Neutron Scattering and Quantum Spins

Bill Buyers

Canadian Neutron Beam Centre

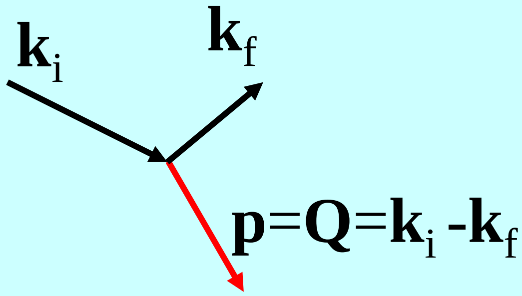
National Research Council,

Chalk River Laboratories, Ontario

Canadian Summer School on Neutron Scattering

Chalk River, 2011 May 12

The scattered neutron reveals



Where atoms are;

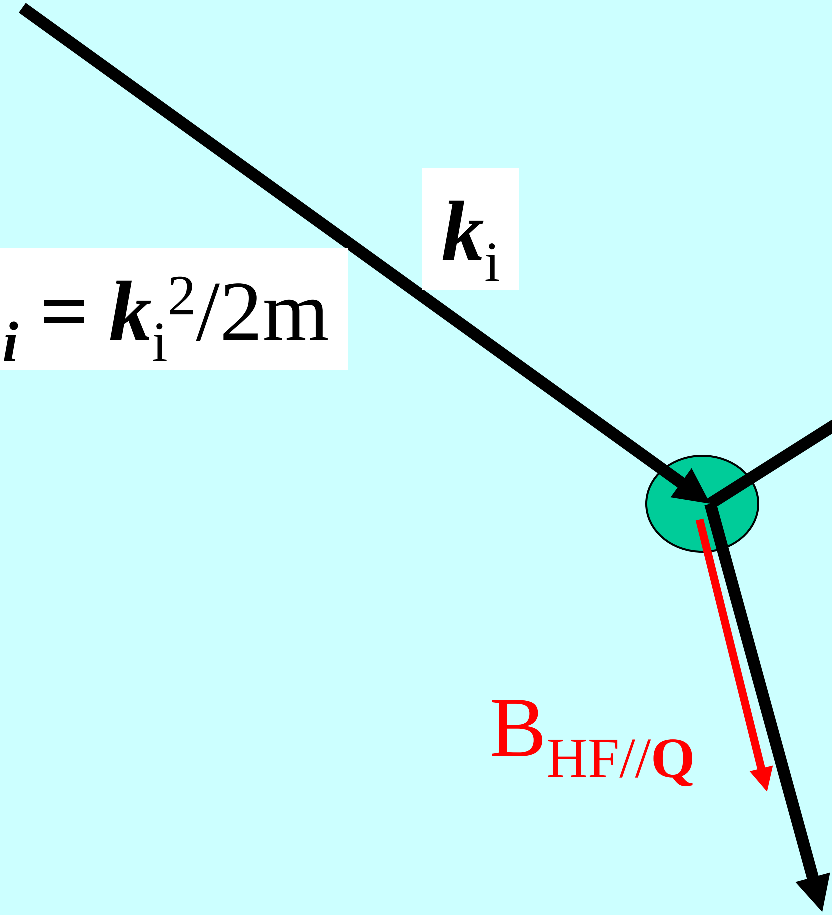
how atoms move;

how atomic spins oscillate;

what is the electronic ground state;

how spins interact with the electron liquid.

Neutron kinematics



$\boldsymbol{E_i} = \boldsymbol{k}_\mathrm{i}^2/2\mathrm{m}$

$\boldsymbol{E_f} = \boldsymbol{k}_\mathrm{f}^2/2\mathrm{m}$

$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f}$

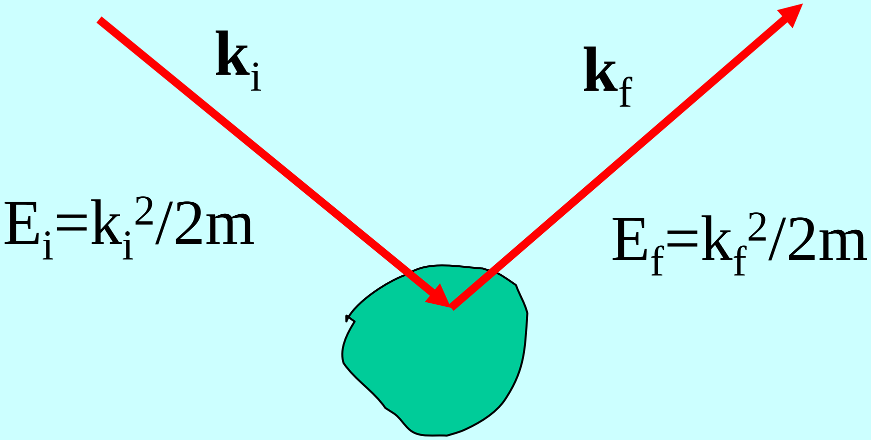
momentum $= \hbar\boldsymbol{Q}$

See Zahra notes on units

$\hbar = 1$

$\boldsymbol{E} = \boldsymbol{E_i} - \boldsymbol{E_f}$ ***energy transfer***

Spin spectrum is determined from neutron scattering by neutron's magnetic moment



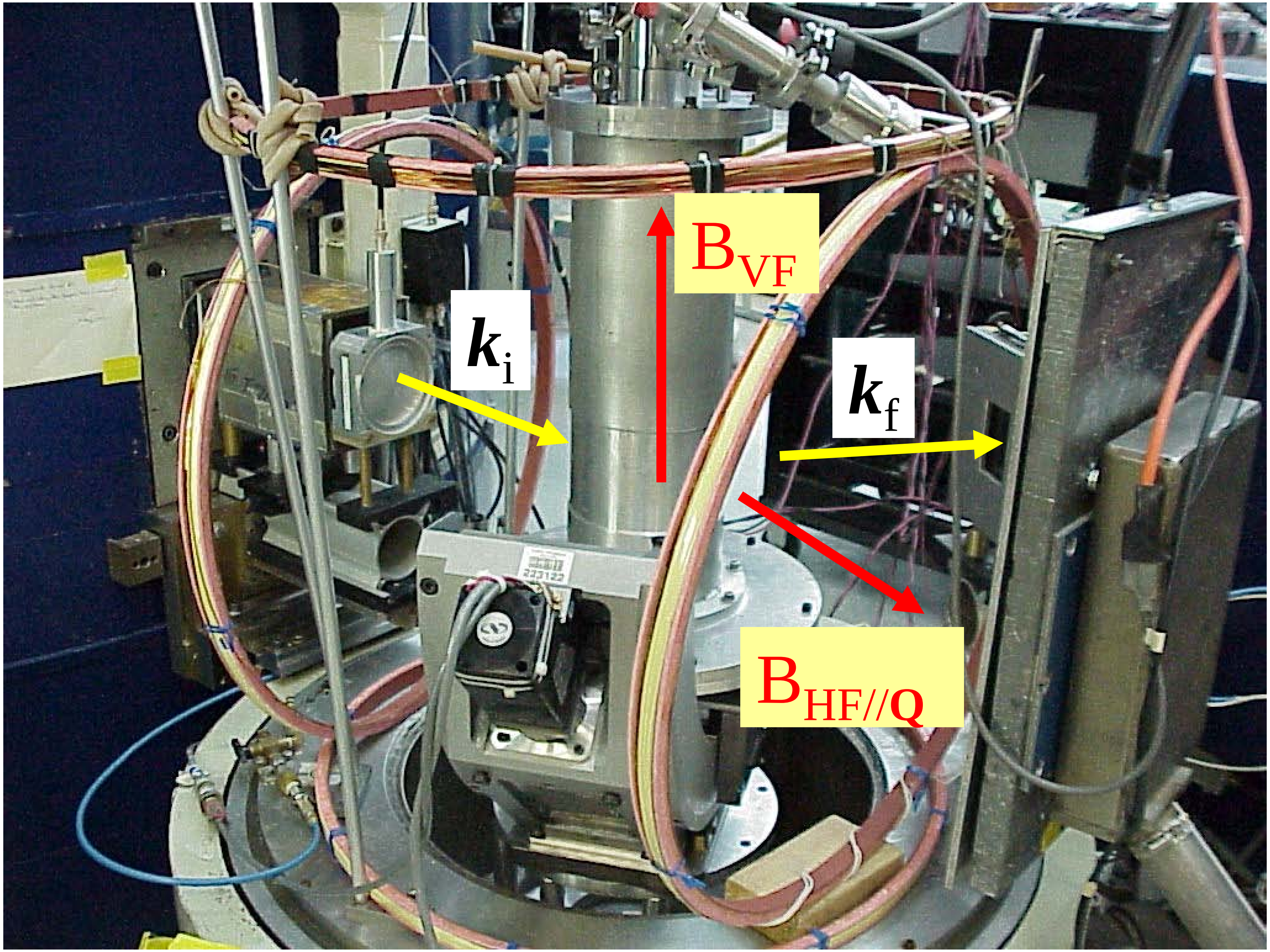
$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

$$\hbar\omega = E_i - E_f$$

Intensity = $S(\mathbf{Q},\omega)$ = FT (in $\mathbf{r}$, t) of $\langle M(\mathbf{r},t)M(0,0)\rangle$

