Spin correlations in $YBa_2Cu_3O_{6+x}$ bulk vs. interface

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outline

new quantum states in bulk?

yes, good evidence for electronic nematic phase

new quantum states at interface?

first step: understand, manipulate carrier concentration

Hwang *et al*., Millis *et al*., Mannhart *et al*., …

second step: understand, manipulate orbital occupation

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Collaborators: Bulk YBCO

neutron scattering	
V. Hinkov, D. Haug	MPI Stuttgart
B. Fauqué, Y. Sidis, P. Bourges	CEA Saclay
C.D. Frost, T.G. Perring	ISIS
A. Ivanov	ILL Grenoble
μSR	
C. Bernhard	Univ. Fribourg
samples	
D.P. Chen, C.T. Lin	MPI Stuttgart

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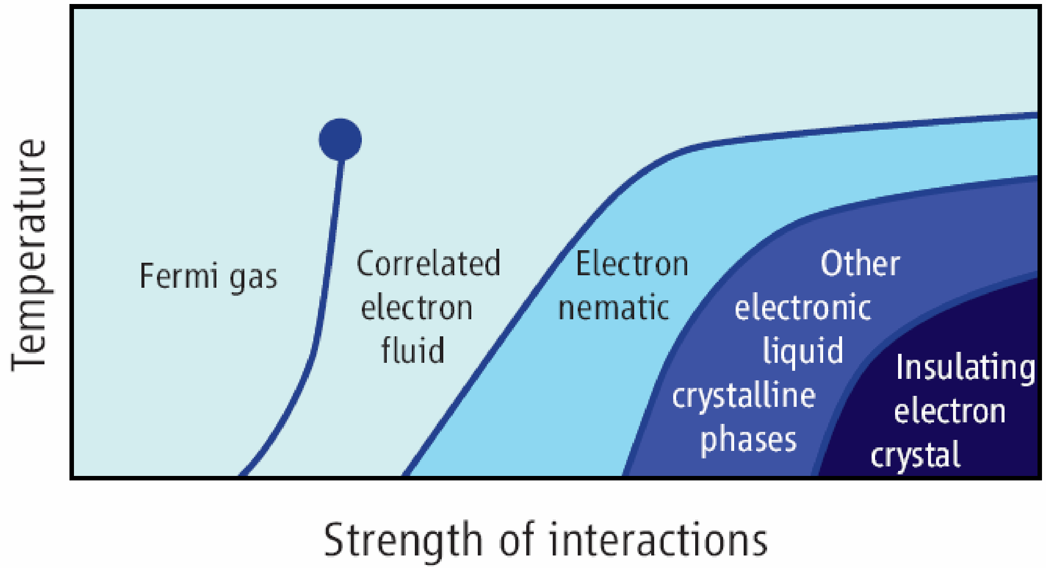
Motivation: electronic liquid crystals ?

electronic nematic phase

- fourfold rotational symmetry spontaneously broken
- translational symmetry unbroken

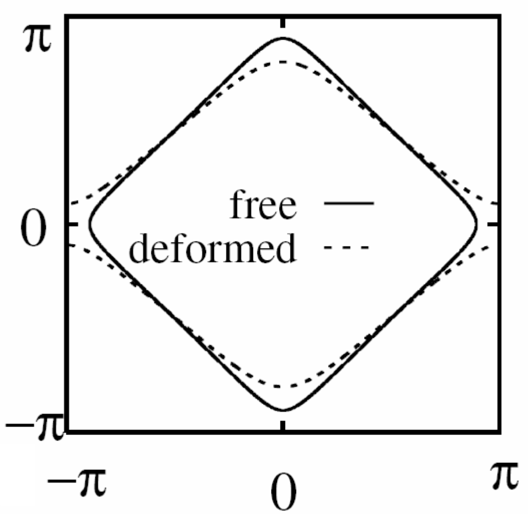


Kivelson et al., Nature 1998

Pomeranchuk instability

in weak-coupling renormalization group calculations
$\rightarrow$ spontaneous formation of open Fermi surface

