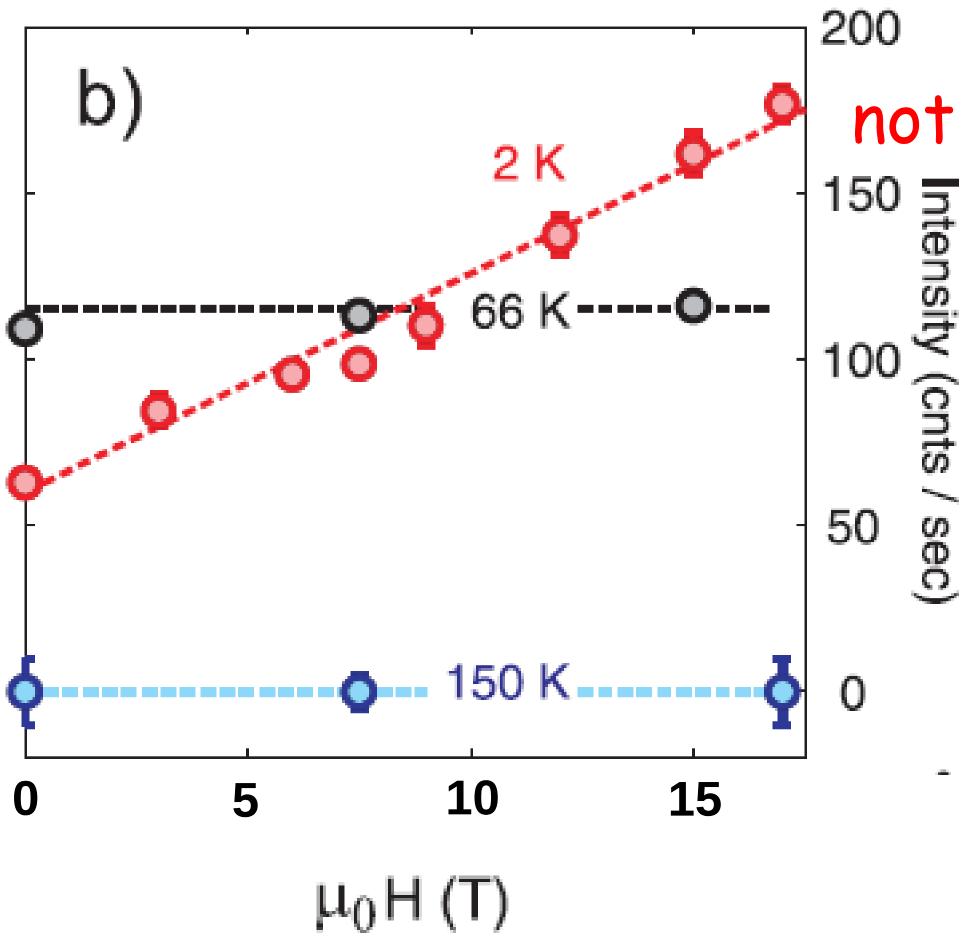


B-field suppresses superconductivity, enhances CDW

Field dependence of CDW Intensity

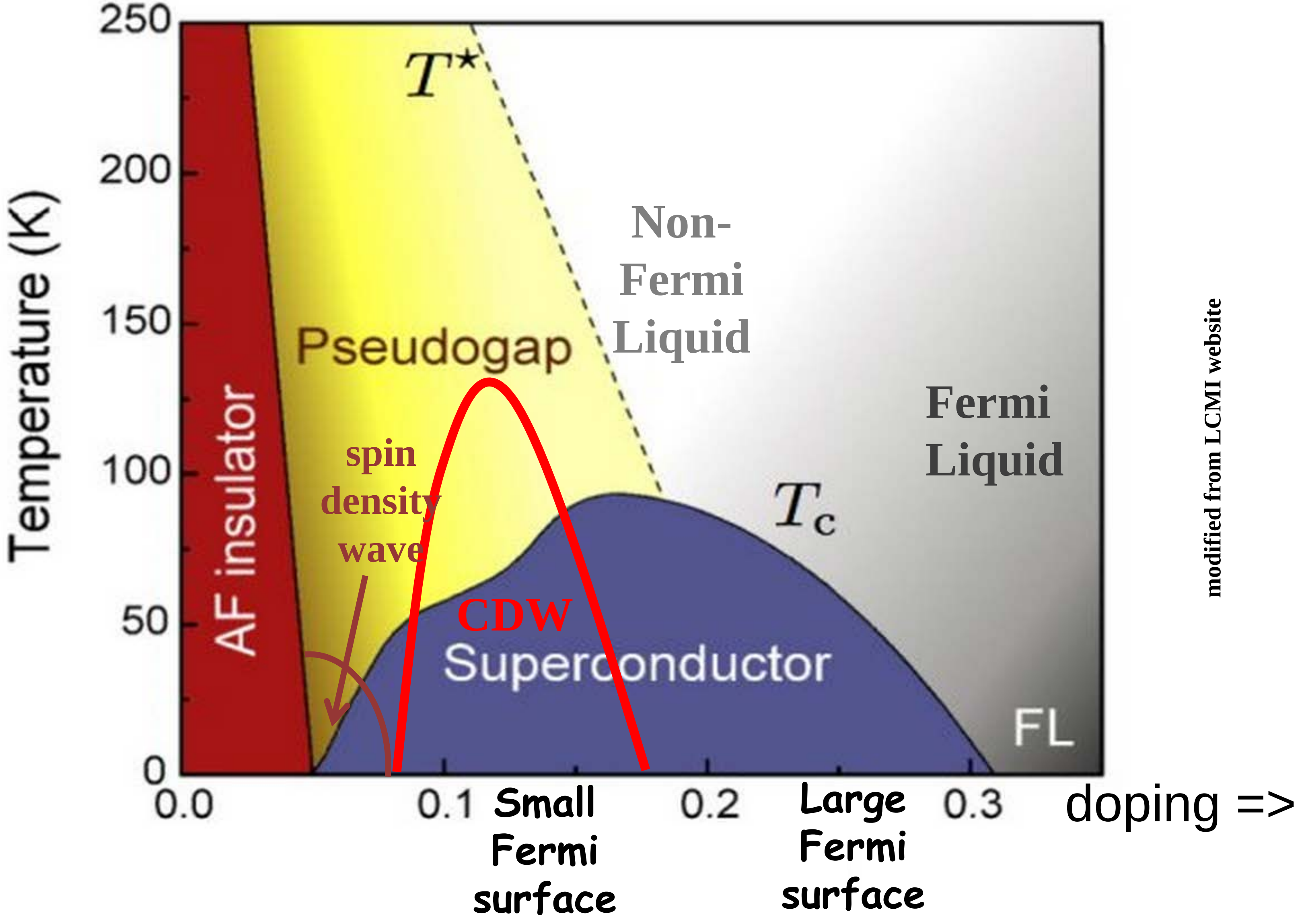


not quite saturated

Above T_c:
no effect of
B-field on CDW

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

High- T_c properties versus hole doping including CDW



modified from LCMI website

What is the *structure* of Charge Density Waves?

Measure sufficiently many (>200) different X-ray diffraction satellites due to the CDWs to derive the atomic displacements that fit the data. Needs zero *B*-field for flexibility

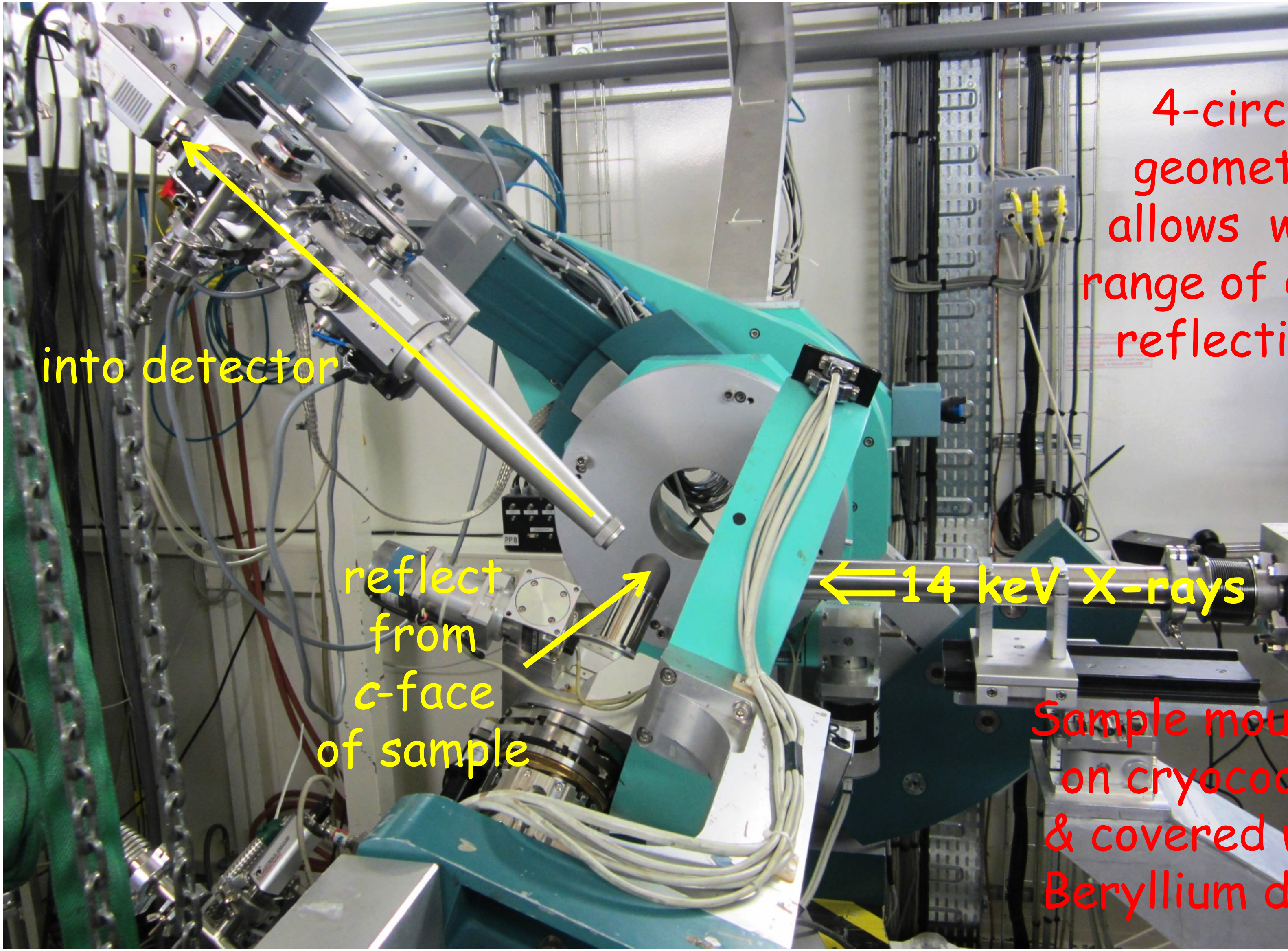
If possible, deduce something about the physics of the CDW from these atomic displacements