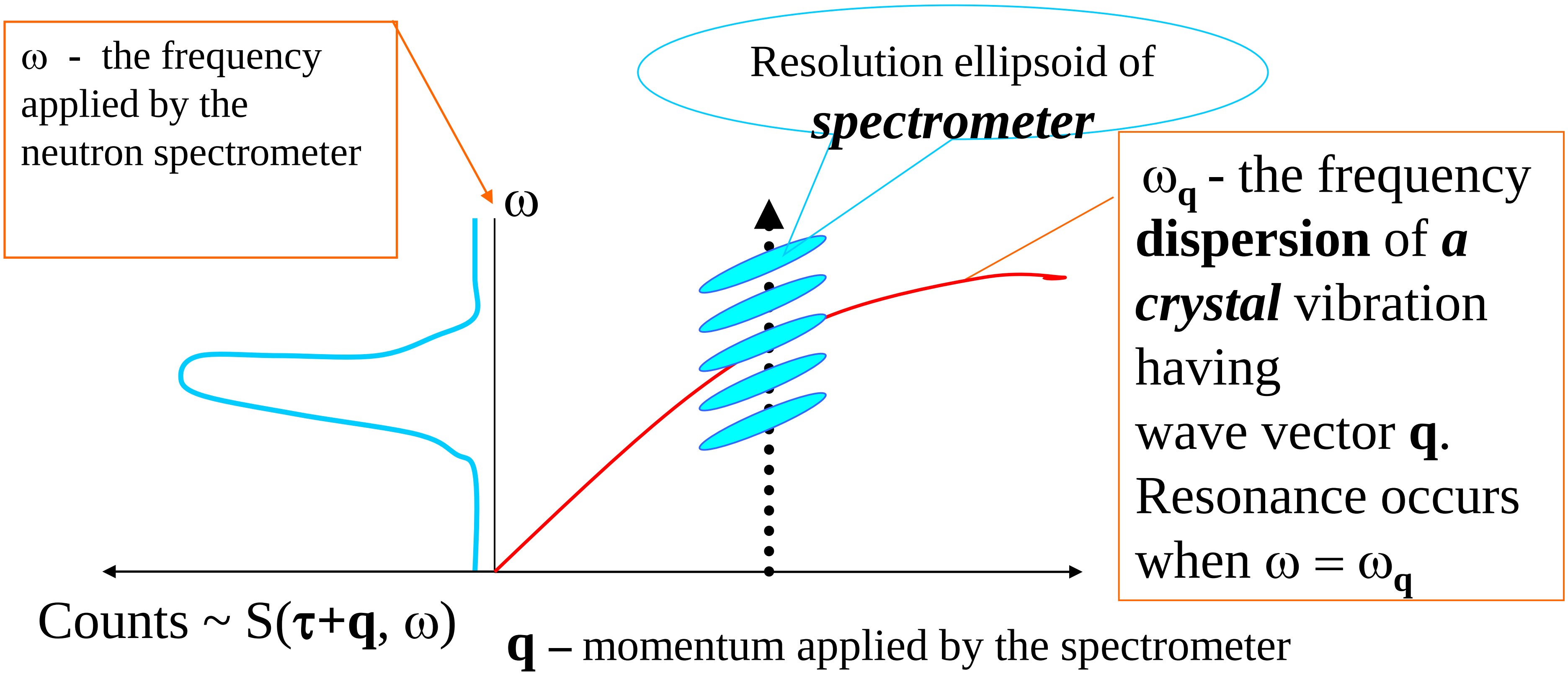
If $M(\mathbf{r},t) = M \quad \exp(i\mathbf{q}.\mathbf{r} - i\omega_c t)$ then scattering peaks at $\omega = \omega_c$ i.e., neutron wave is oscillating at same frequency as a wave of excitation in the crystal or: neutron transfers energy equal to a resonant frequency of the crystal. (Energy = h×frequency)

Polarized neutrons: Spin flip
HF-VF gives only the spin response



Constant-**Q** scan (Brockhouse 1955)

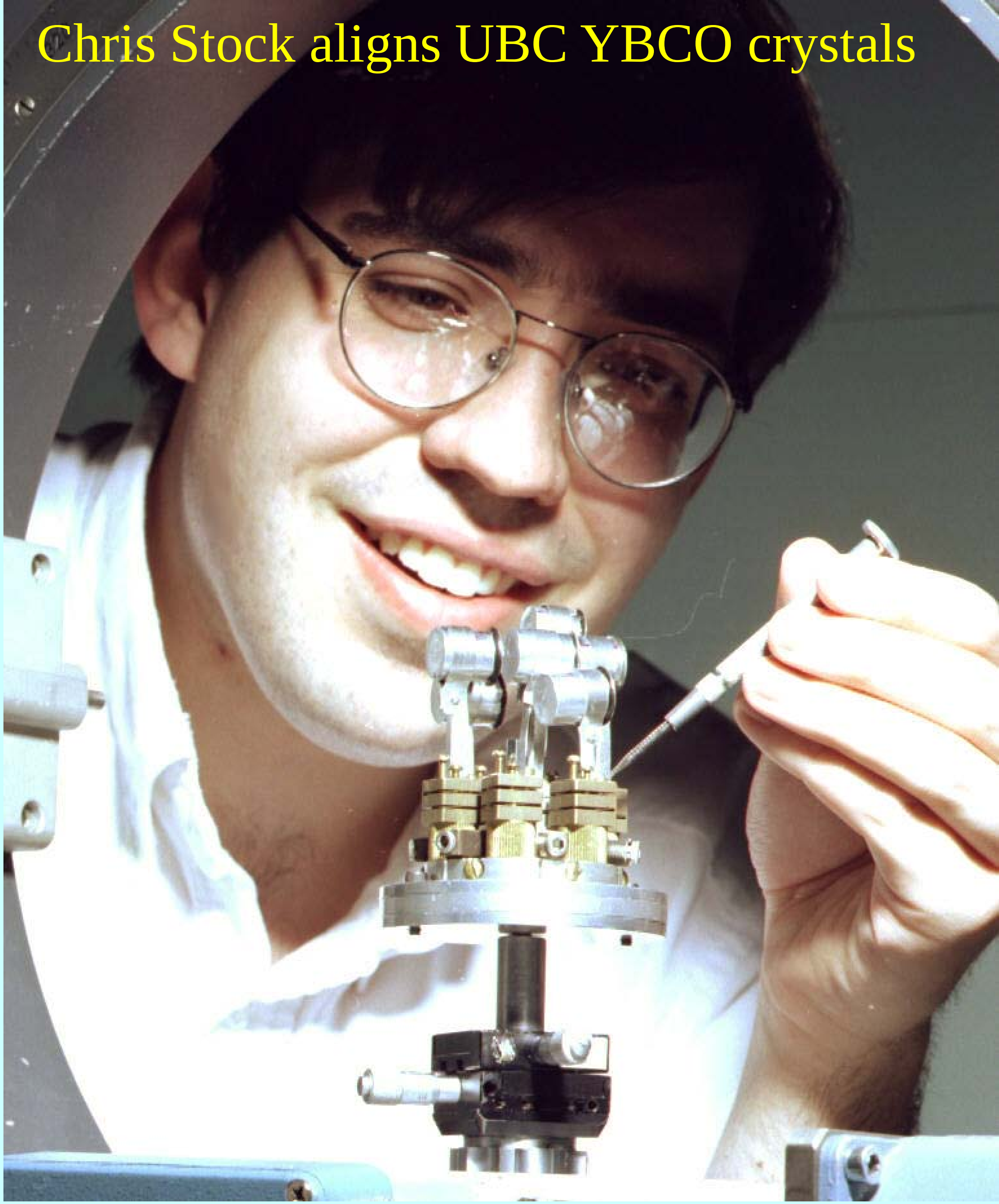
The spectrometer applies a temporal field $e^{i\omega t}$ and a spatial field $e^{i\mathbf{Q.R}}$ and we scan ω. The crystal is set **'ringing'** as the neutron energy transfer creates and matches quanta of vibration or spin oscillation.



Grow crystals!

Aluminum is transparent – neutrons see inside cryostats, SC magnets, pressure cells and furnaces

Chris Stock aligns UBC YBCO crystals



Quick Summary of Qualitative Behaviour

Bragg peaks are from periodic nuclear or magnetic structure

$$S(\mathbf{Q}) \sim b^2 e^{-2W} \delta(\omega = 0) \Delta(\mathbf{Q} = \boldsymbol{\tau}) \left|\mathrm{F}(\mathbf{Q})\right|^2$$

with Debye-Waller $W = B(T)Q^2$ *and* $\mathrm{Q} = 4\pi \sin(\theta)/\lambda$

One Phonon:

$$S(\mathbf{Q},\omega) = b^2 e^{-2W} \left|\mathbf{Q}\cdot\mathbf{e}(\mathbf{q})\right|^2 \frac{n(\omega)+1}{m\omega_{\mathbf{q}}} \delta(\omega - \omega_{\mathbf{q}}) \Delta(\mathbf{Q} = \boldsymbol{\tau} + \mathbf{q})$$

$$\approx Q^2 \cdot T / {\omega_{\mathbf{q}}}^2$$

Magnetic S(**Q,**ω) ~ n(ω)+1 times

$$f(Q)^2 e^{-2W} \left\{ \left\langle M_{\boldsymbol{\tau}}^{\perp} \right\rangle^2 \Delta(\mathbf{Q} = \boldsymbol{\tau}) \delta(\omega) + \left\langle \delta M_{-\mathbf{Q},\omega}^{\perp} \delta M_{\mathbf{Q},\omega}^{\perp} \right\rangle \right\}$$

$\mathbf{M}^{\perp}$ is component of magnetization **M = L**+2**S** perpendicular to **Q.**

What we detect with the neutron

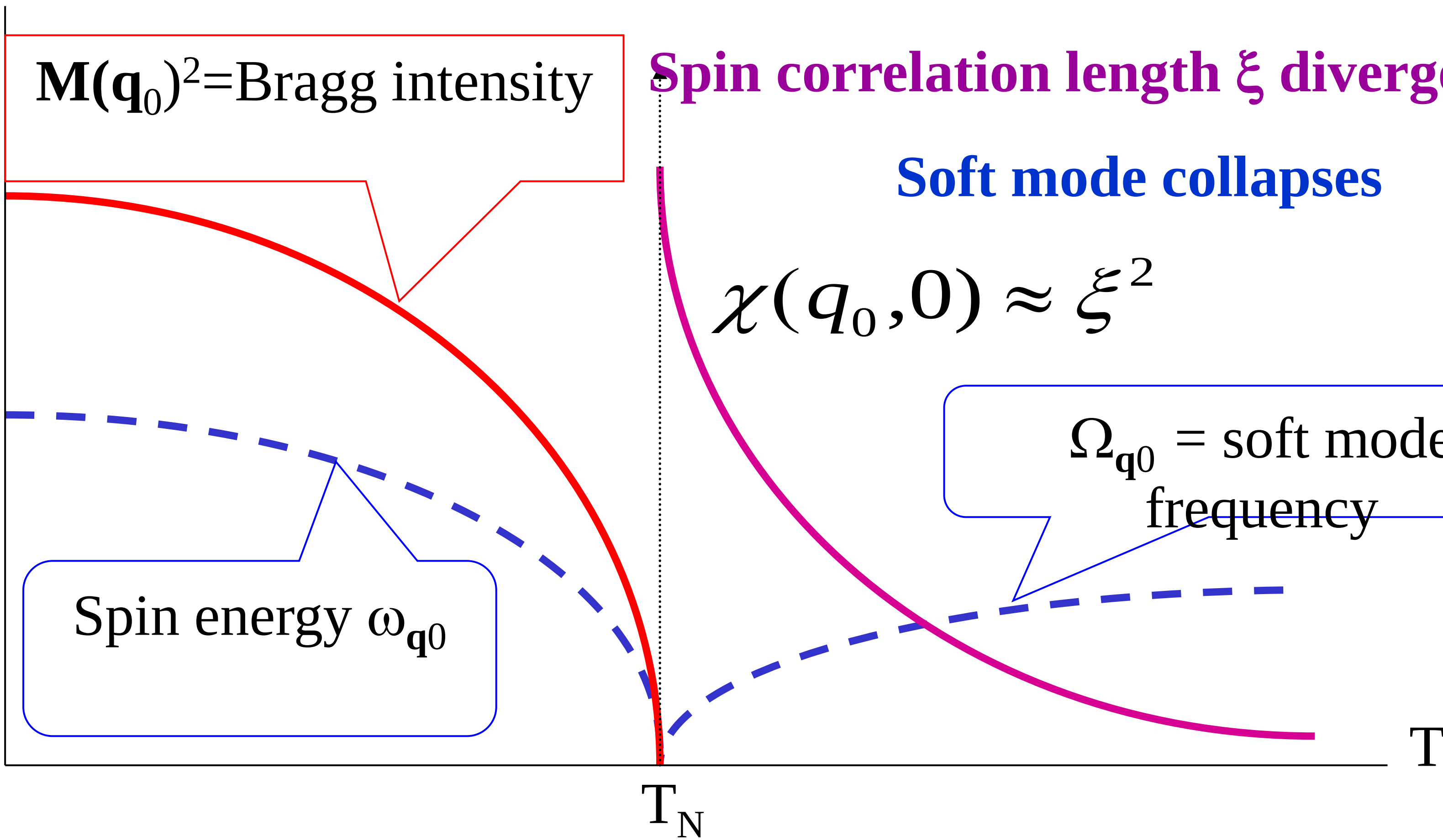
Bragg positions (H,K,L) integer	Symmetry of atomic lattice
Bragg intensities F(H,K,L)	Atom positions in each cell
Sharp elastic peaks non-Bragg	Incommensurate order e.g. Cr
Sharp inelastic peaks	Phonons or spin wave frequency
	- atom-atom interaction strength
Diffuse around Bragg	Disorder (lack of periodicity)
Width in Q of diffuse	Nano scale lengths
Width in frequency of diffuse	-Timescales down to picosecond
	-Relaxation rates
Polarization	Spins – where they point

Near phase transitions at T_N

continuous and second order: soft modes and diverging susceptibility

Condensation of q_0=0 or 2π/a yields a ferromagnet.