Halboth & Metzner, PRL 2000

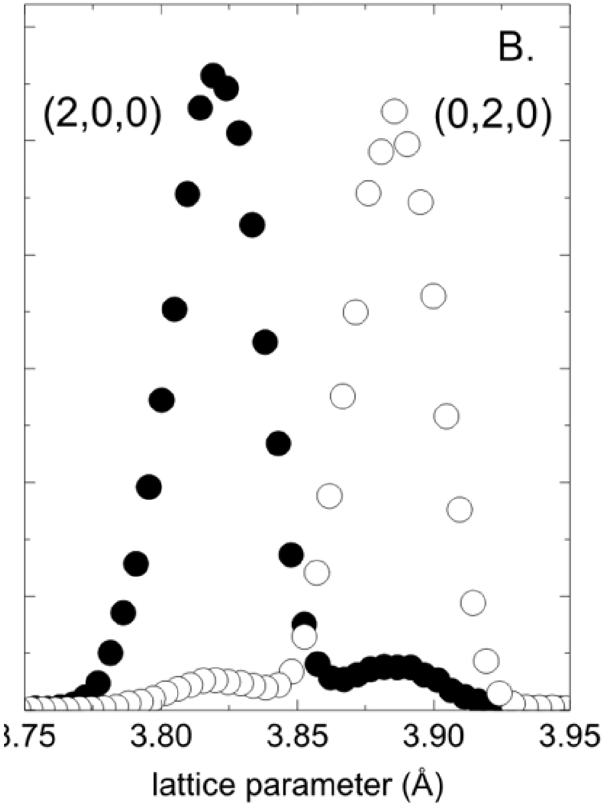


YBCO samples for neutron scattering

- arrays of ~ 200 small single crystals
- individually characterized
- total mass ~ 2g

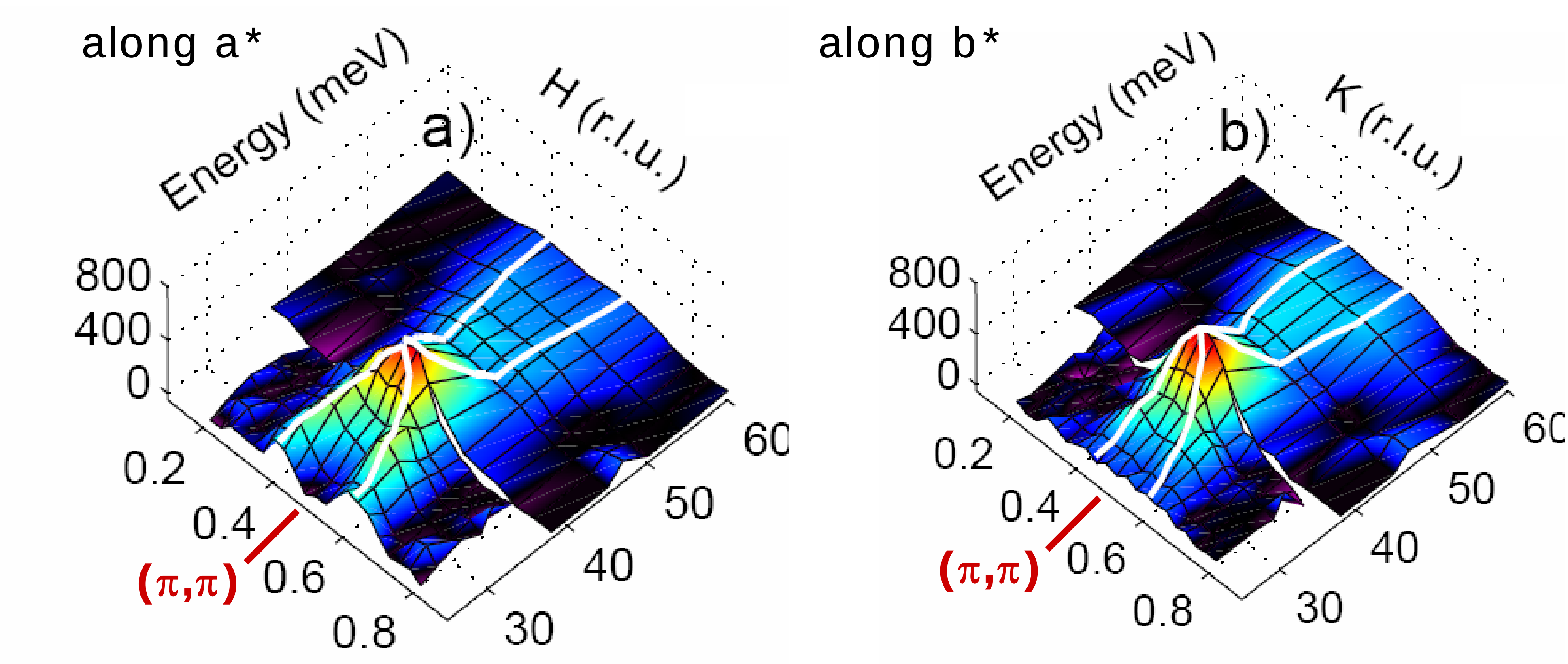
Hinkov et al., Nature 2004

- no impurity phases
- sharp superconducting T_c
- nearly perfectly detwinned



$YBCO_{6.6}$ spin dynamics below T_c

untwinned $YBCO_{6.6}$ (T_c = 61K)