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

Group theory allows us to solve this problem; the symmetry of the derived displacements is quite surprising

We then use the properties of the CDW to propose how the Fermi Surface reconstruction occurs - and learn something about High- T_c

Apparatus: the XMaS (UK) beamline at ESRF



Considerations used in analysis of results

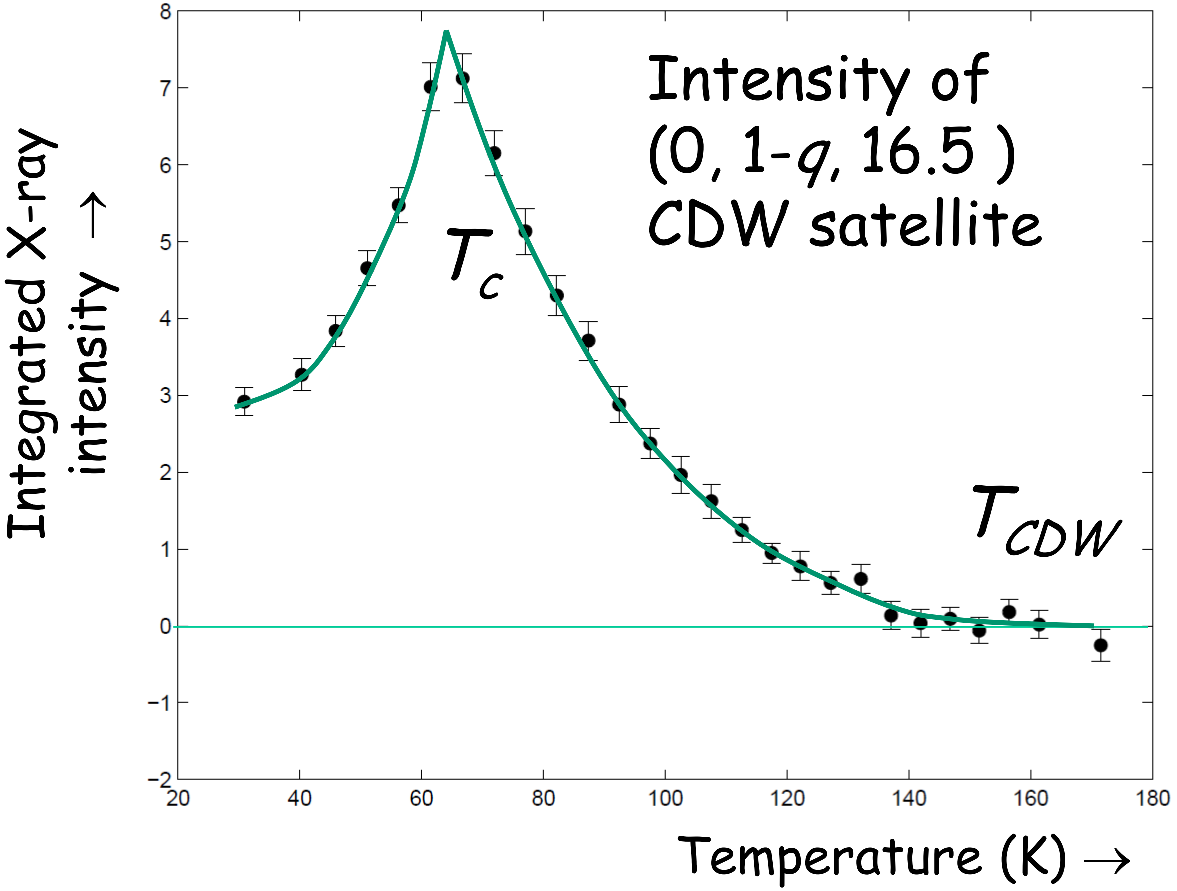
Non-resonant X-rays are insensitive to small charge density changes.
Instead they respond to the associated/resultant atomic *displacements* from their usual positions.
(because ALL the electrons in a displaced atom scatter X-rays)

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)

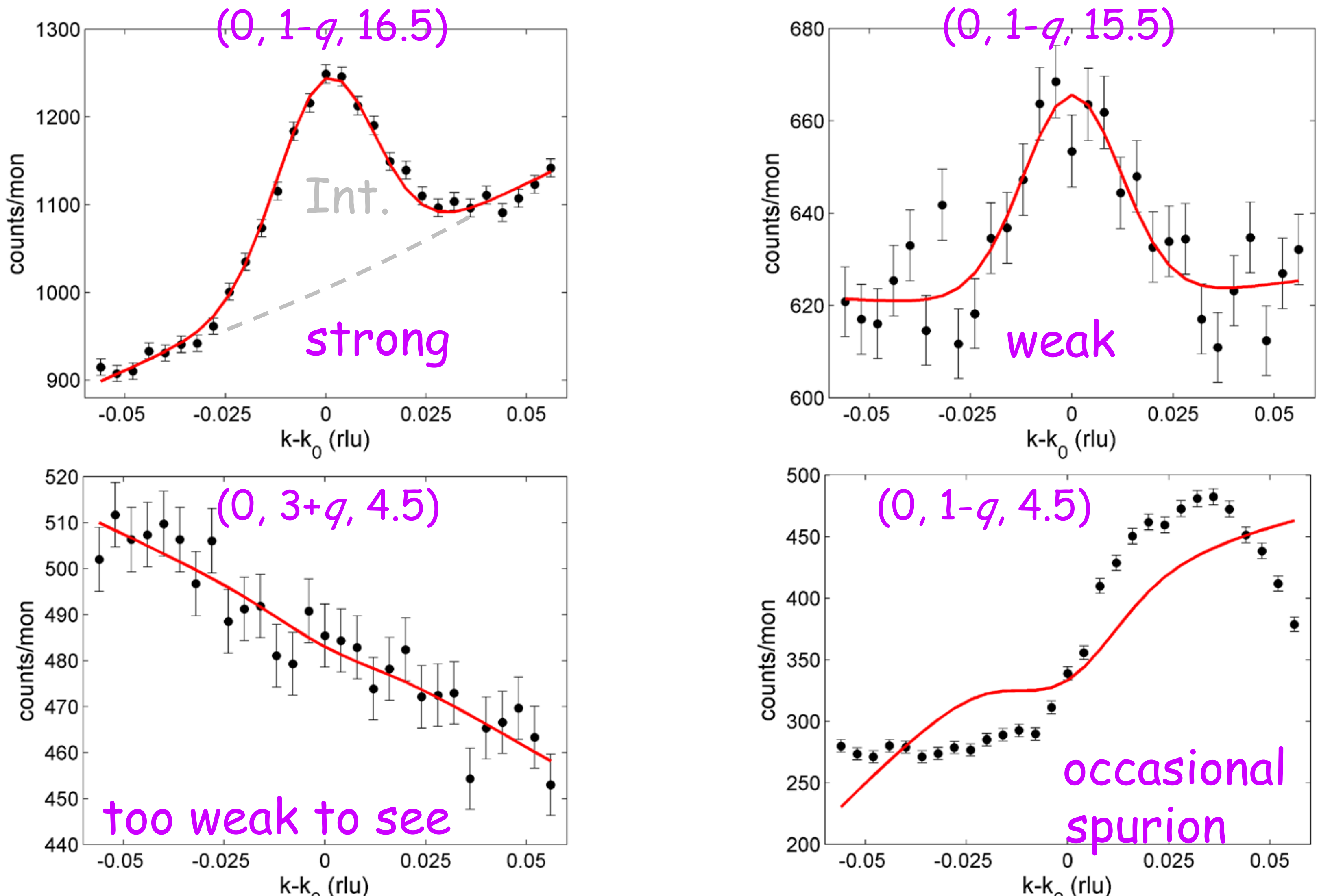
CDWs are longitudinal, with atomic displacements
(e.g. for ***q*** // ***y***) along *both* ***y*** & ***z*** directions.