Condensation of q_0= ½×2π/a yields an antiferromagnet.



What does neutron scattering tell us about HITC superconductors?

None of the above simple physics of phase transitions applies!

– there are competing order parameters.

Structure

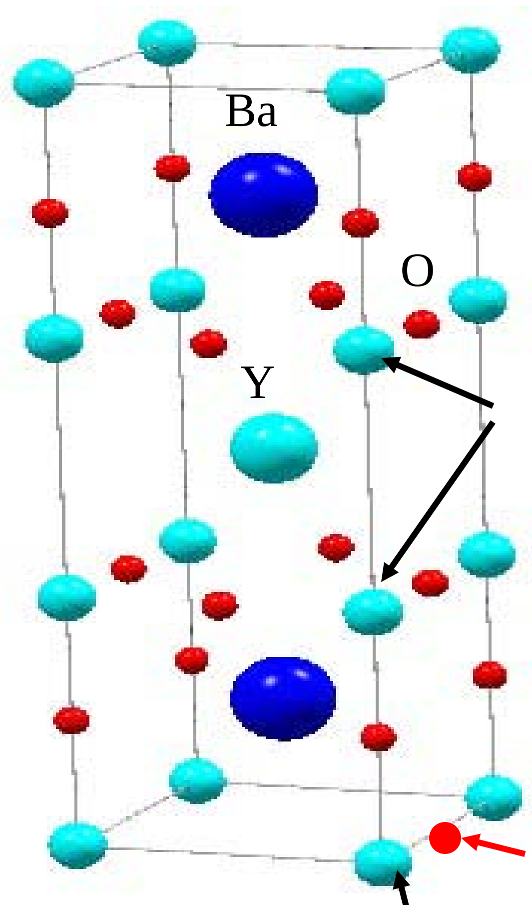
A quantum spin S=1/2 – has only two states

$YBa_2Cu_3O_{6+x}$ contains two CuO_2 planes per unit cell.

Only the **Cu** in the planes are magnetic. For x=0 it is an insulating antiferromagnet.

These CuO_2 bilayers are doped with holes (electrons removed) by doping extra O^{2-} ions in the chains.

The holes destroy the AF order of the Cu spins.

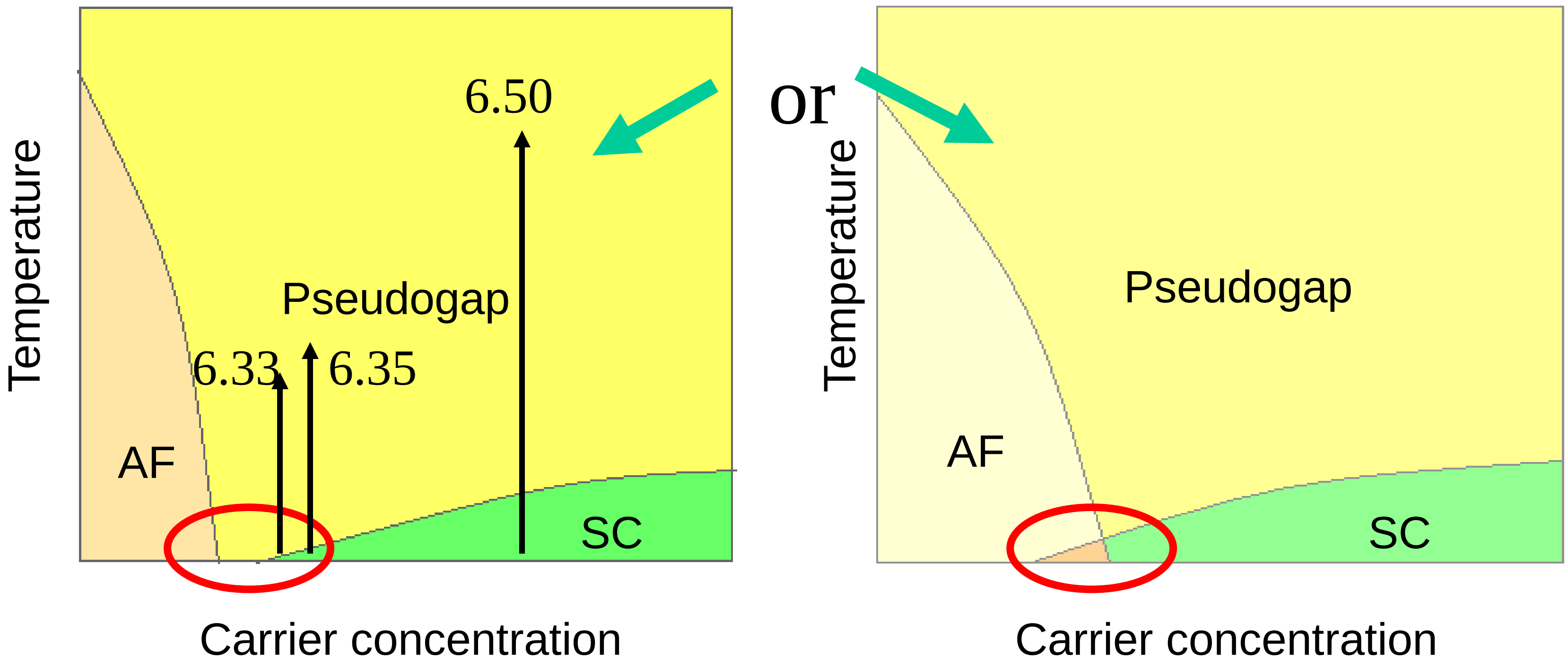


Precursor state to superconductivity

Metallic or insulator? AF order or spin glass?

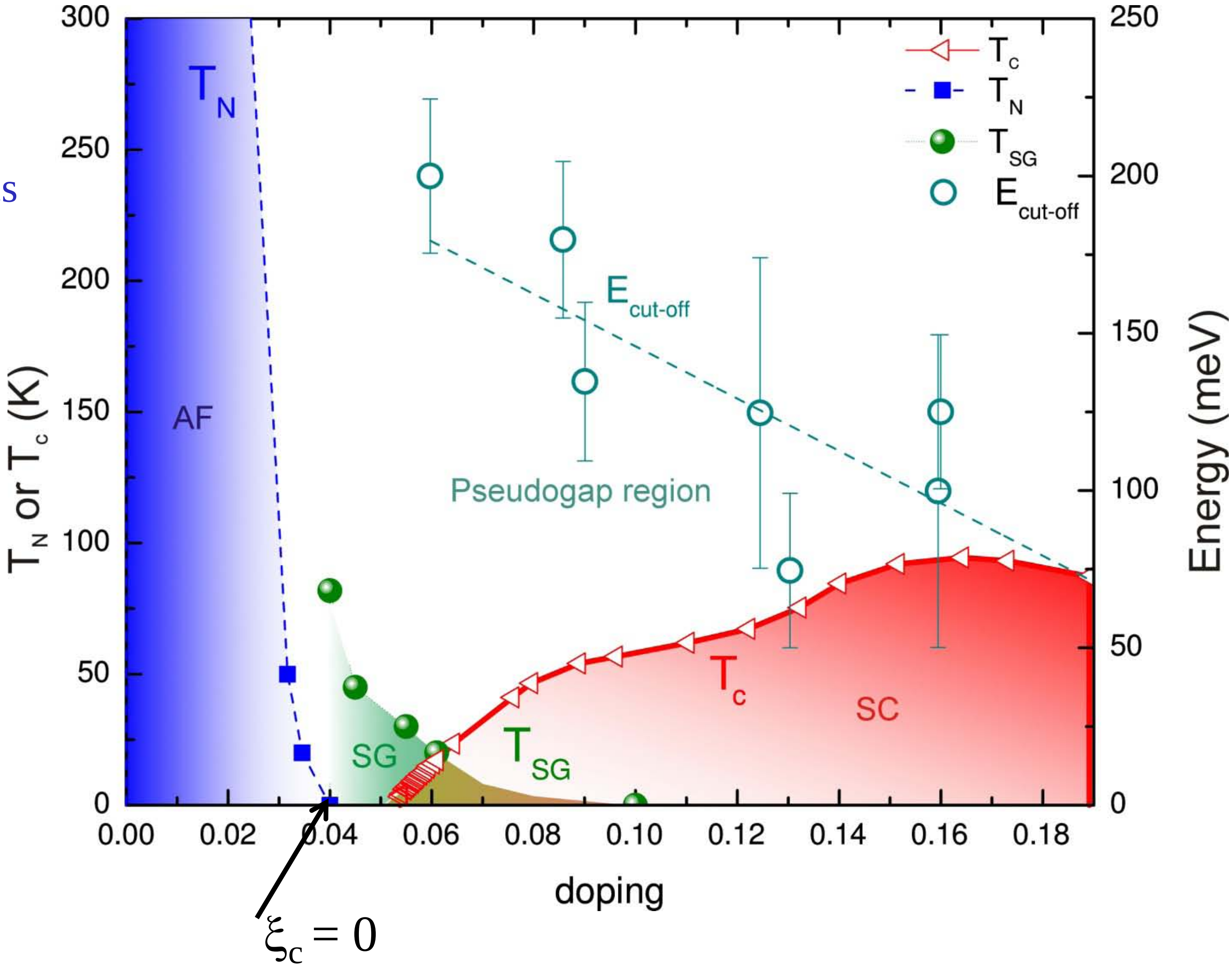
QPT: Are AF and SC states separated, contiguous, or coexistent?

Do holes destroy spins?