two-dimensional “hour glass” dispersion

also seen in $YBCO_7$ and other high-T_c cuprates

Hinkov et al.,
Nature 2004
Nature Phys. 2007

für Festkörperforschung

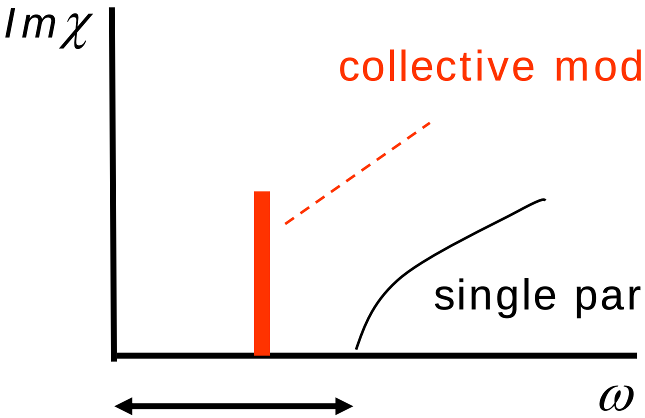
Spin exciton model

simplest formalism: RPA

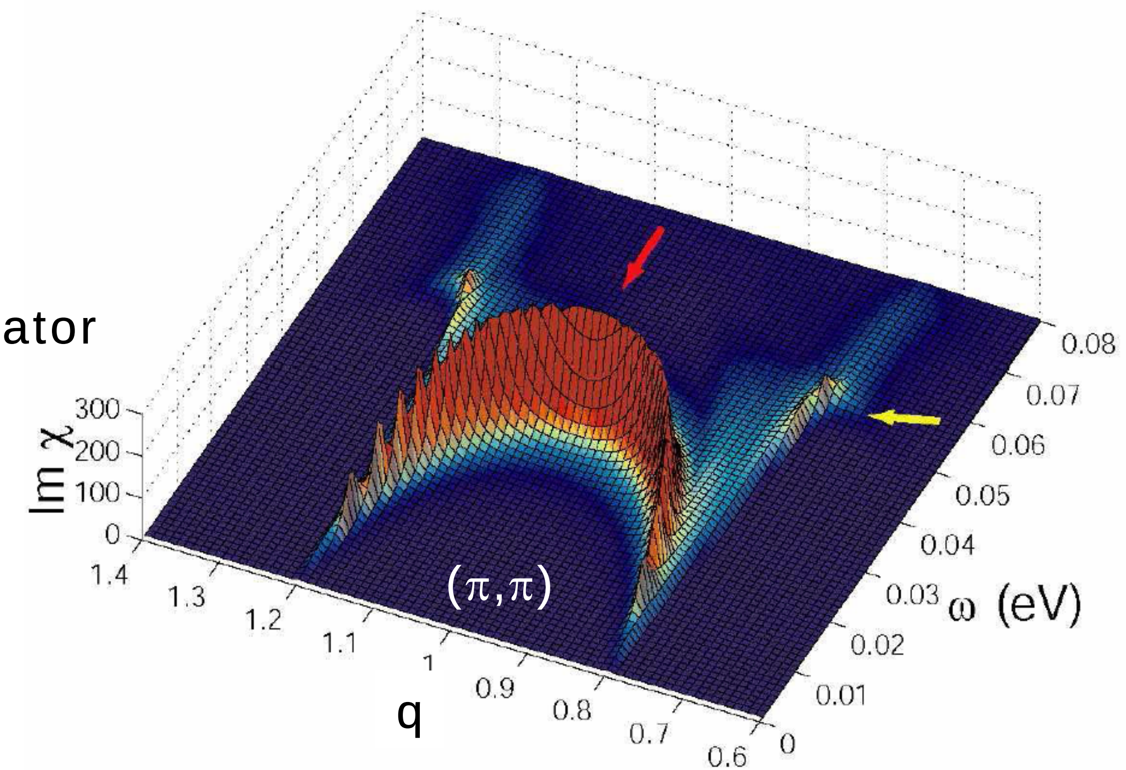
$$\chi(\mathrm{q},\omega) = \frac{\chi_0(\mathrm{q},\omega)}{1 - J(\mathrm{q})\ \chi_0(\mathrm{q},\omega)}$$