Temp-dependence of CDW order in $YBCO_{6.54}$

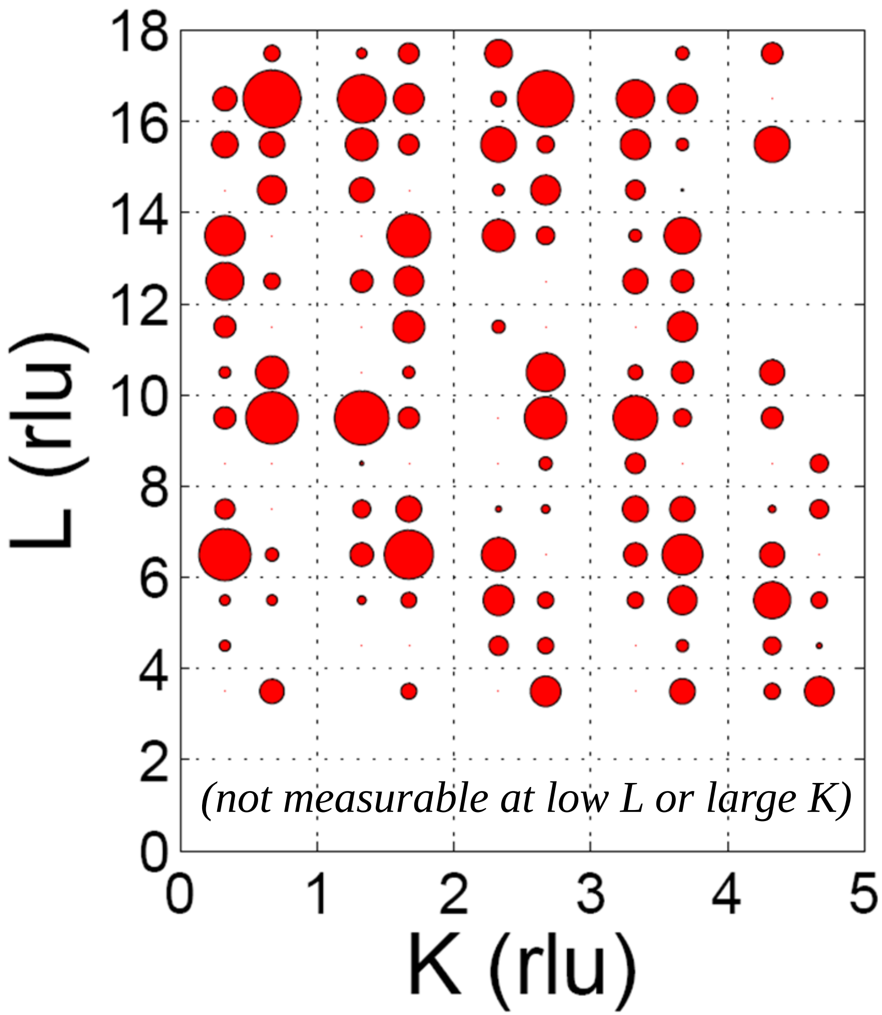


Make all observations of CDW intensities at T_c (superconductivity) = 60 K

Typical observations of CDW satellites at 60 K



A typical CDW satellite intensity pattern



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

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

A total of 269 satellite positions observed for q_b and 193 for q_a

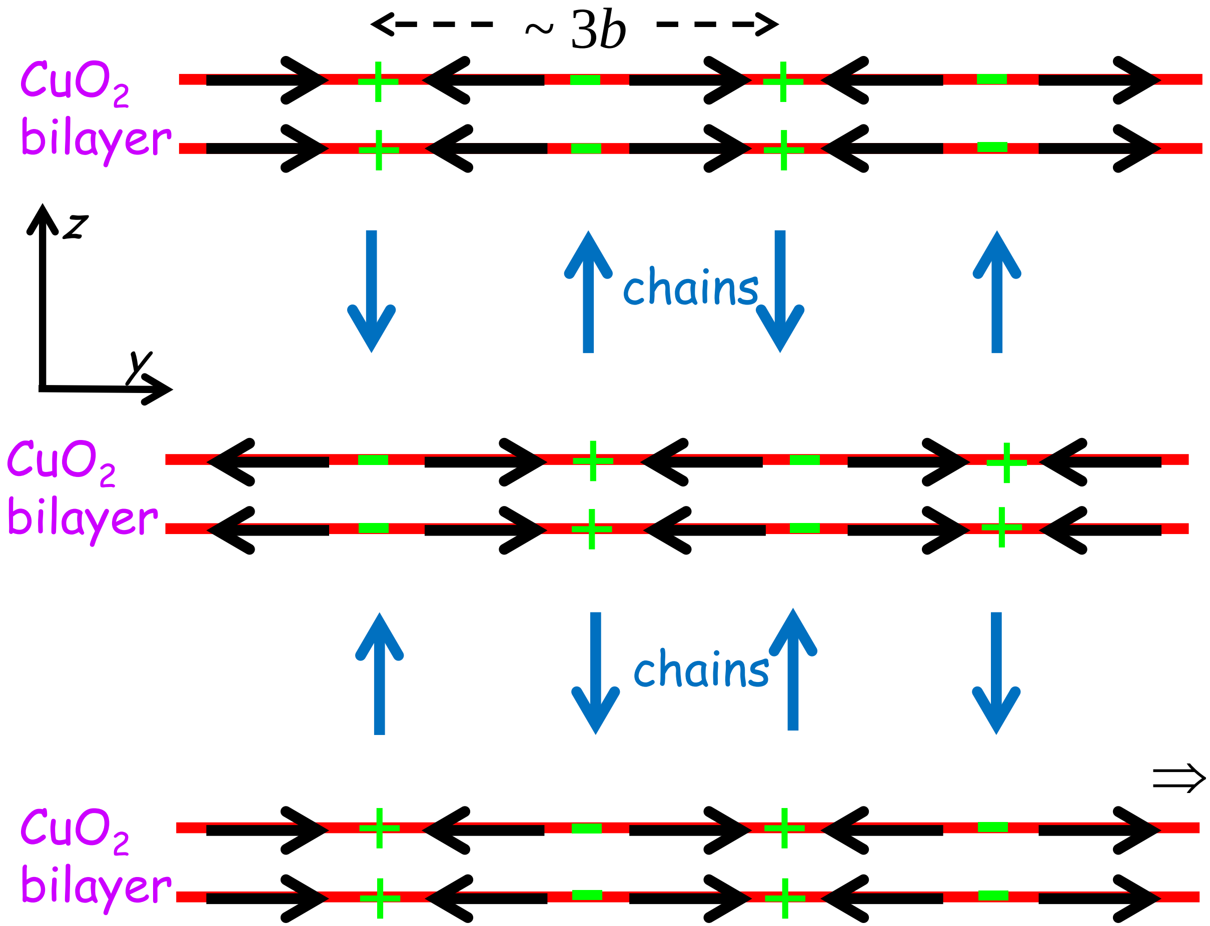
Area of circle ∝ Intensity

blank = not measured

Expected structure of the CDW order

We expect atomic displacements with this *symmetry*

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



CDW ⇔ atomic displacements

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

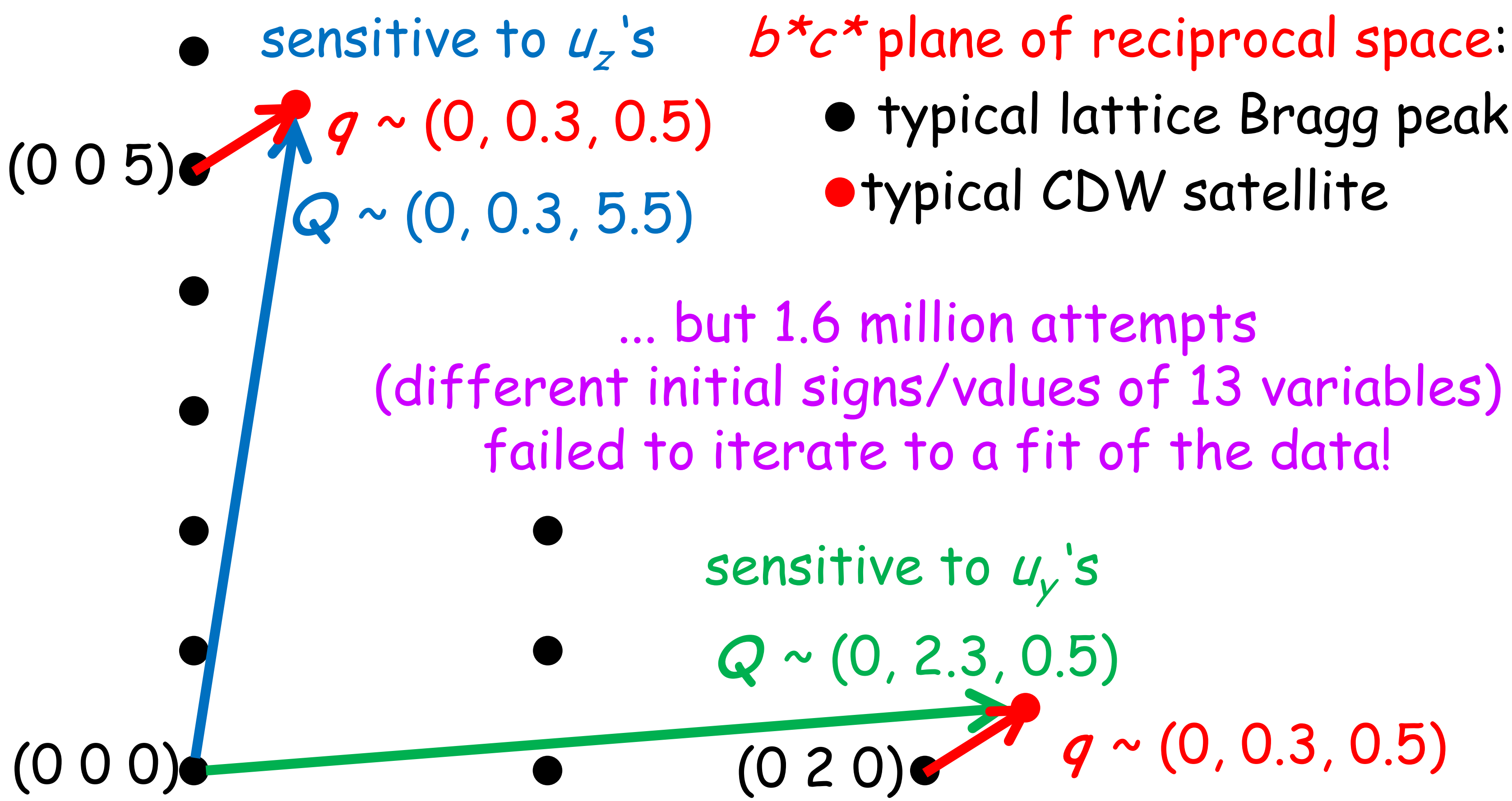
also ∃ *c*-axis displacements

⇒ total of 13 atomic motion variables to fit the data

How to deduce atomic displacements *u* in the CDW

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

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

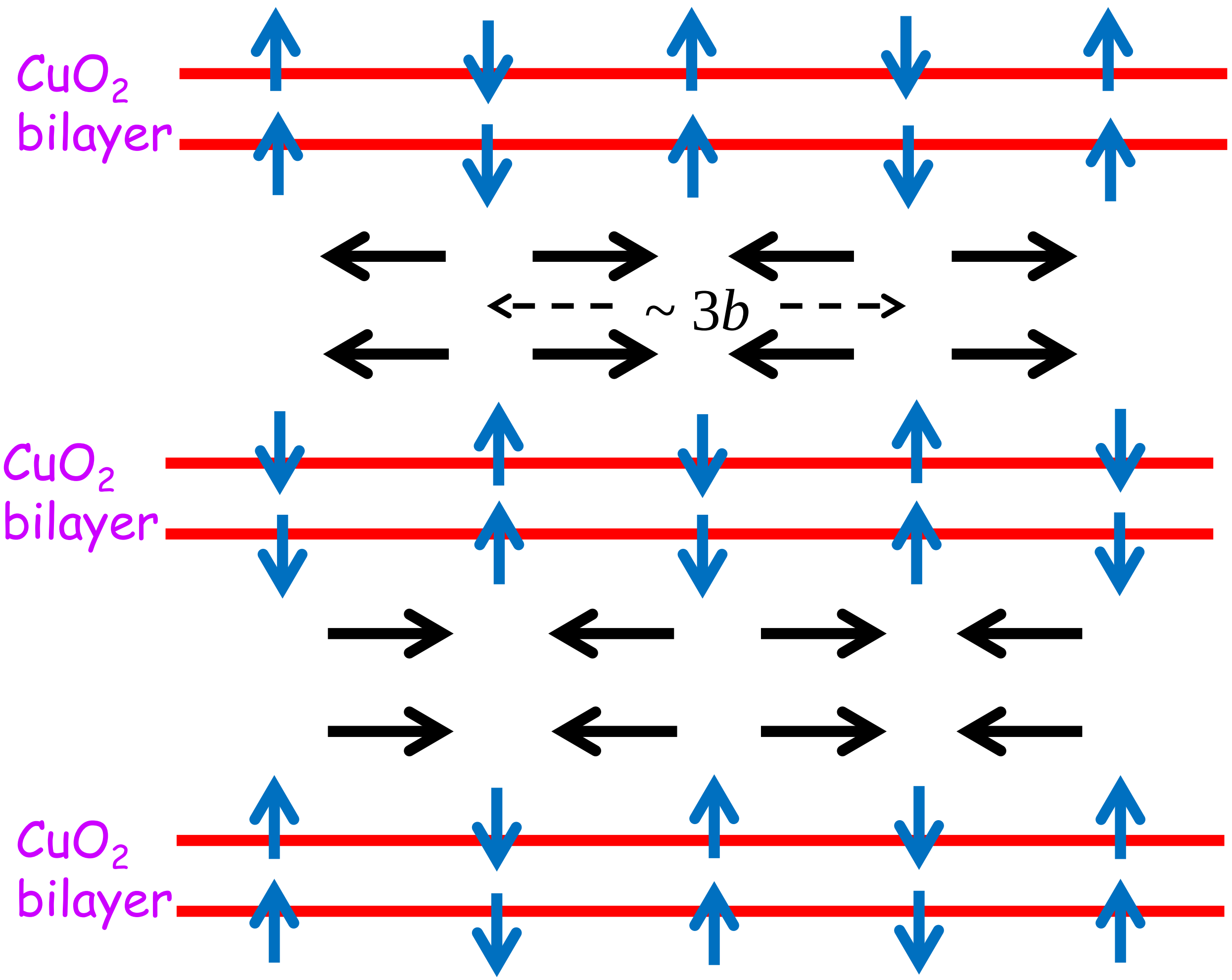