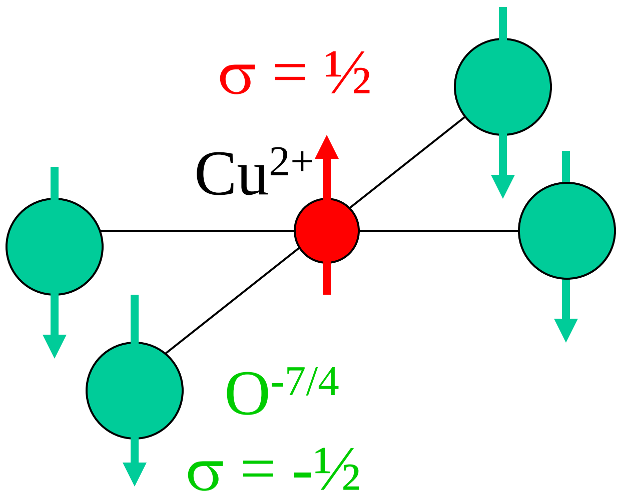
The cuprate phase diagram: $YBa_2Cu_3O_{6+x}$

Yamani and Buyers, Can J. Physics 2011



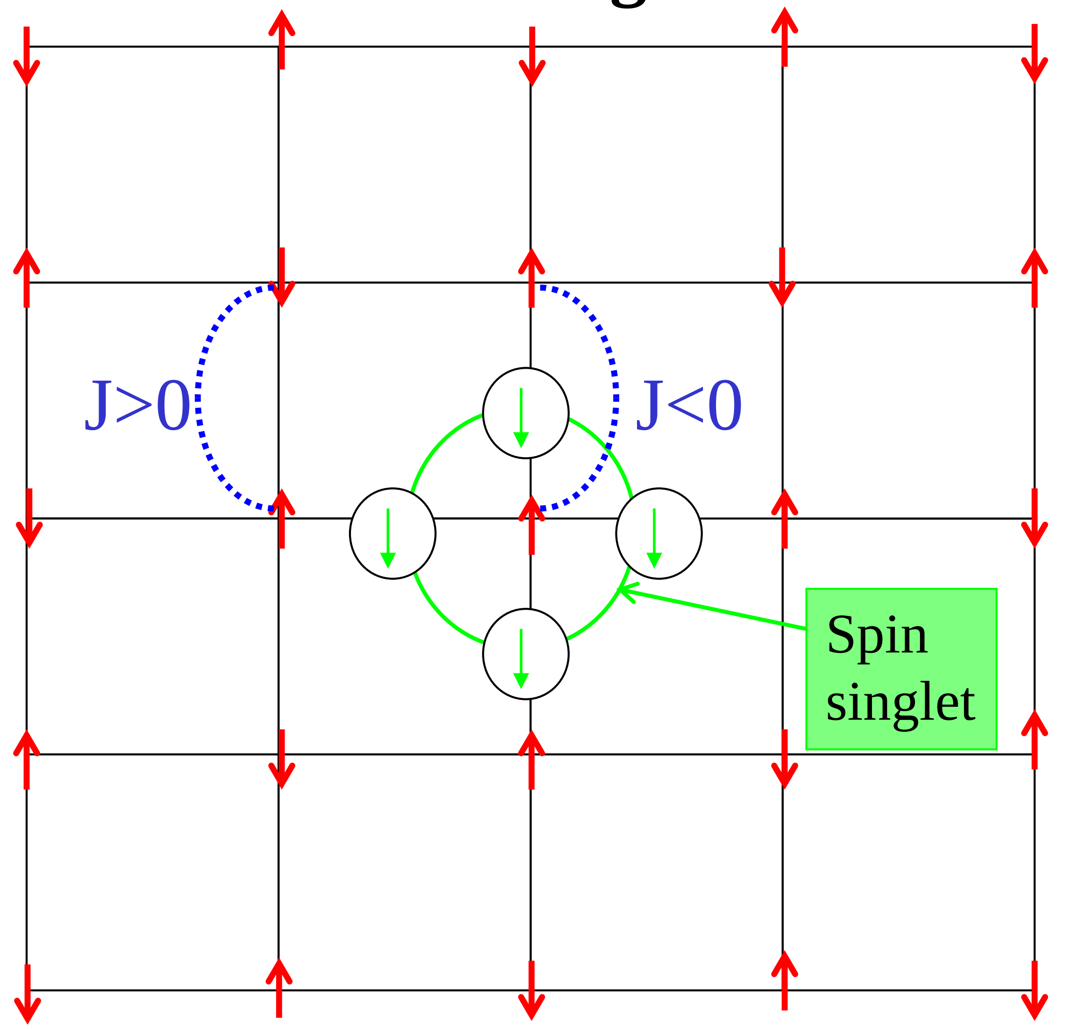
Singlet formation destroys order

Hole on O puts $Cu\text{-}O_4$ into singlet state.



AF order destroyed at low doping p < 4% because each hole affects ***many*** sites

Holes cause **ferromagnetic bonds**.