J(q) antiferromagnetic

amplitude ~ 100 meV, as in AF insulator



reproduces "hour glass" dispersion



Eremin et al., PRL 2005

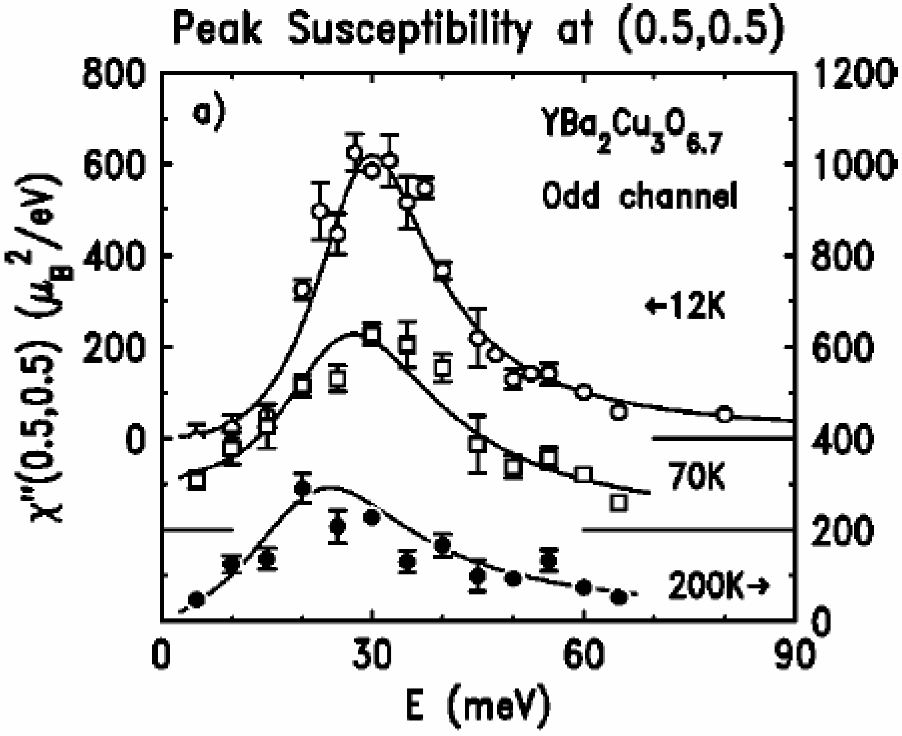
see also:

- many other RPA calculations
- memory-function approach

$YBCO_{6.6}$ spin dynamics in pseudogap state

prevailing wisdom

incoherent precursor of superconducting state

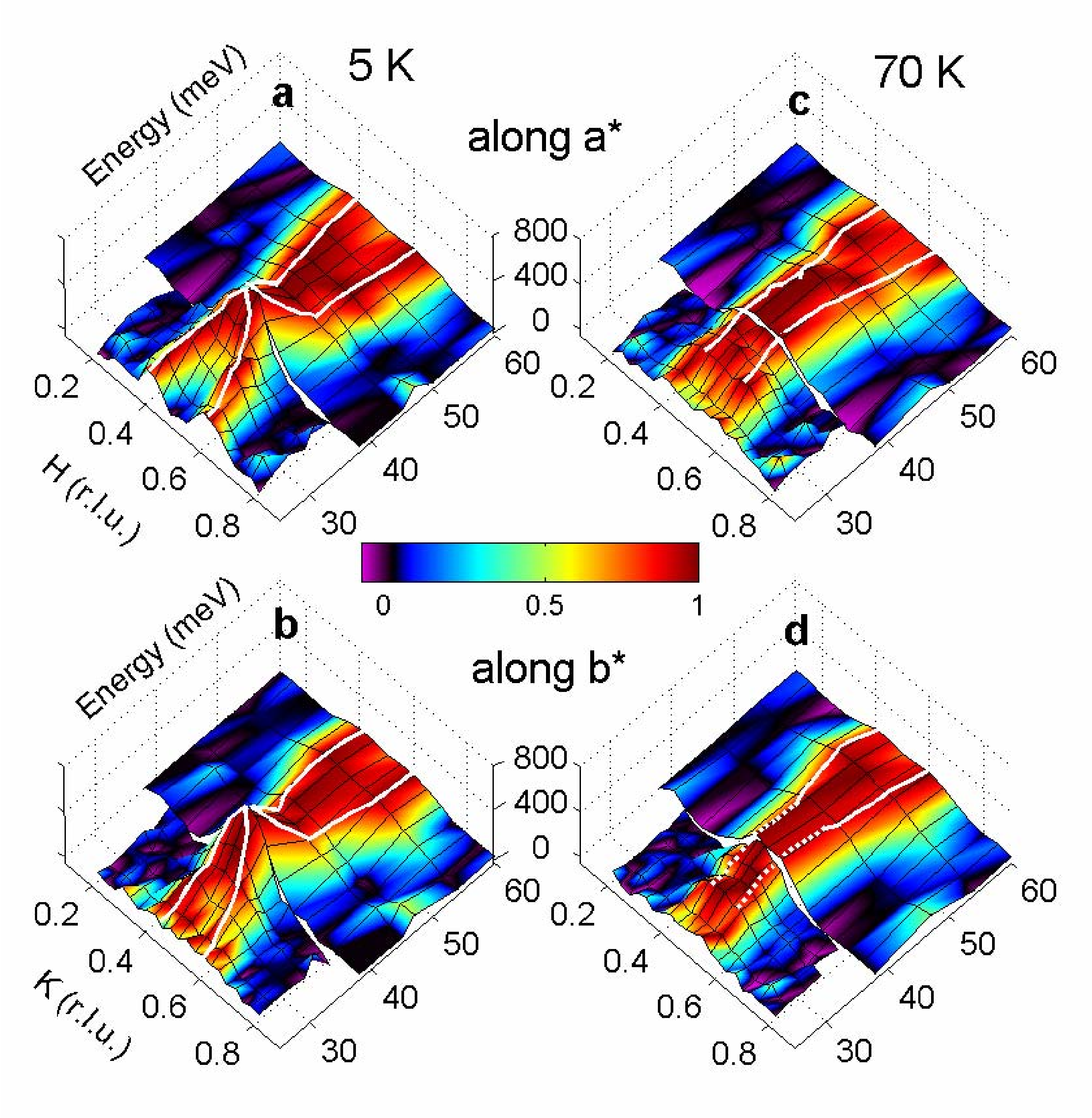


Fong et al., PRB 2000

new measurements on untwinned crystals

qualitative difference between superconducting and pseudogap states

$YBCO_{6.6}$ spin dynamics in pseudogap state



superconducting state

- "hour glass" dispersion
- many aspects described by RPA

pseudogap state

- "hour glass" replaced by "vertical" dispersion
- large in-plane anisotropy not described by RPA

Hinkov et al., Nature Phys. 2007

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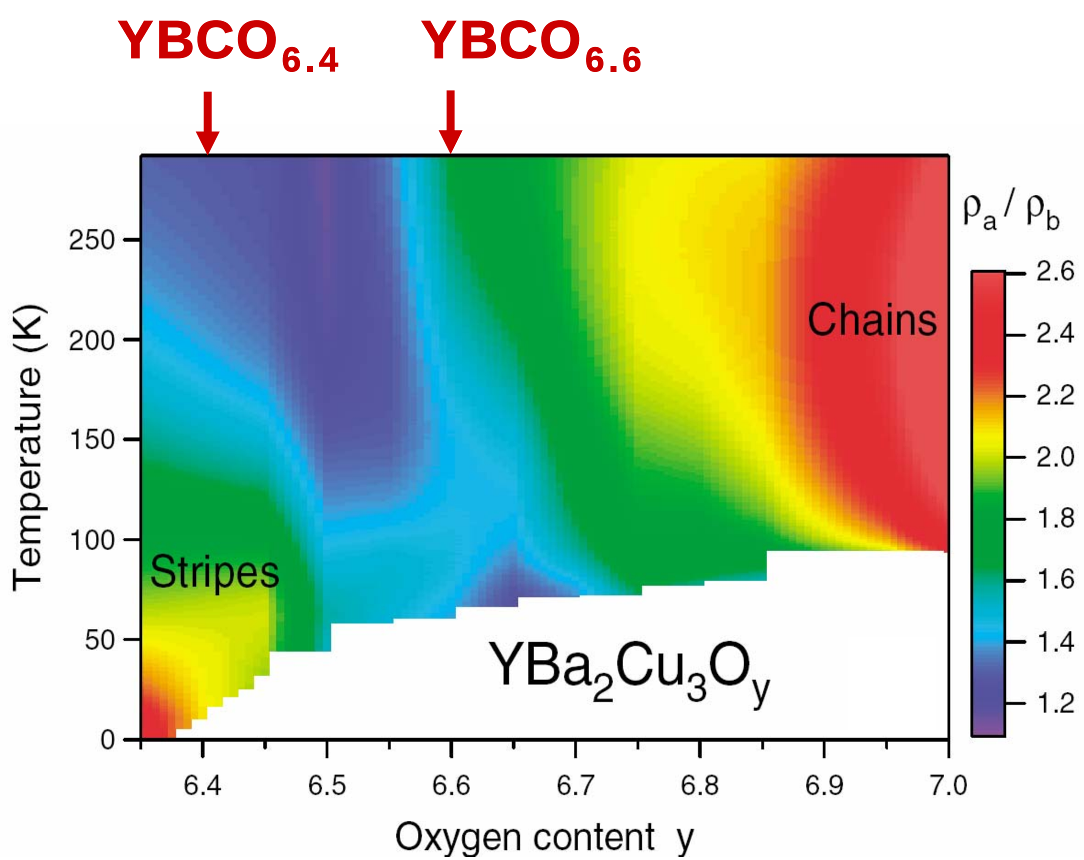
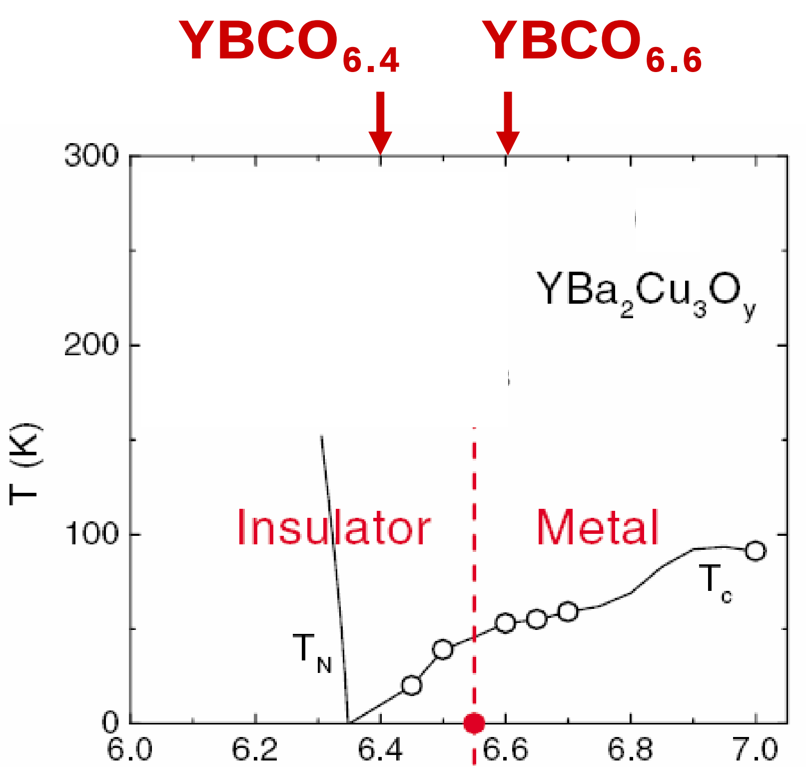
$YBCO_{6+x}$ transport properties