... but 1.6 million attempts
(different initial signs/values of 13 variables)
failed to iterate to a fit of the data!

Only other possible model for the atomic movements

We are forced to consider displacements of this *symmetry*

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



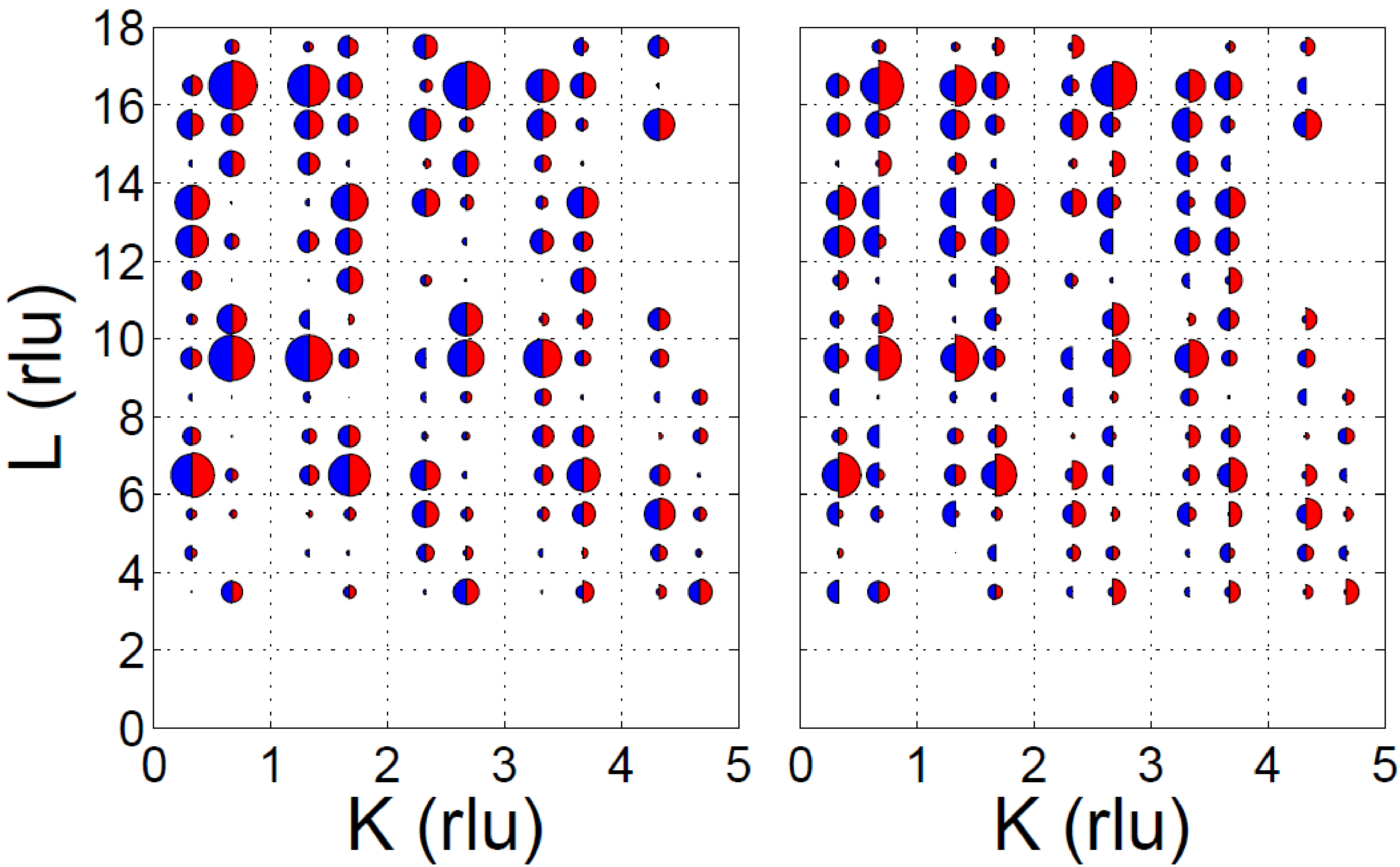
CuO_2 bilayers *sheared* - not compressed

Next unit cell in antiphase (≡ *ℓ* = 0.5)

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

fits the data!

Good fit - bad fit...

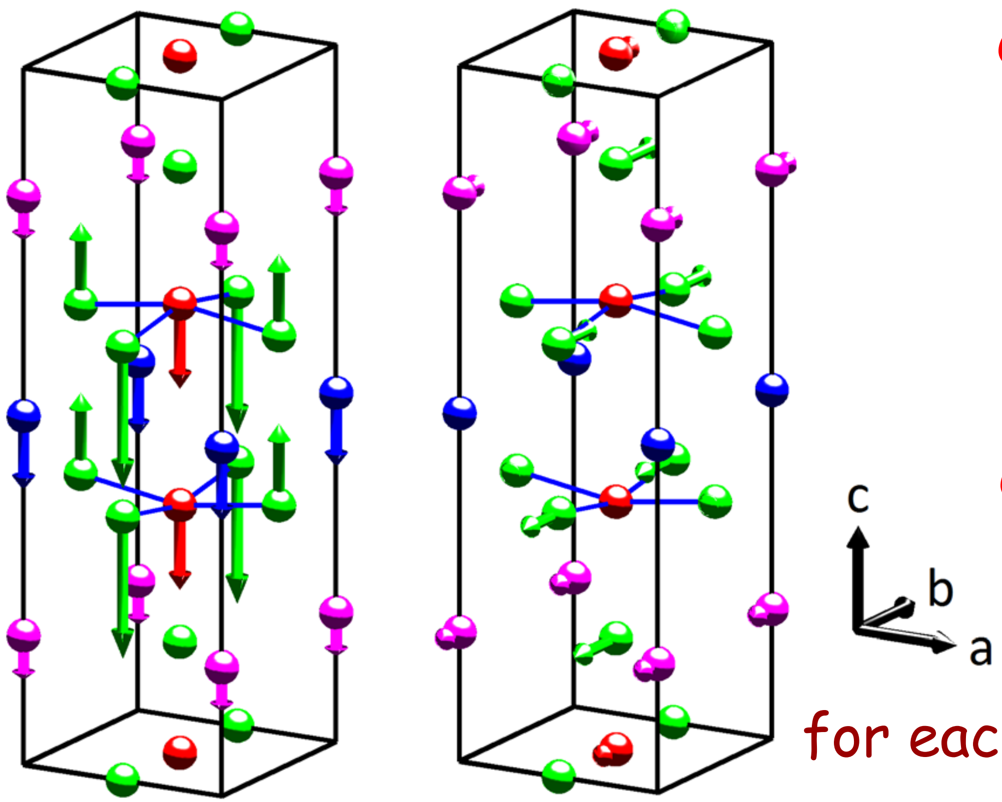


CuO_2 bilayers sheared

CuO_2 bilayers compressed

The motif which is modulated to form the CDW

- from the results of the good fit to the q_b mode



u_c u_b

CuO chains

BaO layer

CuO_2 plane

Y layer

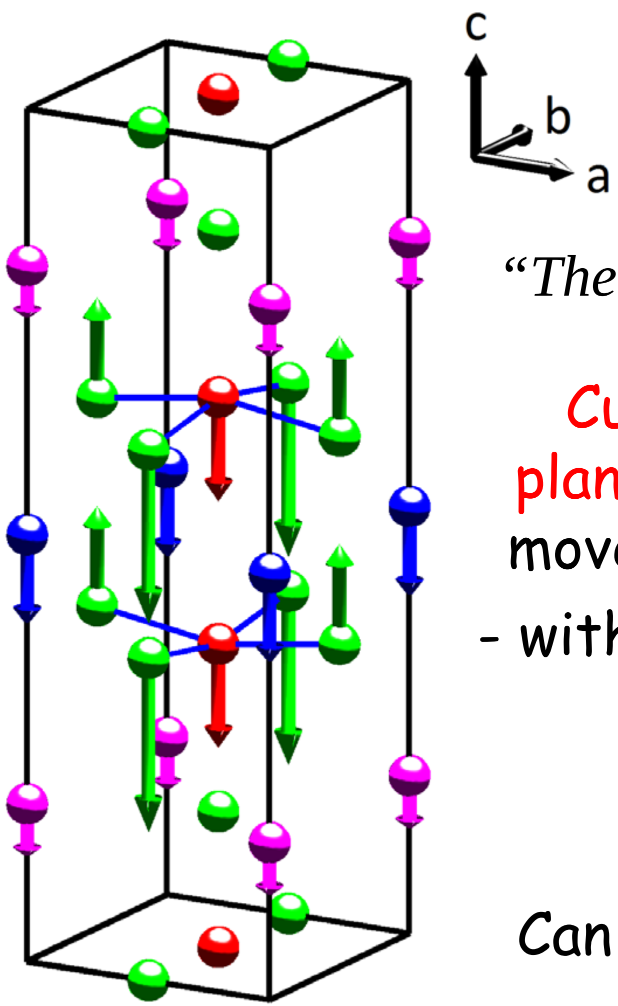
CuO_2 plane

for each atom, $r_0 \Rightarrow r_0 + u(r_0)$

$u(r_0) = u_c \cos(q.r_0) + u_b \sin(q.r_0)$

In zero field, next unit cell along *c* is in antiphase

The motif which is modulated to form the CDW



- concentrating on the *c*-axis displacements which dominate

"The change in strain is mainly out of plane"