Spin spectral map x=6.5 – damped spin waves AF

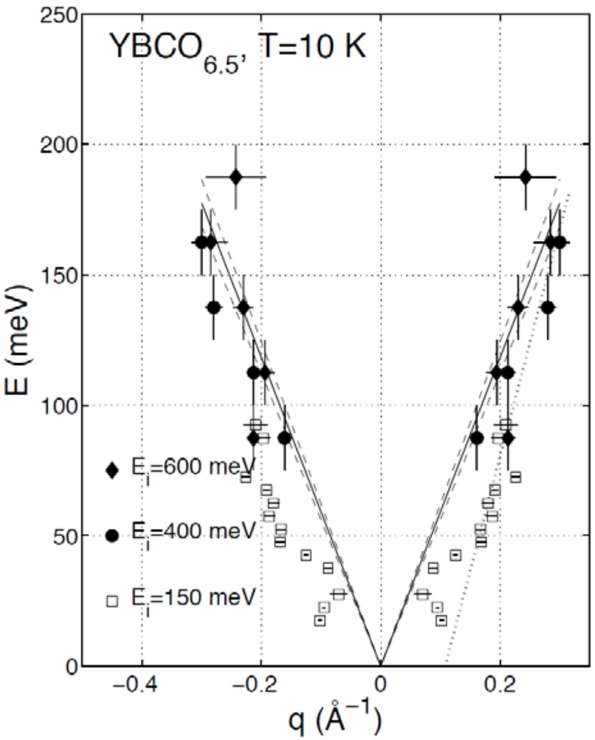
$YBCO_{6.5}$

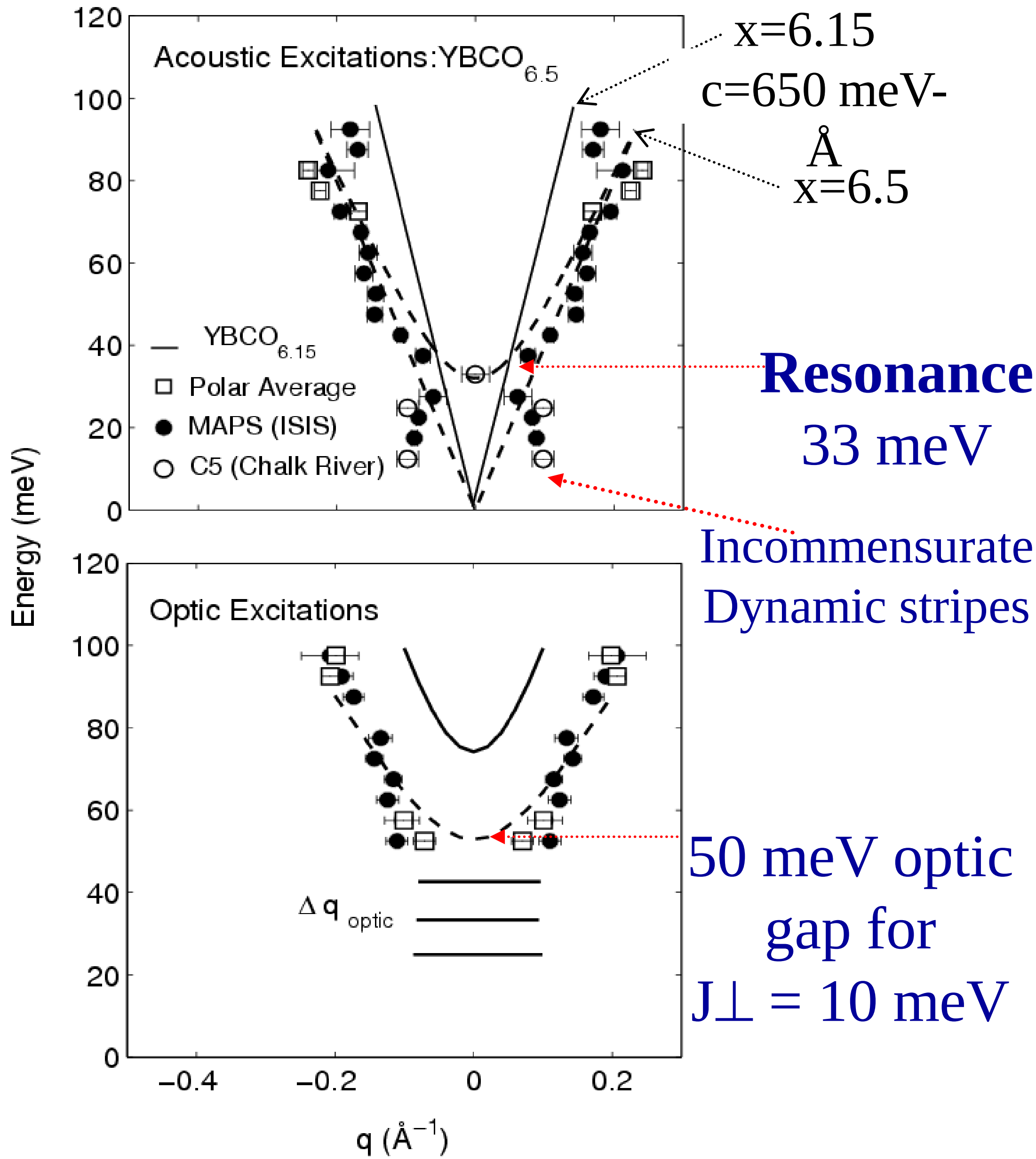
E increases with **q**

E = cq

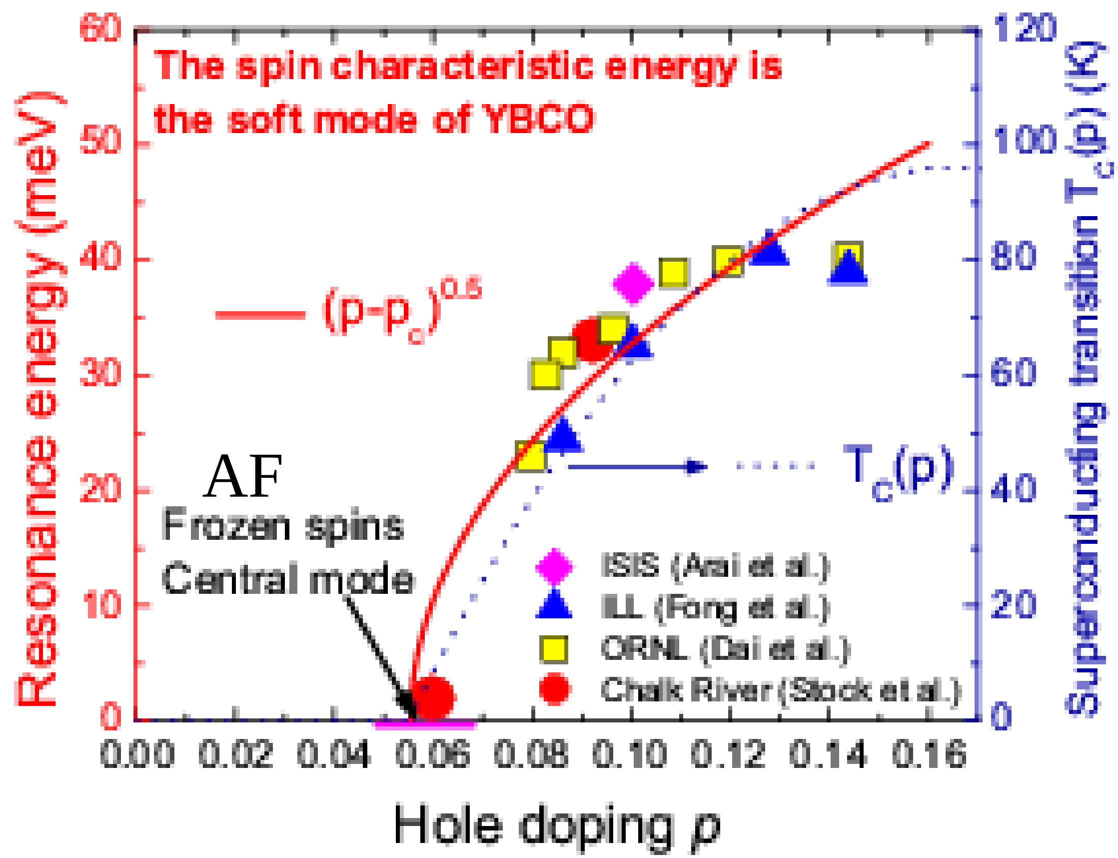
Stripes at low energy

Total moment² conserved S(S+1).



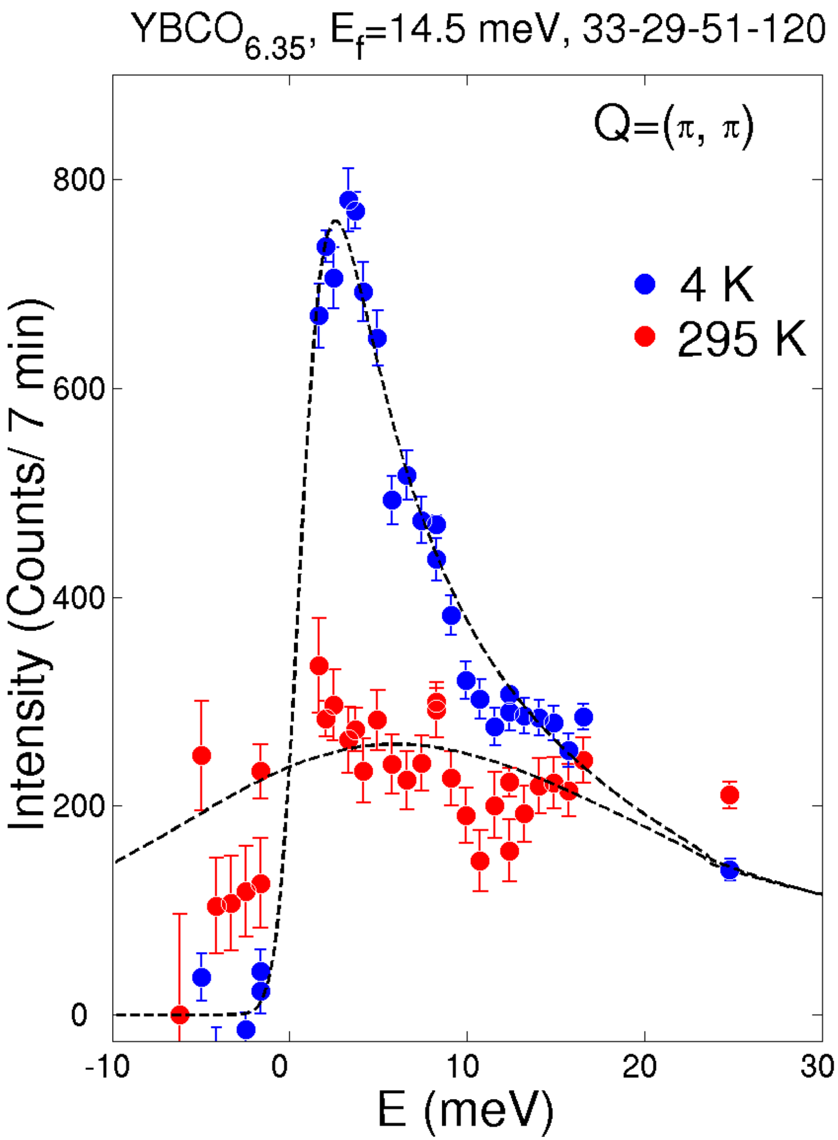


For large doping the resonance energy *looks* like ***the soft-mode*** of the SC phase – but is not. Below p ~ 0.08 there is a metal to insulator transition and ***no*** resonance. The spin oscillations collapse for lower doping to give an intense **central mode**. Is it critical at p_c?

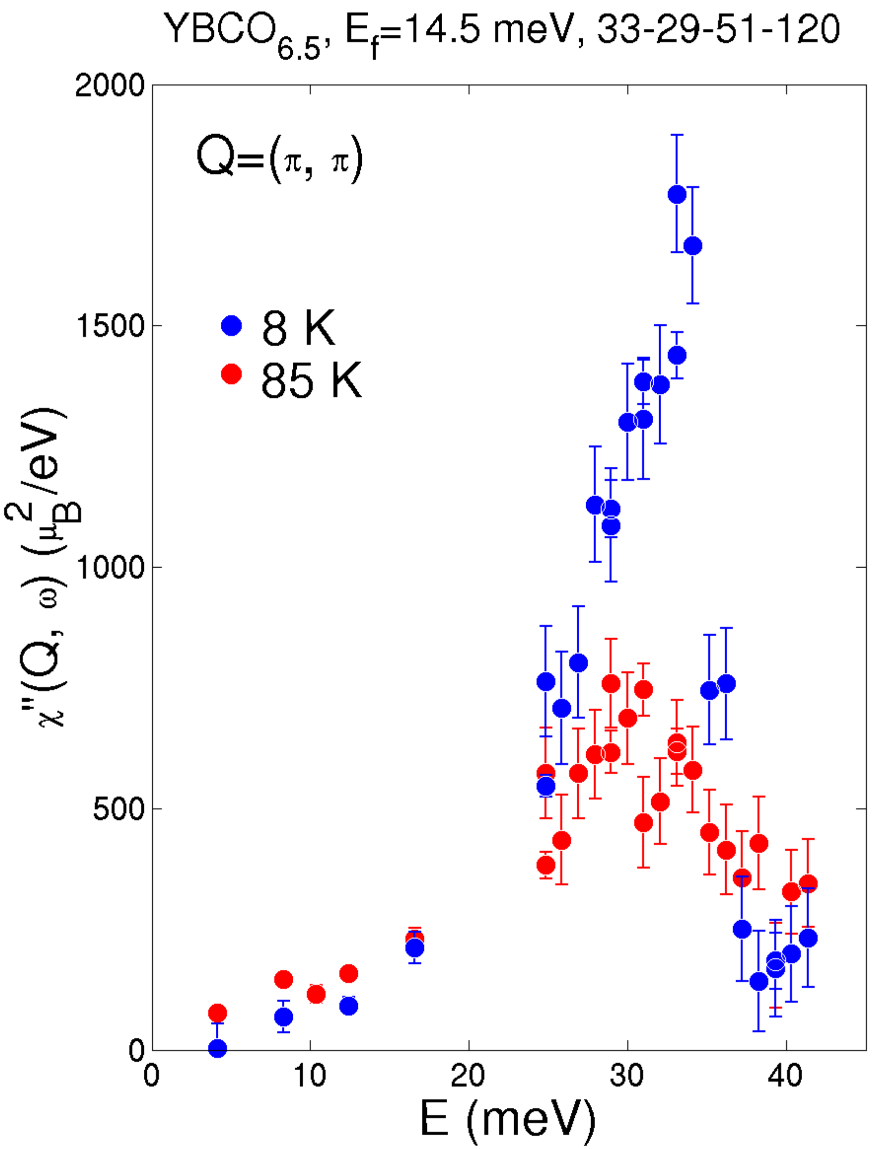


Approach to SC boundary: Spectrum for x=6.35 and 6.5

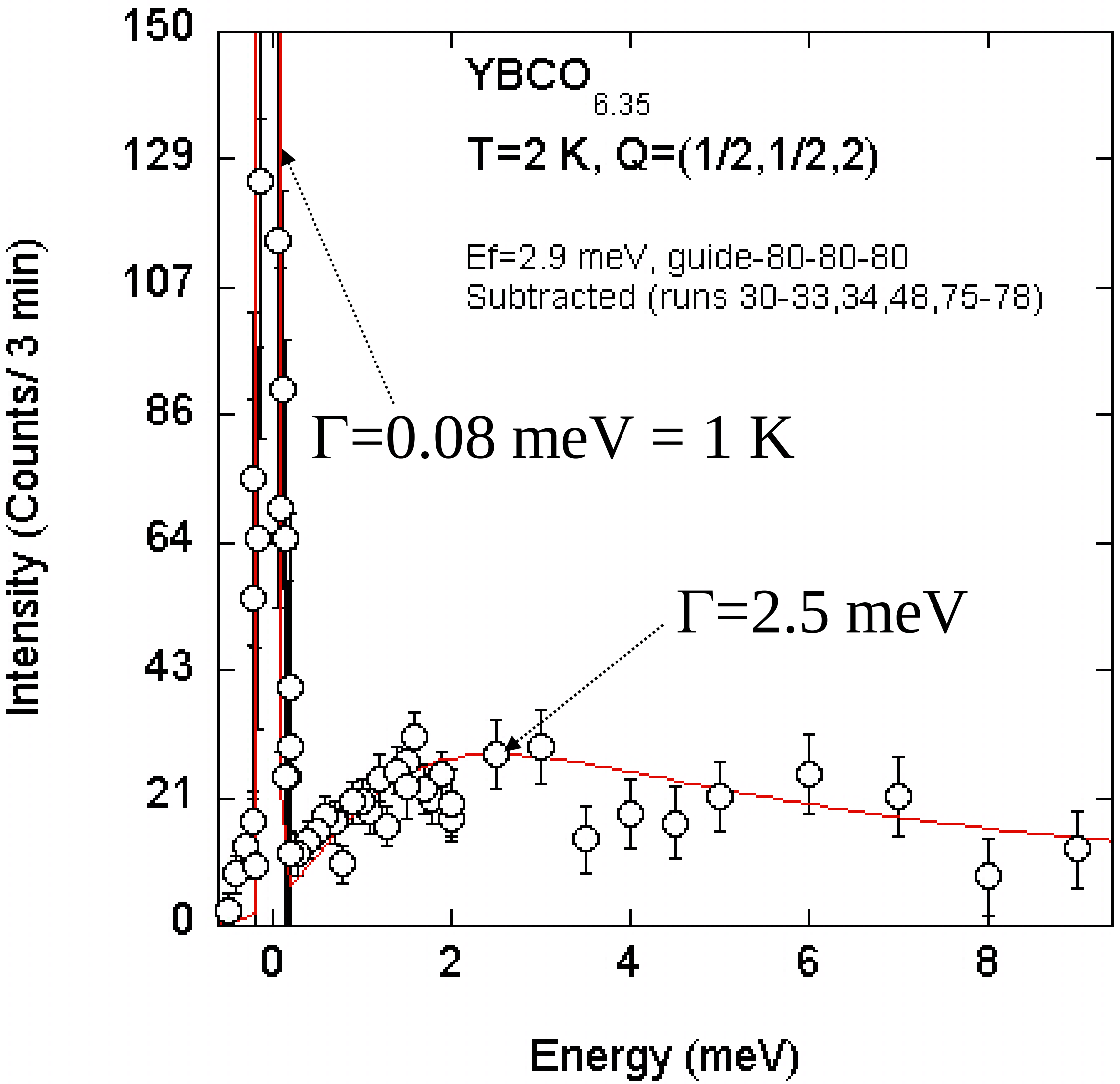
T_c=18 K   3 meV   'insulator'



T_c=59 K   33 meV   'metallic'



Two energy scales - a new lower energy scale:
a **central mode**: 30 times lower energy & 150 times stronger.