in-plane resistivity anisotropy

high-field phase diagram



Ando et al., PRL 2002



Sun et al., PRL 2005

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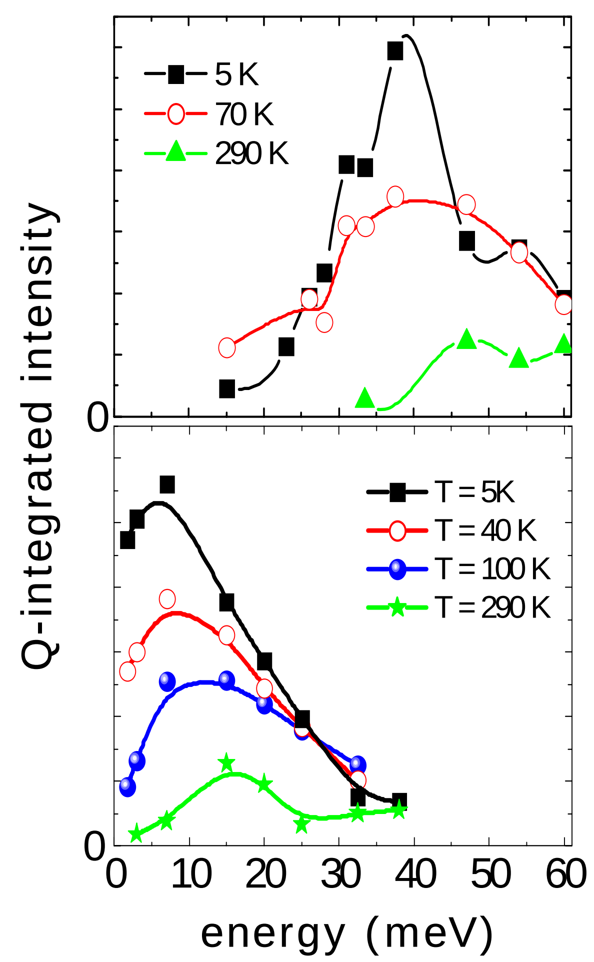
Comparison: $YBCO_{6.4}$ and $YBCO_{6.6}$

$YBa_2Cu_3O_{6.6}$ (T_c = 61 K)

- large spin gap
- qualitative difference between superconducting and normal states

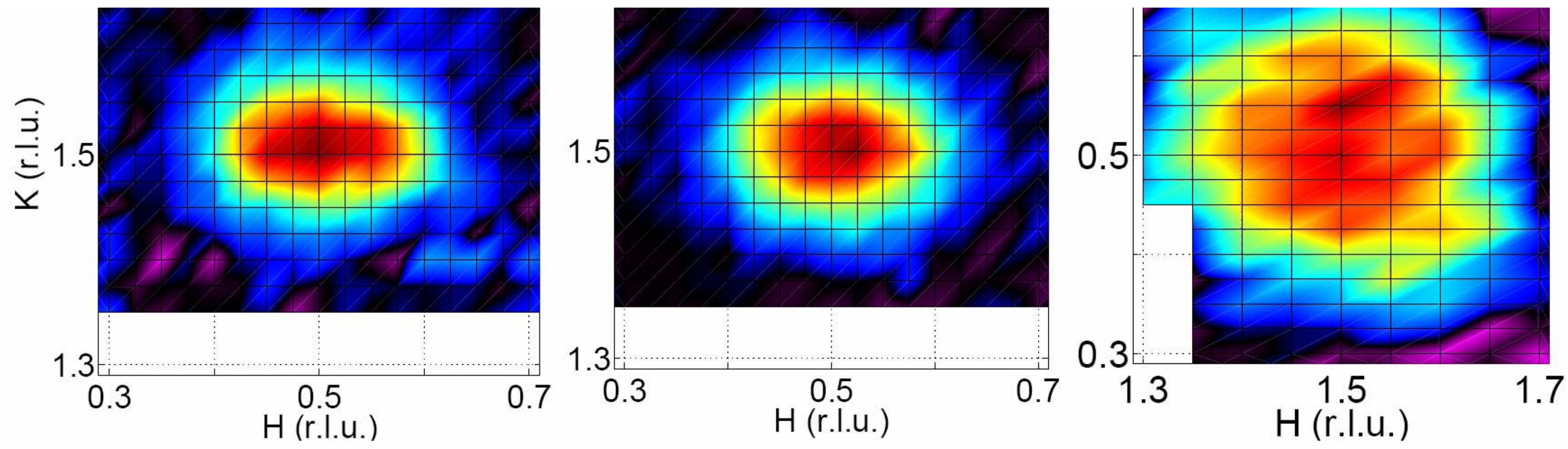
$YBa_2Cu_3O_{6.4}$ (T_c = 35 K)