Cu's in the planar bilayers move together

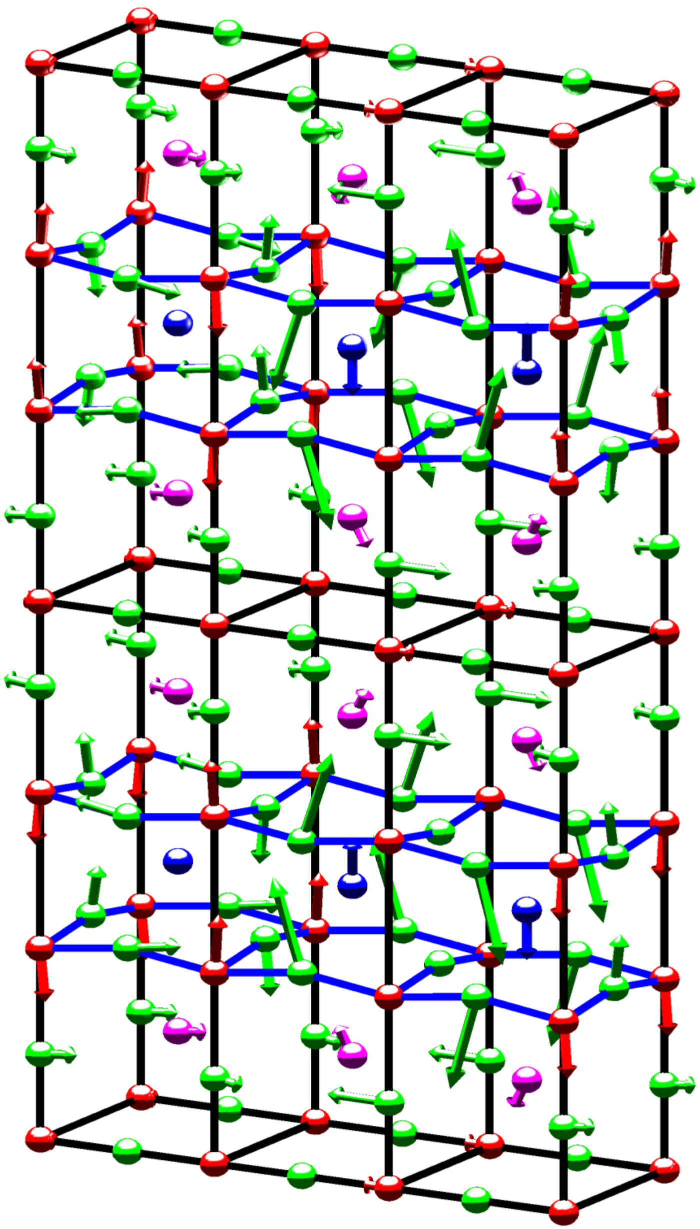
- with the Y's

O_x & O_y move *oppositely* to each other

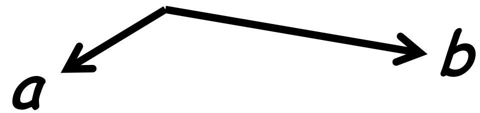
Actual amplitude ~ 10^{-3} of an atomic spacing!

Can this tiny effect be important? Yes!

CuO chains don't move (symmetry)



Resulting modulated ionic displacements



period only ~ 3 unit cells
so π phase change in only $1\frac{1}{2}$ cells

not tilted CuO_5 half-octahedra

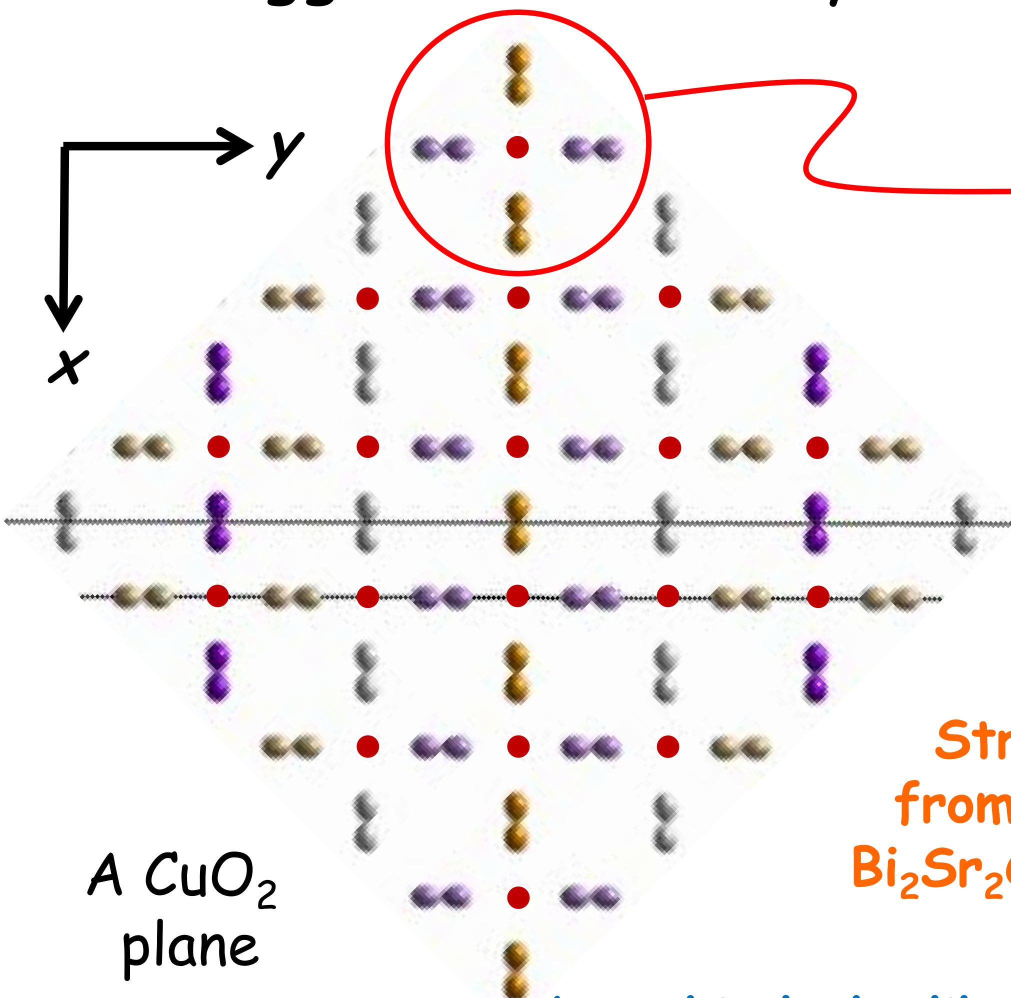
Plus a similar modulation in the perpendicular direction

Almost certainly in the same region of space:

"double-*q*" or "biaxial" order

=> Fermi surface reconstruction

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



a small charge transfer from one pair of oxygen orbitals to the other

Cu
O_x
O_y

Spatially modulated along y

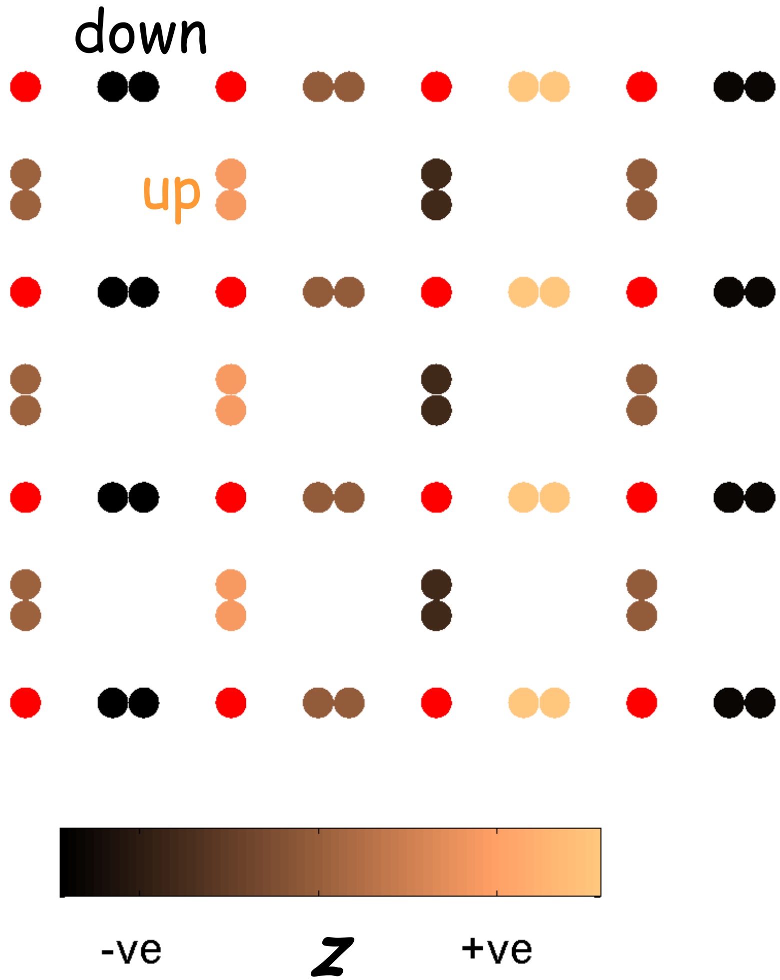
A CuO_2 plane

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 2014

A plot of the modulated oxygen *z*-displacements



for a single CDW mode

modulation direction ➔

You have seen this pattern before...