Two energy scales:

• Central Peak

< 0.08 meV

• Damped excitations

2.5 meV

•They are coupled

Spin structure: commensurate
Elastic scattering

No break at T_c.

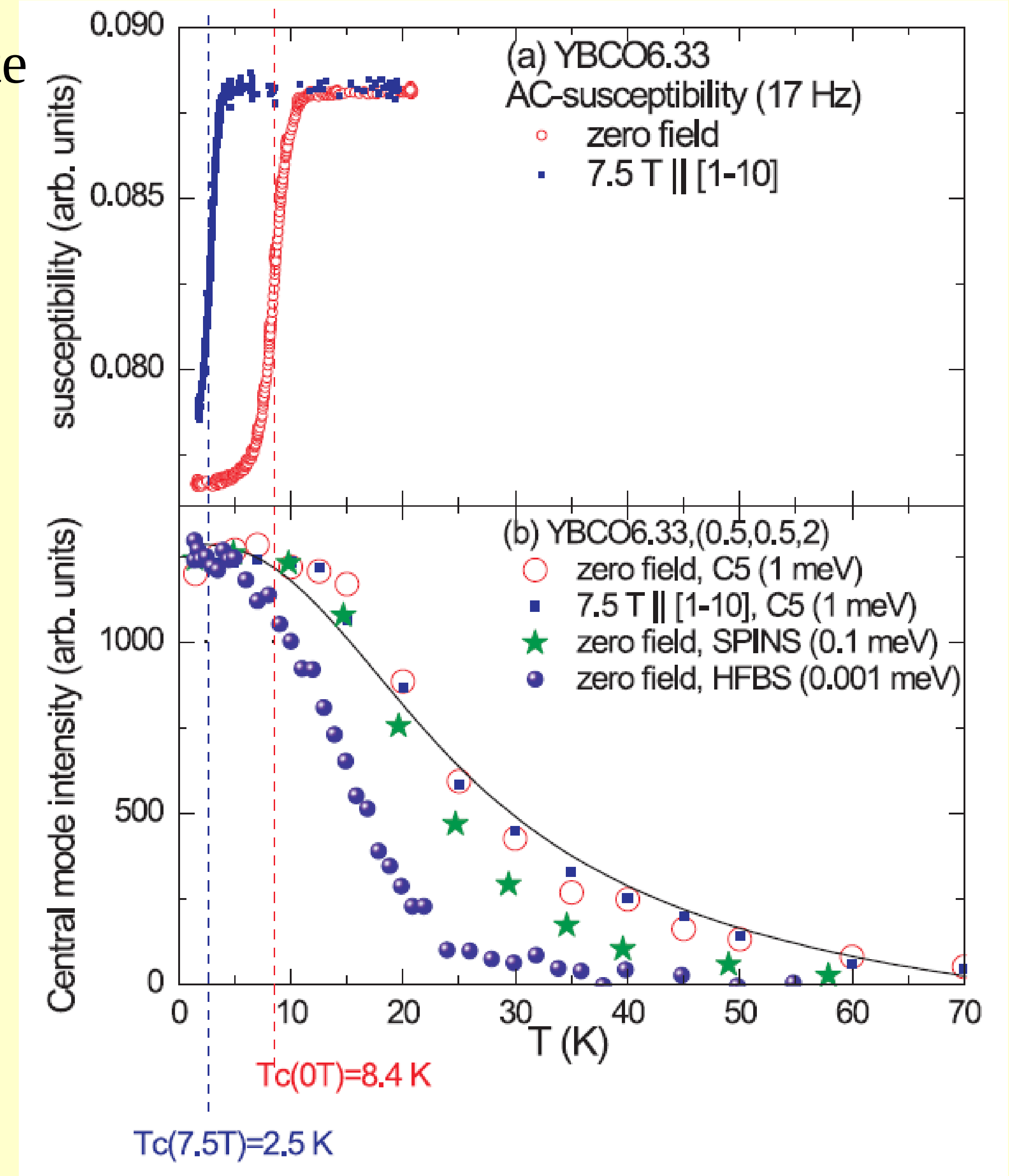
Spins and charged SC pairs

evolve **independently**.

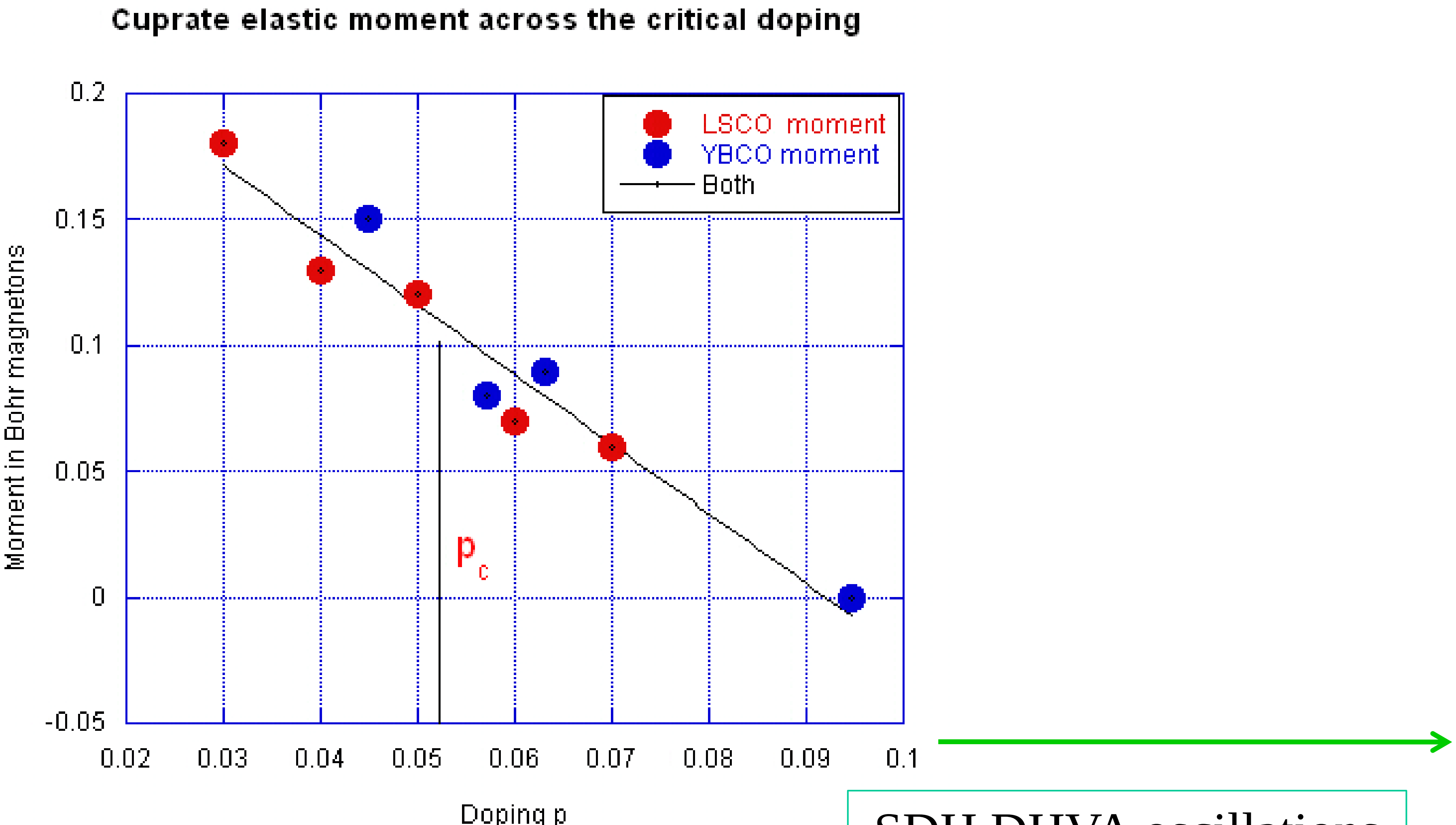
No spin stripes.

Conclude that superconductivity does not require stripes nor a resonance

Do spins still pair the charges?