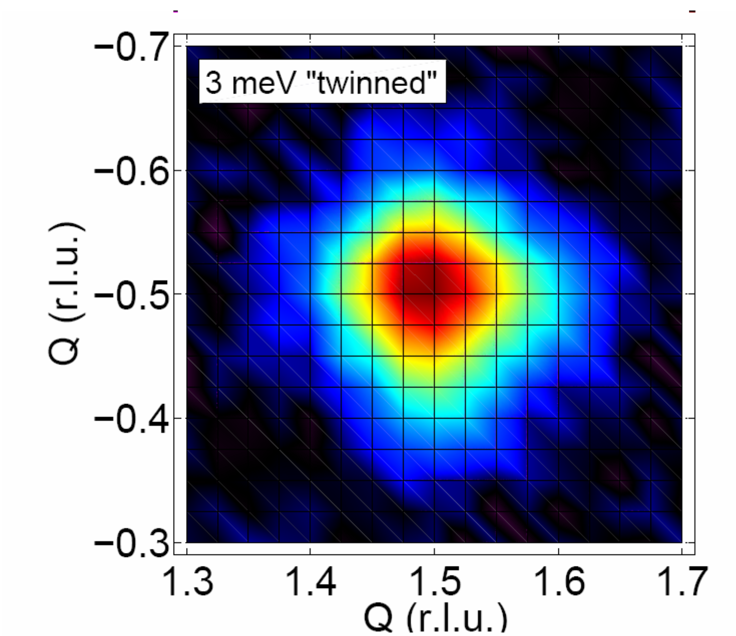
- small or absent spin gap
- spectrum evolves smoothly through T_c



$YBCO_{6.4}$ constant-energy cuts

3 meV **7 meV** **50 meV**





E > 15 meV isotropic

E < 15 meV large anisotropy

can only be seen in untwinned samples

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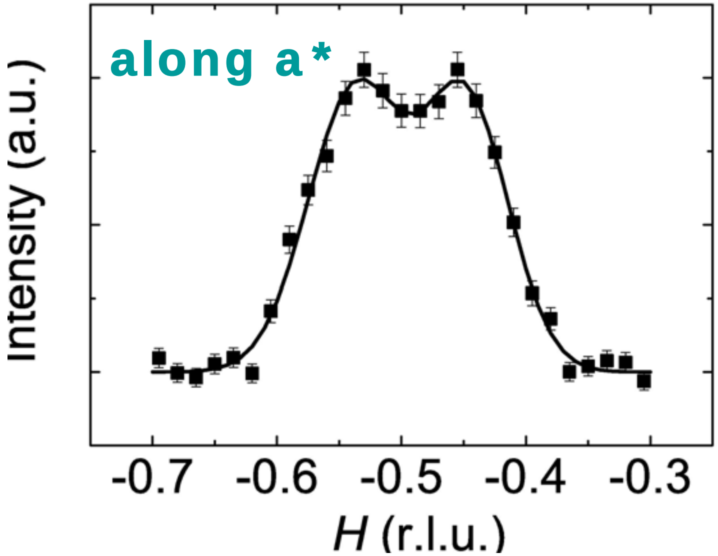
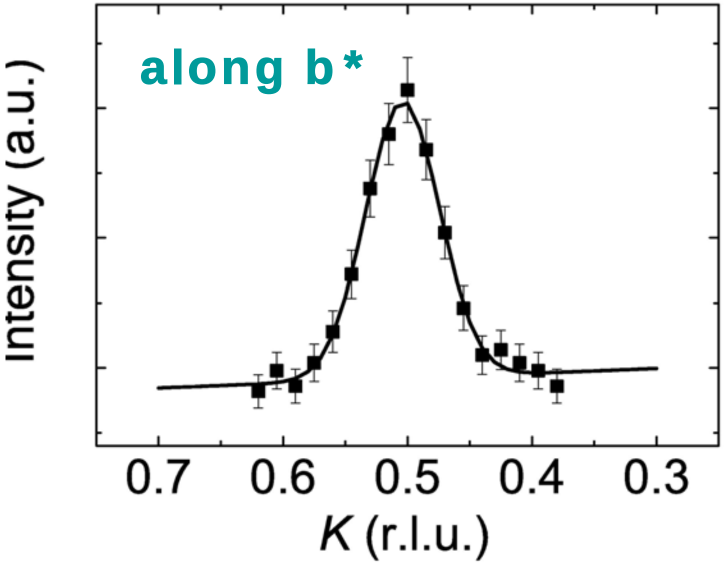
$YBCO_{6.4}$ high-resolution measurements