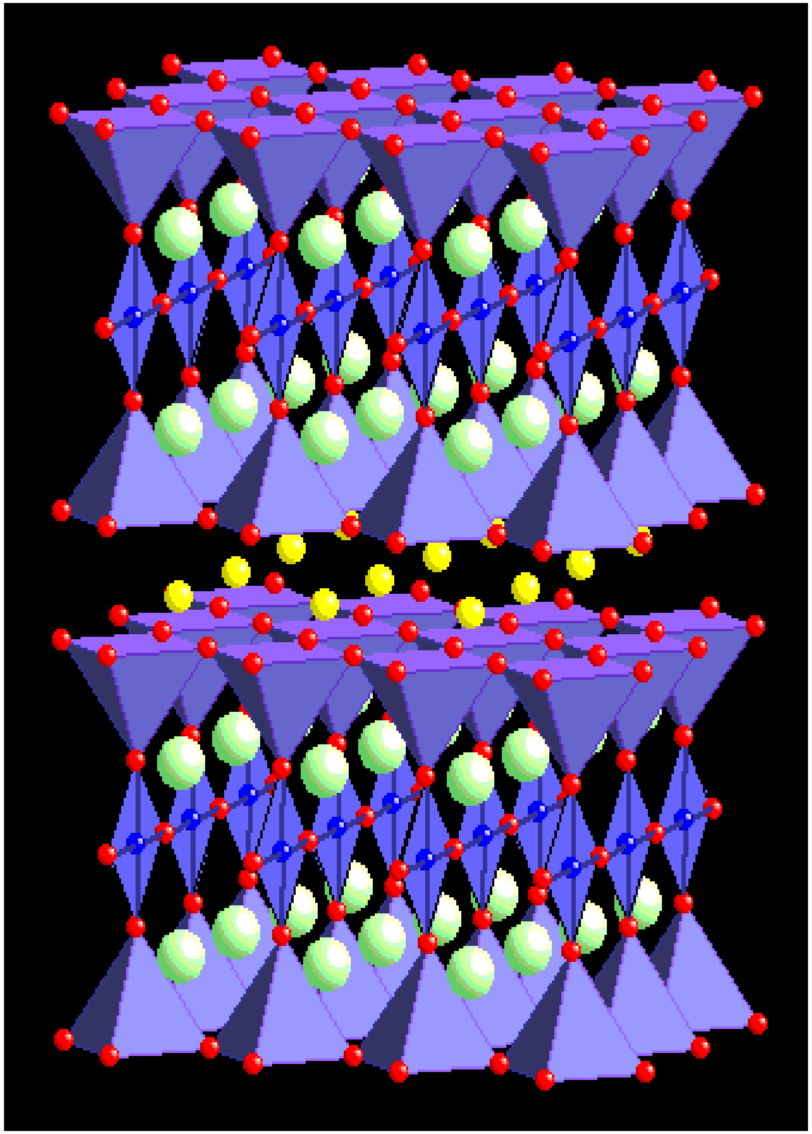
Motion of an ion in the *z*-direction can alter the local doping

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

CDW Structure determination: Nature Comms. 2015

Electron states in a CuO_2 bilayer in $YBCO_{6.5}$

YBCO structure from: www.ncl.ox.ac.uk/icl/heyes/structure_of_solids/lecture4/lec4.html



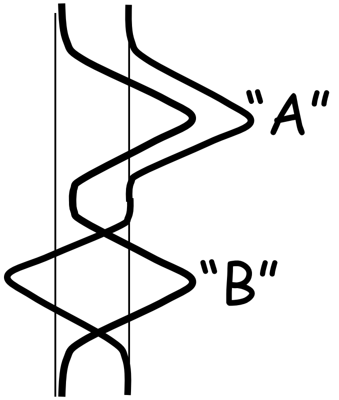
Superconductivity resides mainly in the CuO_2 planes

Cu O chains: O ½ occupied – electrically inactive

Cu O_2 plane

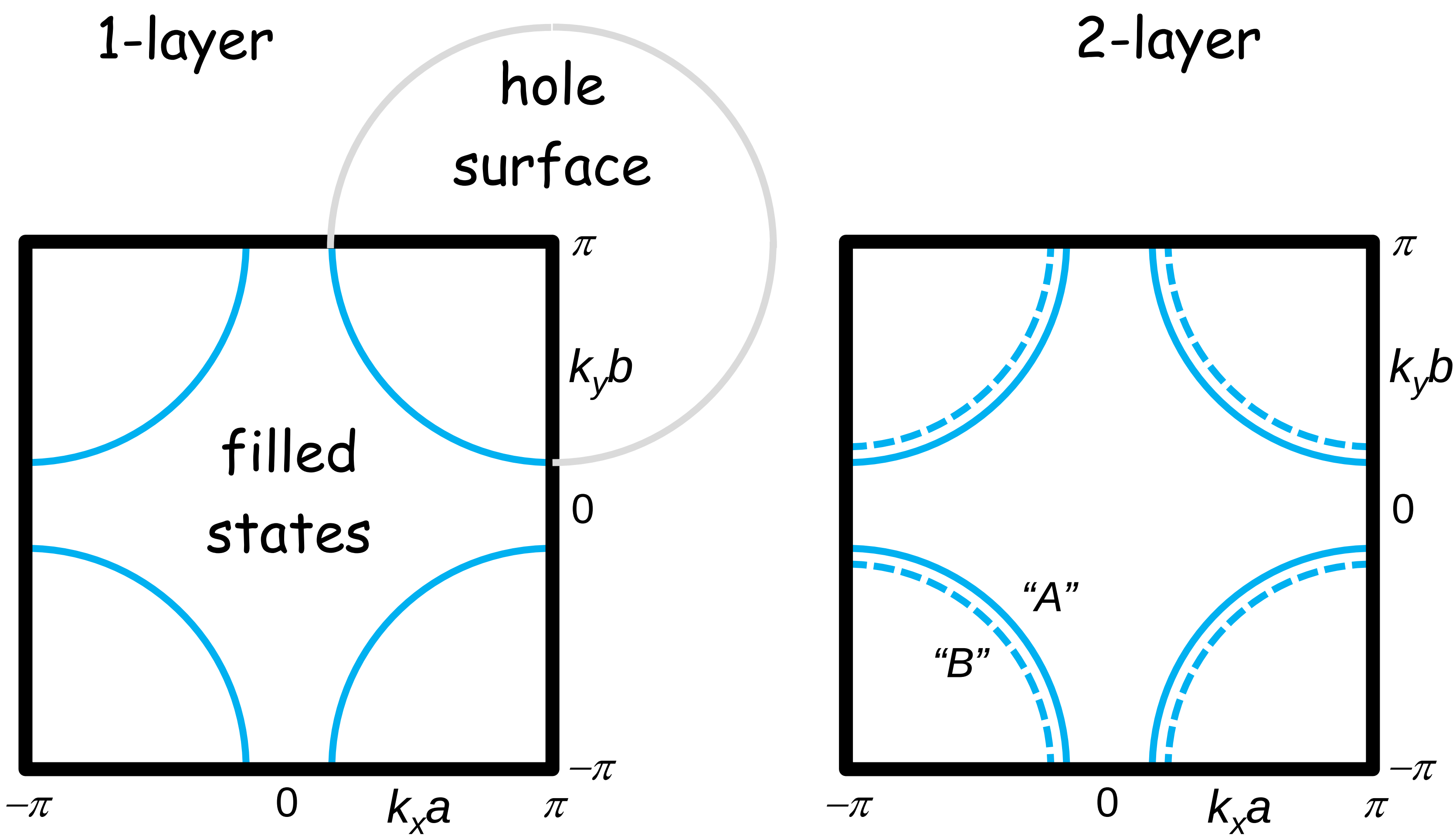
Y layer

Cu O_2 plane



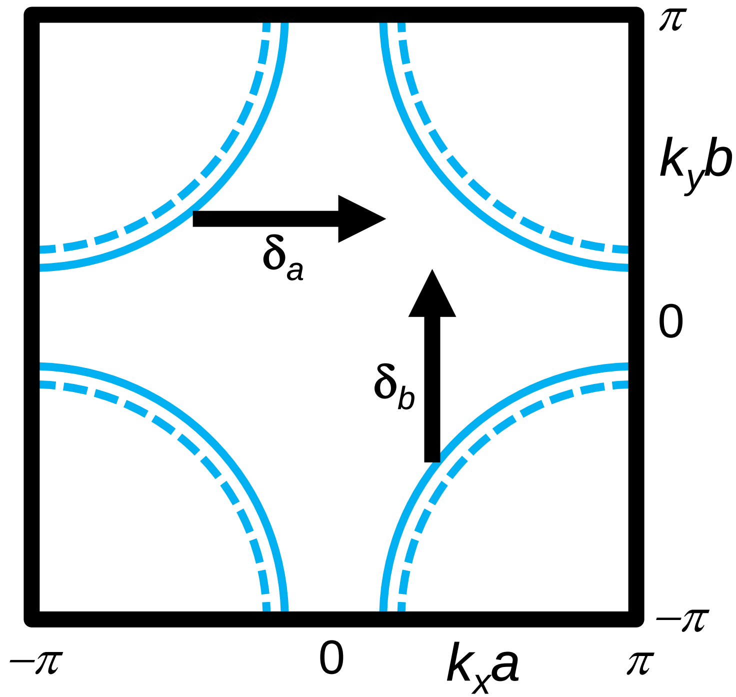
There are two ways of combining the wavefunctions of the states in the two halves of a bilayer

Single-layer & Bilayer Fermi Surfaces – no reconstruction



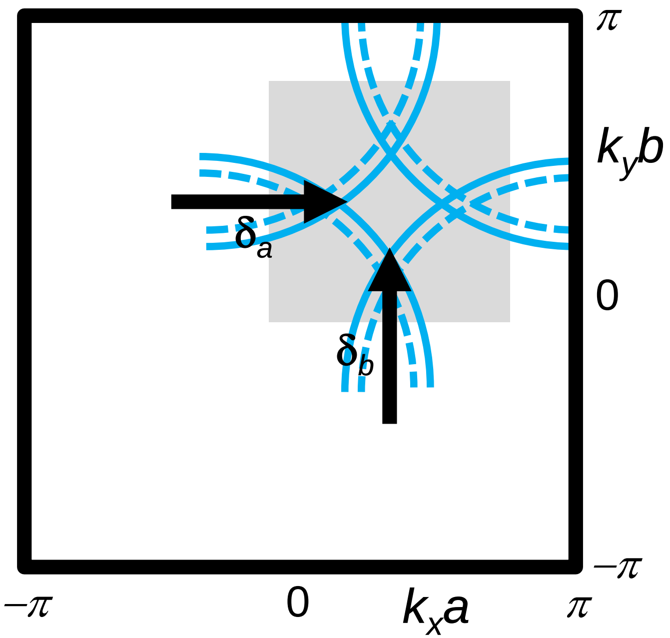
Reconstruction by CDW with basal wavevectors δ_a & δ_b