Yamani *et.al* tbp 2011 YBCO6.33 YBCO6.35 Stock *et.al* 2008



No oscillations – ‘insulating’

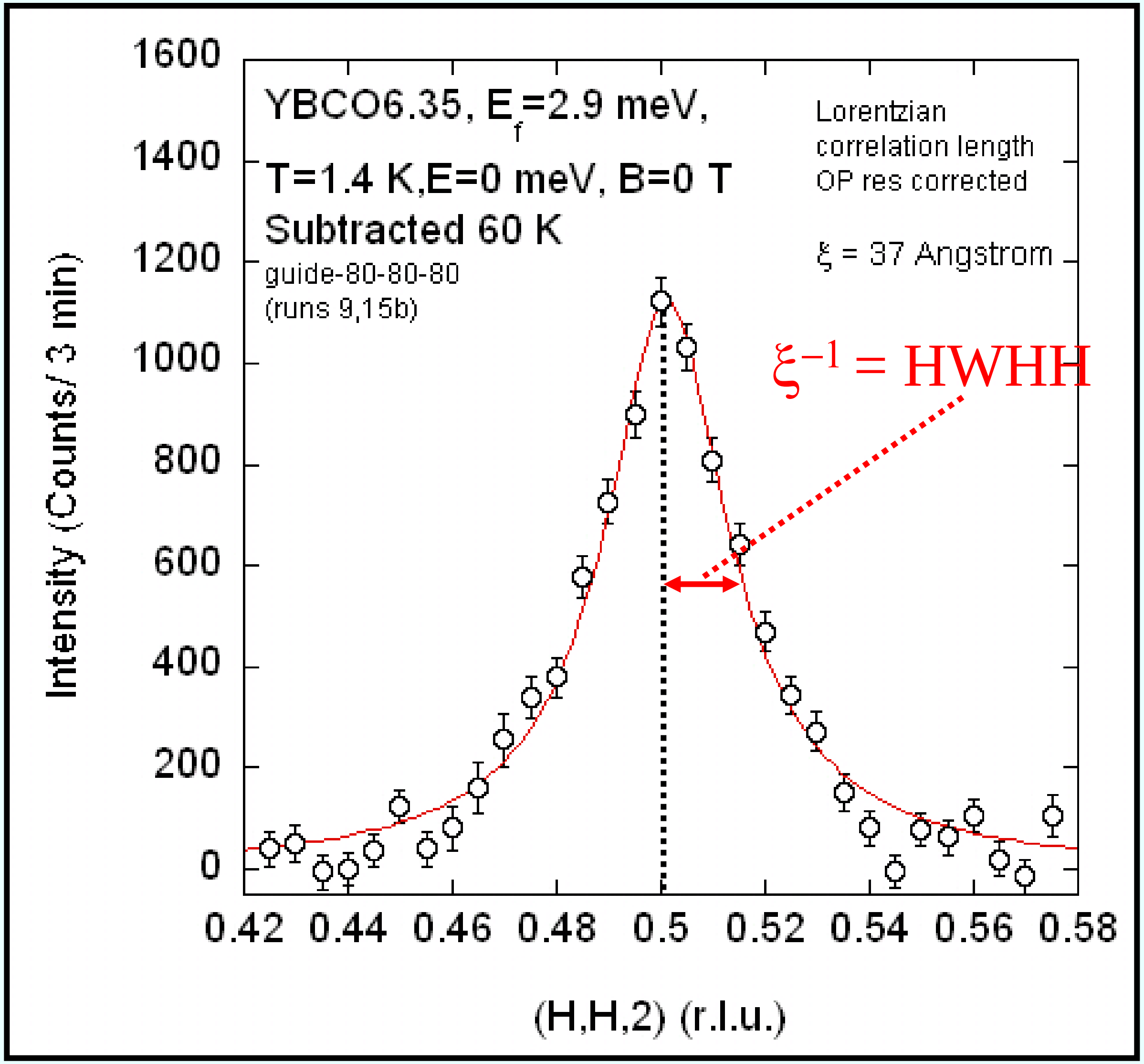
For p < 0.8

SDH DHVA oscillations – fermi surface orbits ‘metallic’

Neutrons measure **nanoscale** lengths with ease!

The elastic scattering shows the spins are correlated over 37 Å or ~10 cells in-plane.!

Spin frustration.



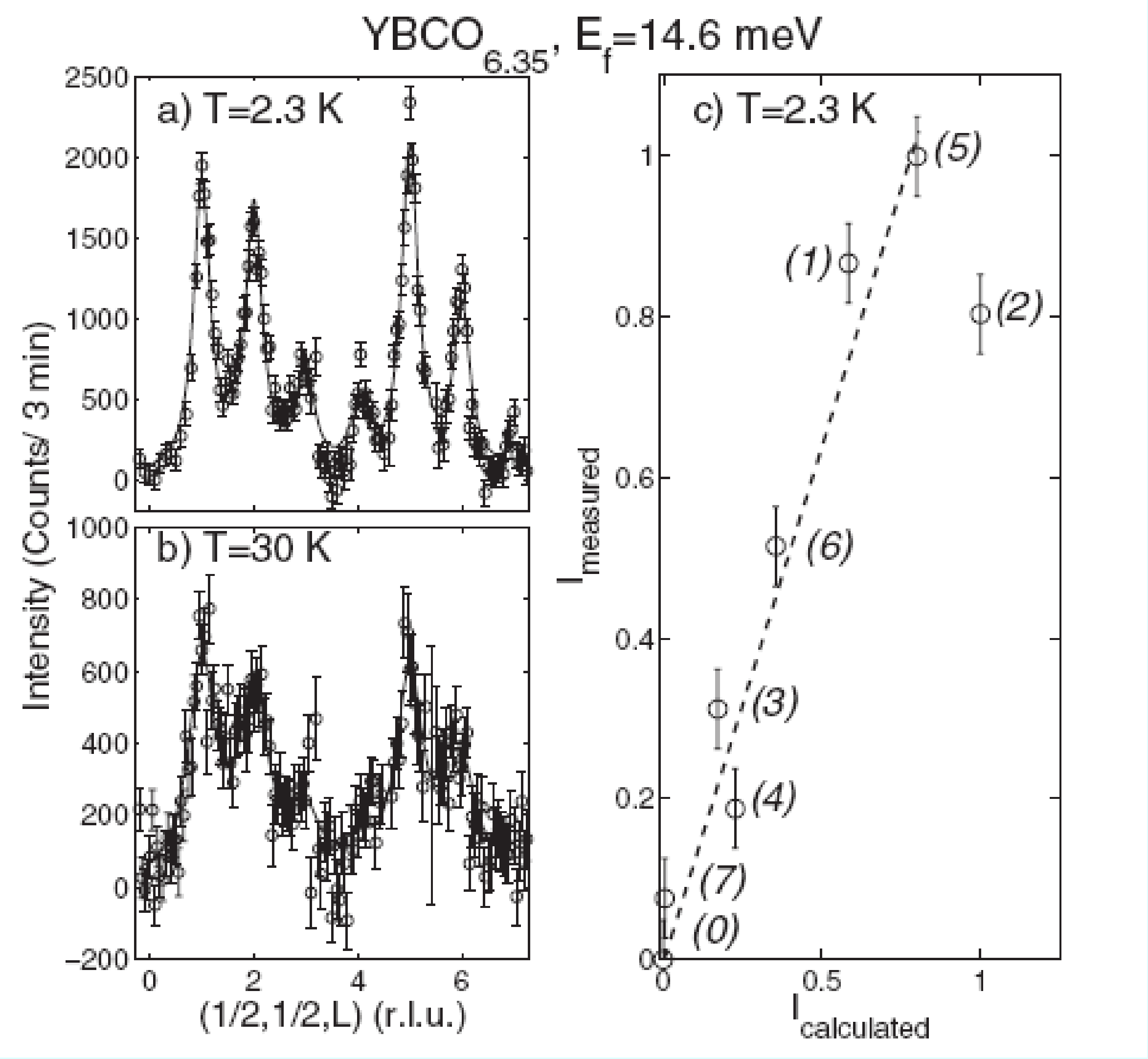
Correlations **between** cells along c axis extend over only

ξ= 1 cell = 12 Å

for T_c = 18 K.

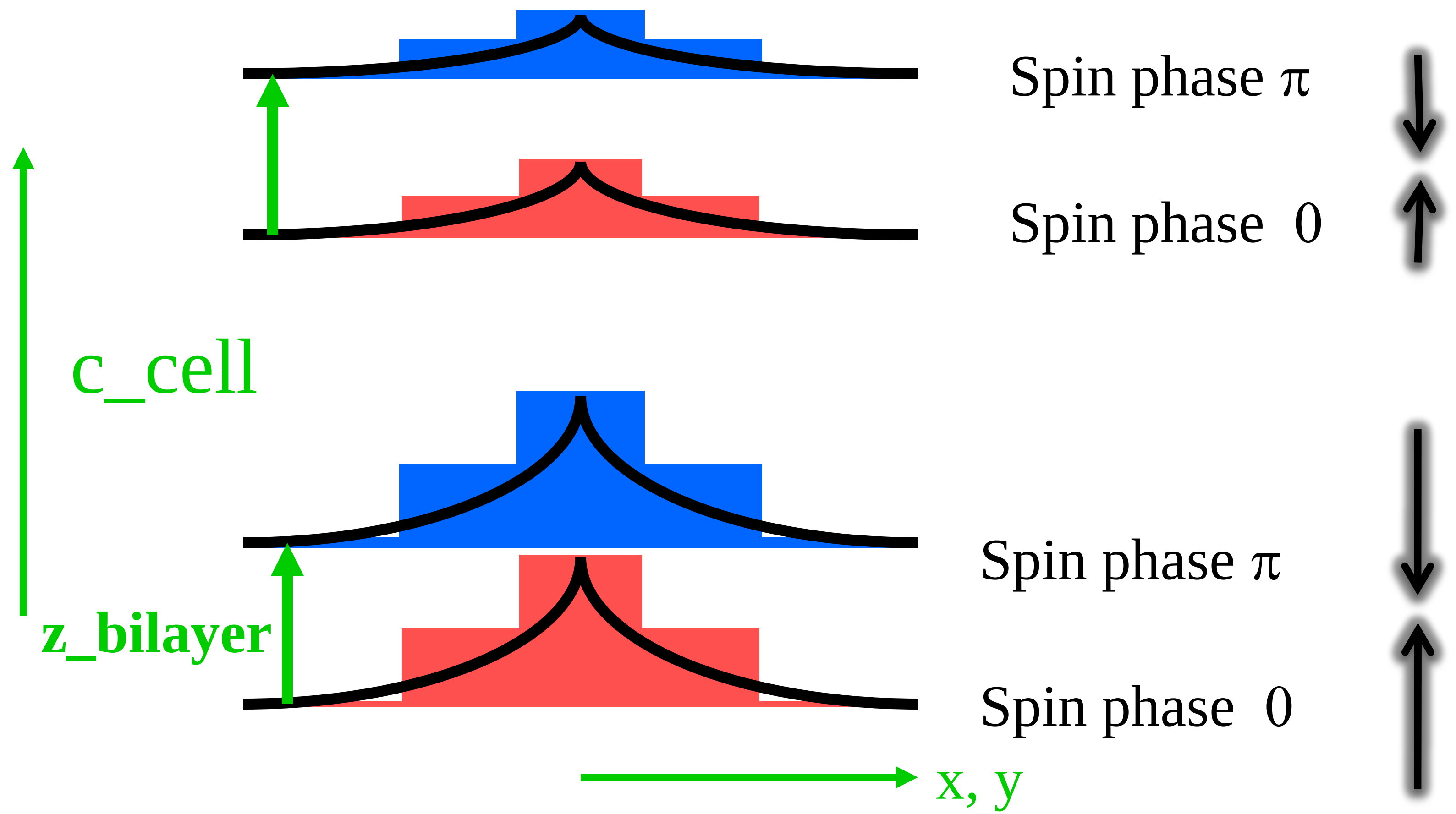
The spins are antiparallel in each bilayer and in-phase between cells.