states can pick up wavevector of CDW



Reconstruction by CDW with basal wavevectors δ_a & δ_b

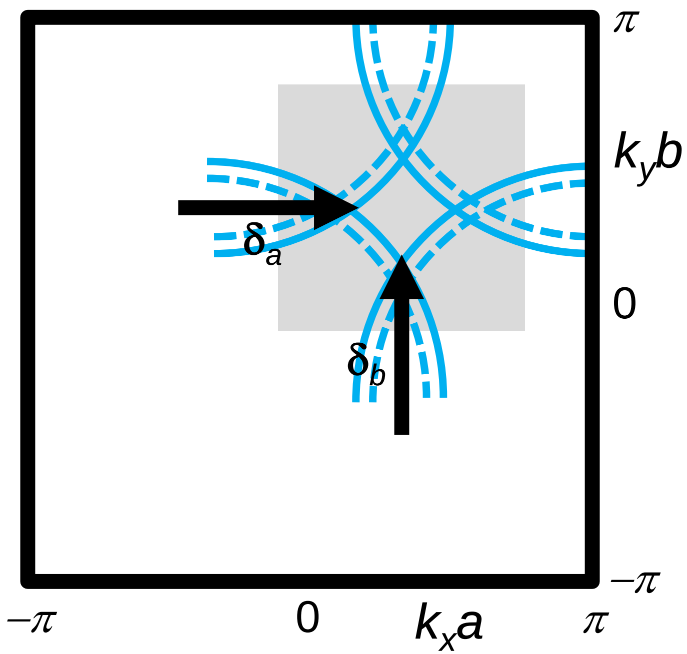
states can pick up wavevector of CDW

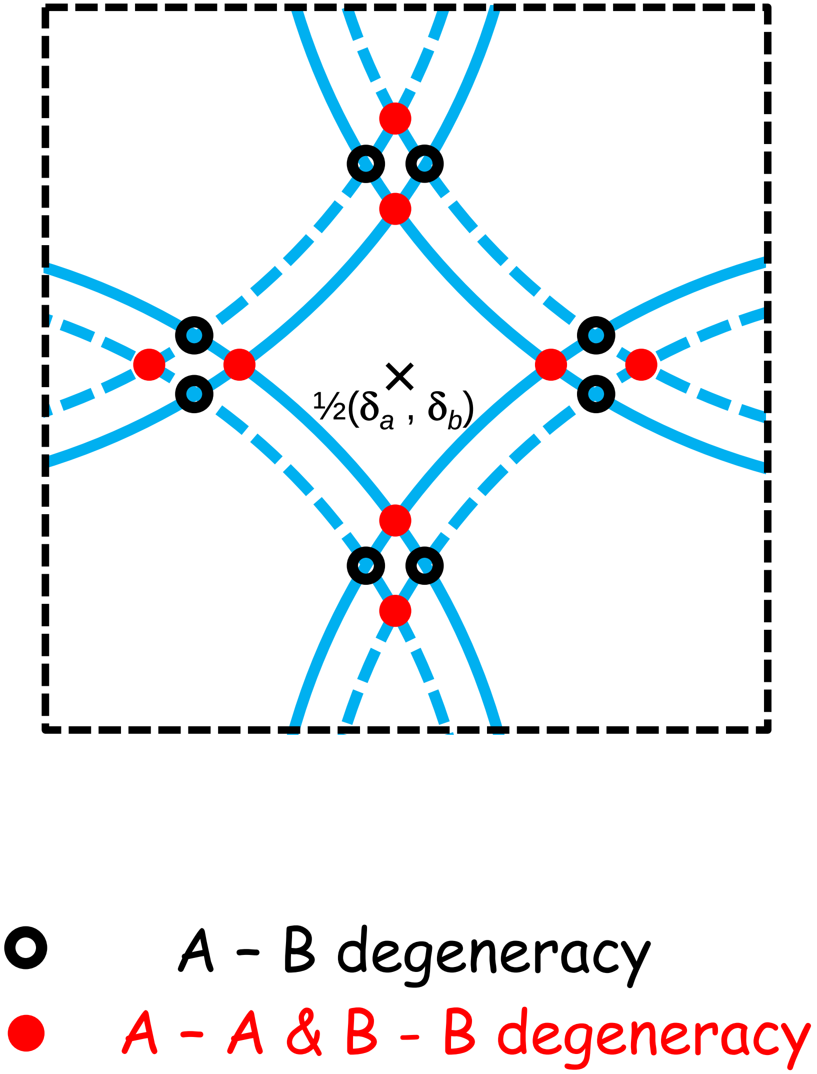


and may hybridise where degenerate

Reconstruction by CDW with basal wavevectors δ_a & δ_b

states can pick up wavevector of CDW





and may hybridise where degenerate

Reconstruction by CDW with basal wavevectors δ_a & δ_b

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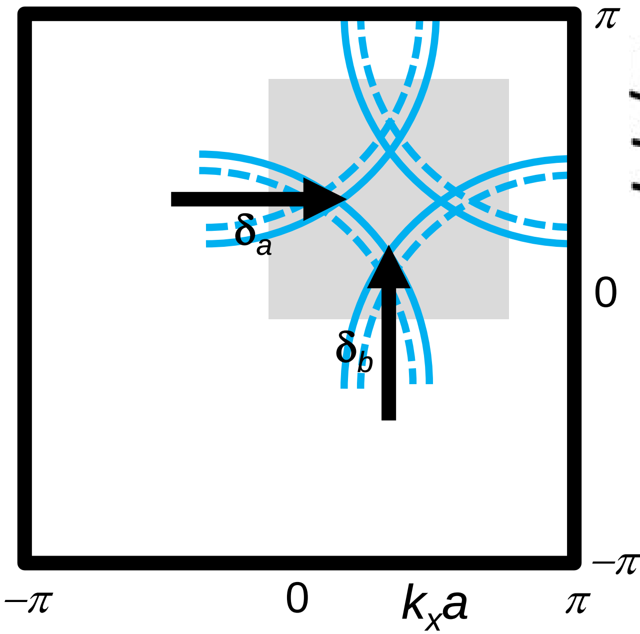
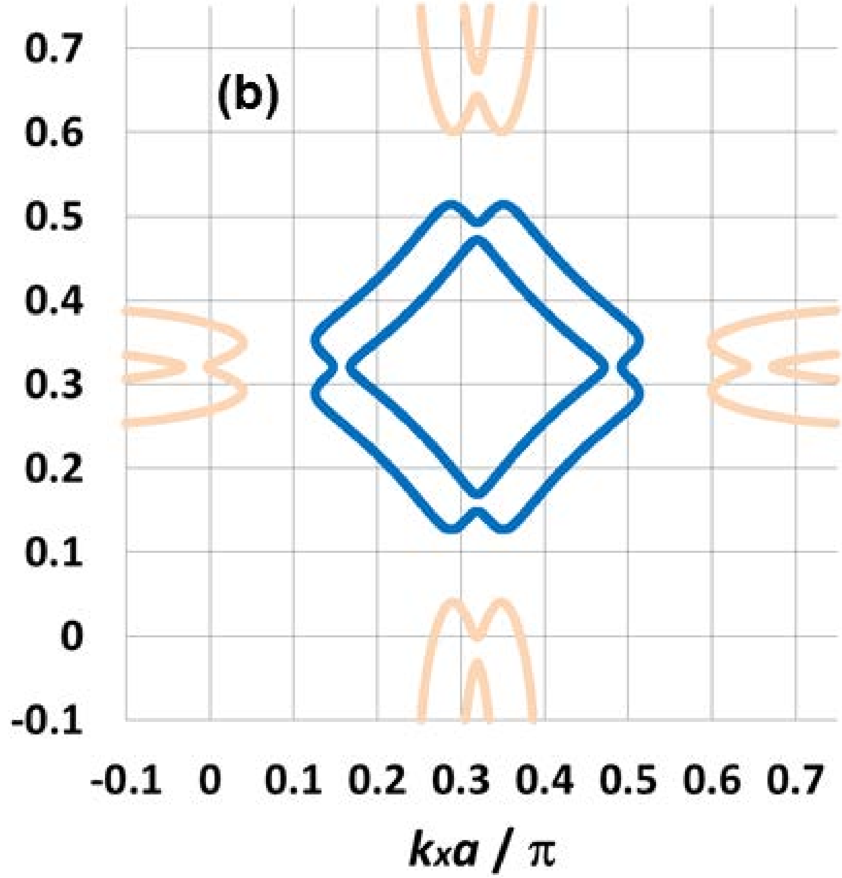