Frustrated phase transition nearly critical



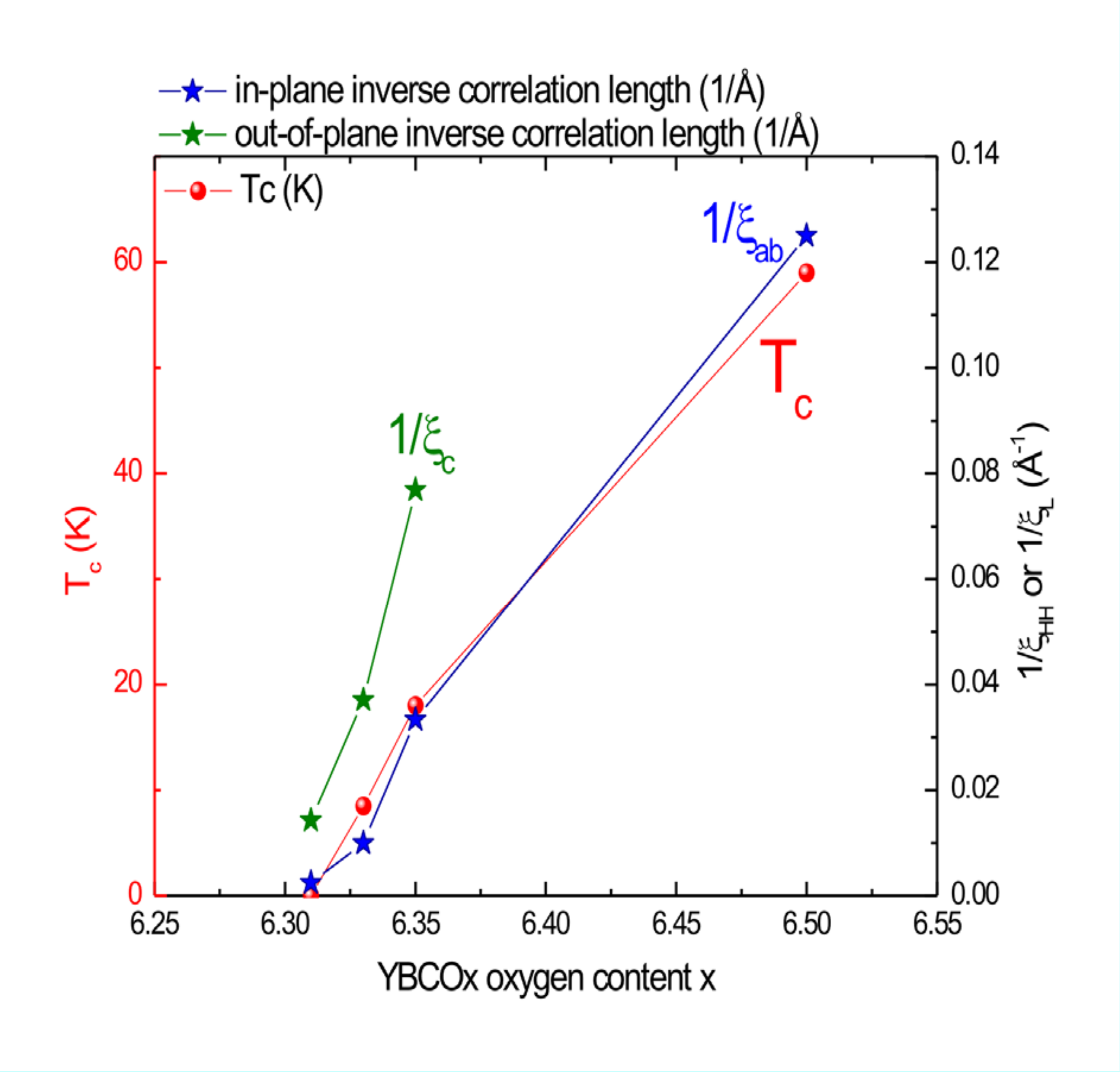
Stock *et.al* Phys Rev **B 77**, 104513 2008

Bilayer remains AF coupled.
Spin islands are aligned along c



Approaching a quantum phase transition: the T→0 correlation length in $YBCO_{6+x}$

The correlation lengths track T_c



Anisotropy: hence far from universality near AF QCP.

What is the role of **the pseudogap**?

Energy below which the charge spectrum is suppressed – and the spin fluctuation is a collective mode.

Spins may be ***damped*** by conduction density and their peaks disappear.

e.g. Landau damping of spins in metals

Spin waves ***die*** above the pseudogap energy

Do spin waves 'bore a hole' in the weak conduction band as it forms gradually with doping?

Spins survive at low doping.

At large doping, charges destroy collective spin waves.

Stock *et al* 2010 PhysRev B17

Grey points from Hufner & Sawatsky Rep Prog Phys 2008

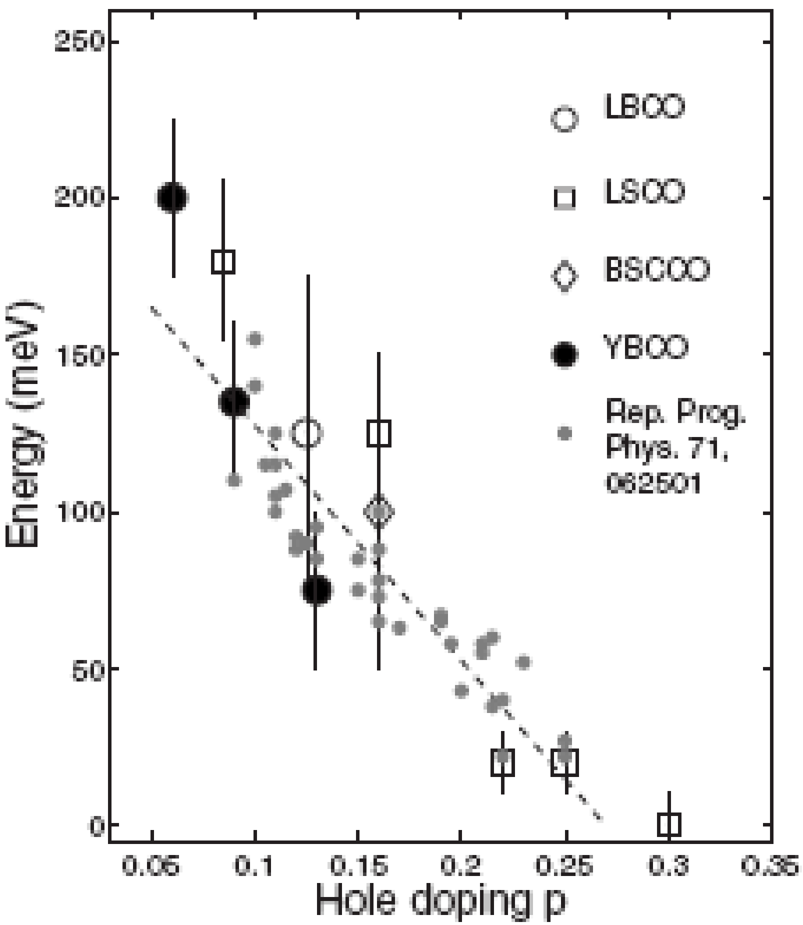
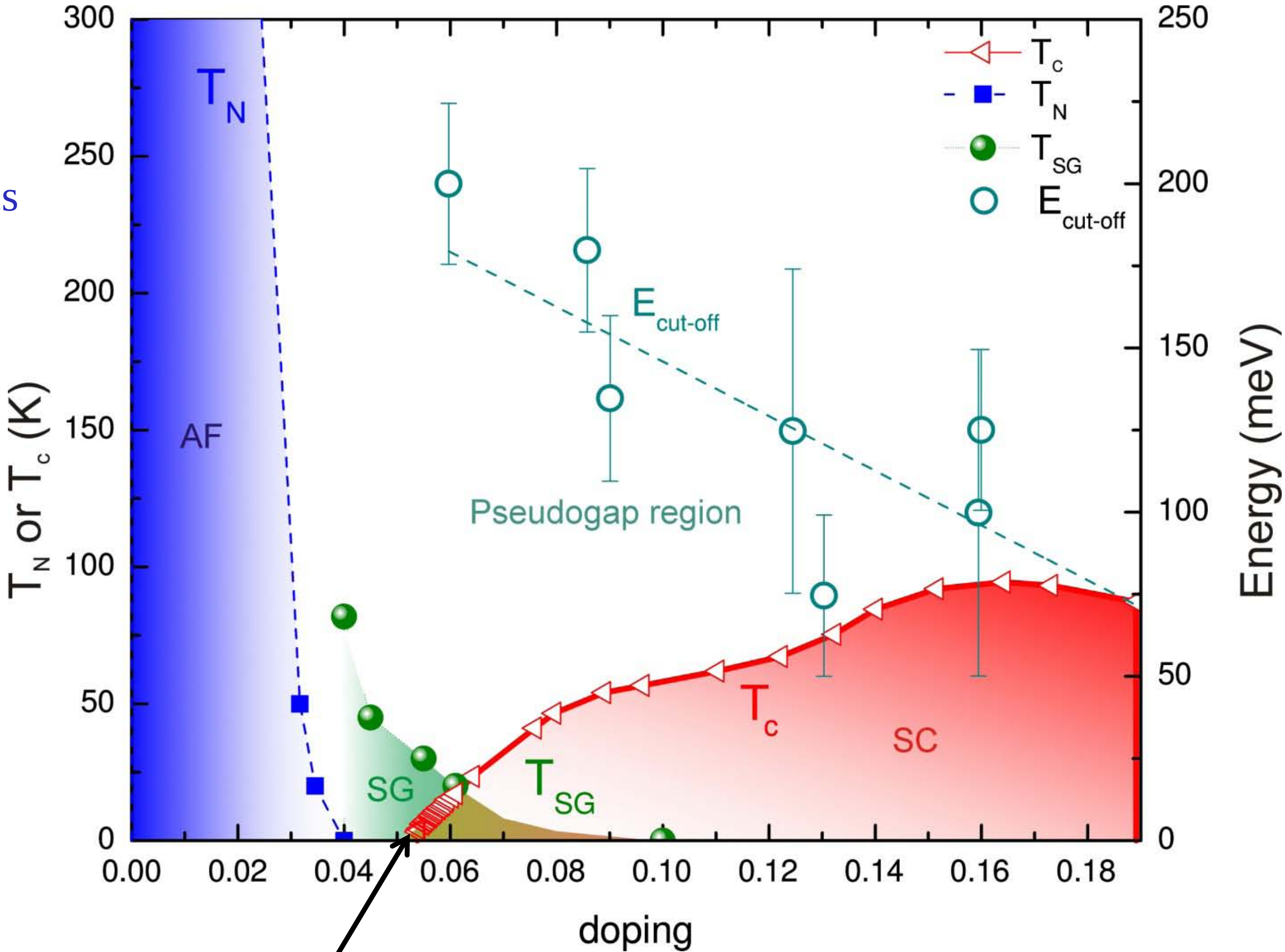


FIG. 6. A summary of the energy value at which the momentum-integrated susceptibility $[\chi''(\omega)]$ falls to half the value predicted by spin-wave theory (taken to be 1.75 $\mu_B^2/eV \times 1/2$ =0.88 μ_B^2/eV per copper spin) for a variety of hole doped cuprate materials. The light gray symbols are taken from a variety of techniques and summarized in Ref. 65.

The cuprate phase diagram: $YBa_2Cu_3O_{6+x}$

Yamani and Buyers, Can J. Physics 2011



ξ_c = large: strong pairing force, few carriers

Neutrons can reveal the space and time scales of the nascent superconductor – and of most other materials.

Neutron beams are an ***essential tool*** in the armory of a materials scientist.