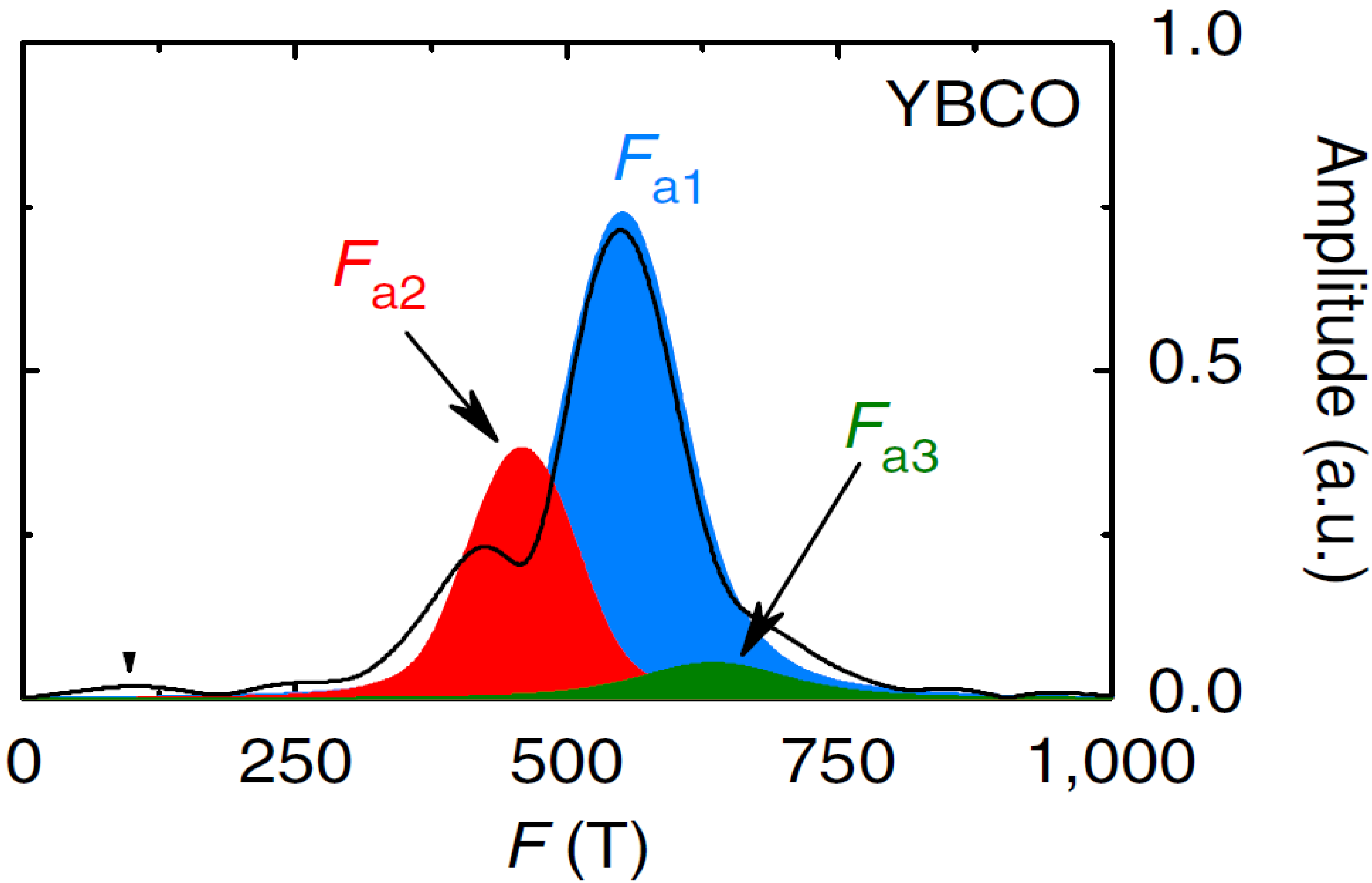


and may hybridise where degenerate

○ A – B degeneracy

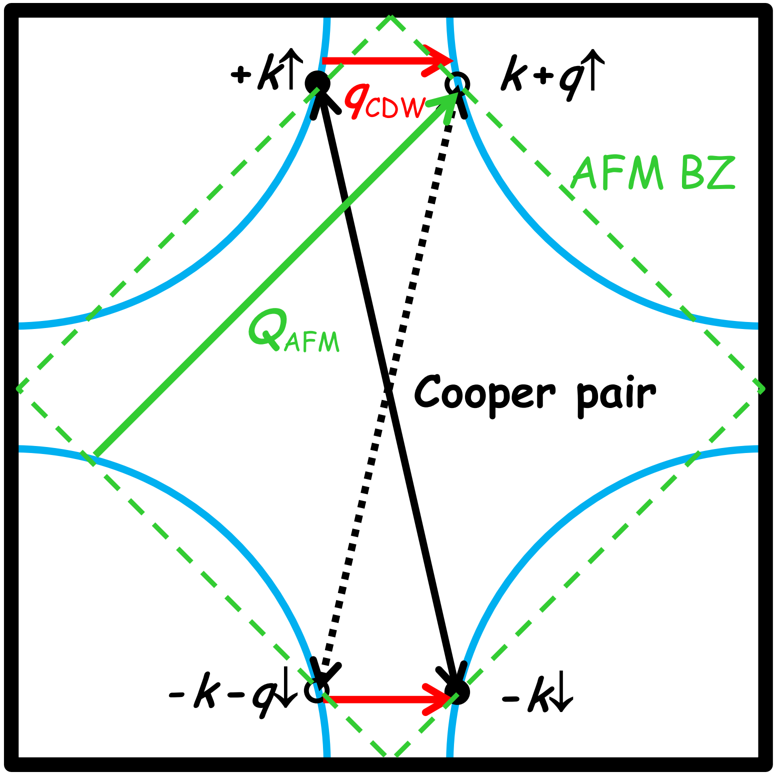
● A – A & B – B degeneracy

Due to bilayer-split FS, QO results in YBCO show multiple Fermi Surface areas



Fermi Surface Reconstruction: Phys Rev B 2016

How does this all hold together? "SU(2) theory"



A CDW can be regarded as the Bose condensation of electron-hole pairs

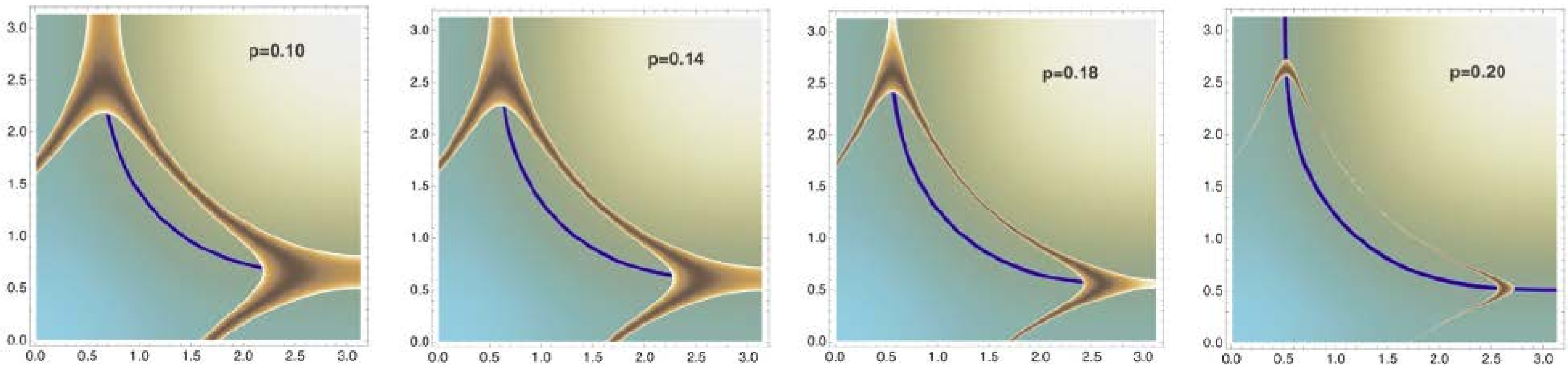
A superconductor can be regarded as the Bose condensation of electron-electron (Cooper) pairs

An underdoped cuprate has a superposition of both orders related by an SU(2) symmetry

How does antiferromagnetism come in?
The CDW occurs near the AFM "hot spots" where the SU(2) symmetry is exact and AFM fluctuations cause pairing

How does this all hold together? "SU(2) theory"

calculation* of SU(2) fluctuations *vs.* doping =>



It is proposed that these fluctuations create the pseudogap

- which removes the ends of the "Fermi arcs"

-and creates the conditions for the CDW
and Fermi Surface reconstruction to occur

*C. Pepin group, Phys Rev. B **95** 104510 (2017)

How High- T_c theory appears to me in 2017

CDW appears in fairly flat parallel regions of Fermi surface

Antiferromagnetic fluctuations link CDW & Superconductivity

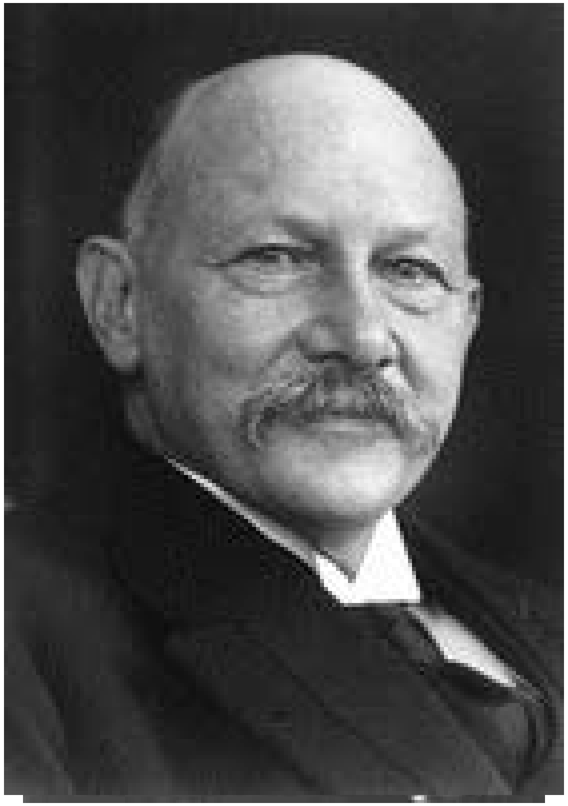
The CDW and the superconductivity share the same *d*-wave symmetry (though they don't need to by theory), and they compete for the same electrons

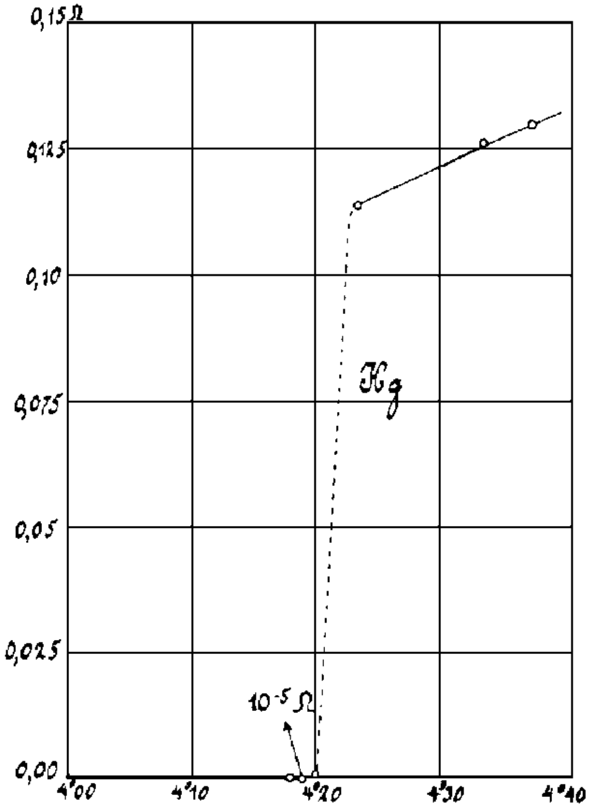
Highest T_c where SU(2) fluctuations/pseudogap are reduced

Workers on LBCO or LSCO who see antiferromagnetic + CDW **stripes** as important would not agree!

Some numerology

http://superconductors.org/history.htm#resist





Kamerlingh Onnes 1911 - explained 46 years later

- or 32 years after Quantum Mechanics came along in 1925

Some numerology

John Bardeen, Leon Cooper & Bob Schrieffer 1957

http://superconductors.org/history.htm#resist
http://www.nobel.se/physics/laureates/1913/onnes-bio.html

Kamerlingh Onnes 1911 - explained 46 years later

- or 32 years after Quantum Mechanics came along in 1925

- 1986 + 32 = 2018 - are we approaching the explanation of HiTc?

That's all Folks!