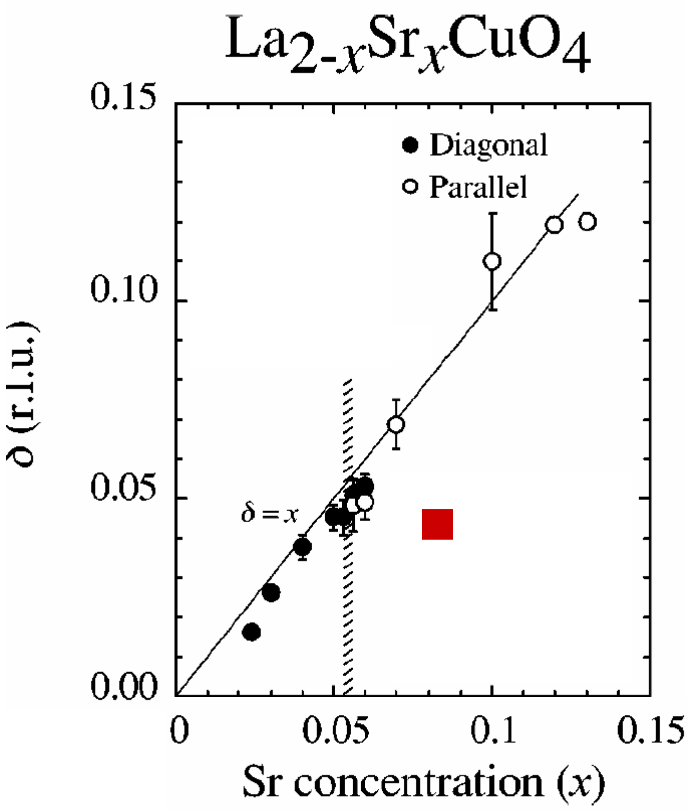
E = 3 meV, T = 5 K





incommensurate along a*, commensurate along b*

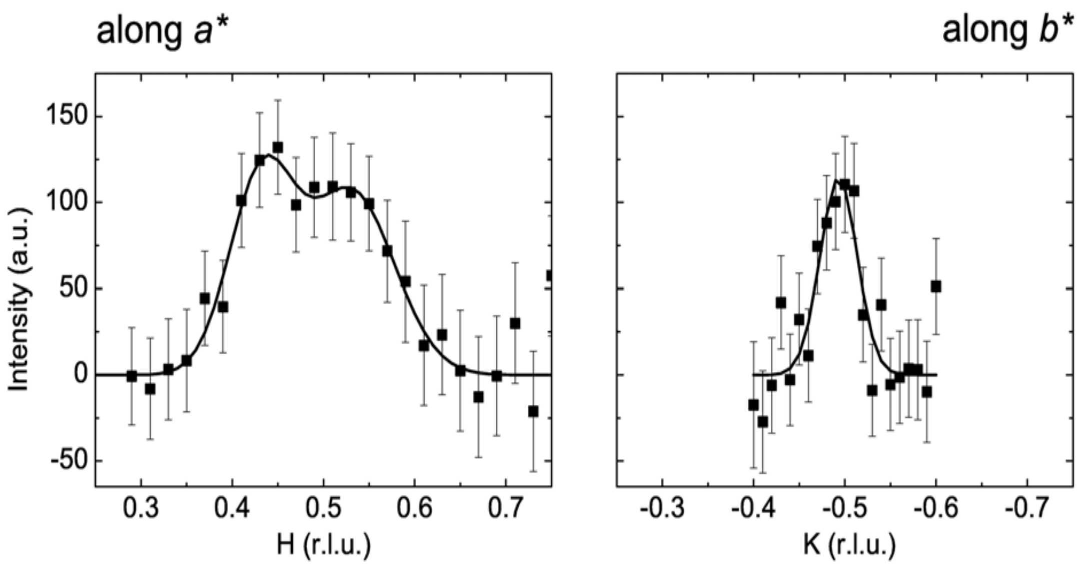
→ **one-dimensional geometry at low energies**



Fujita et al.
PRB 2002

modulation along Cu-O bond direction
but magnitude matches “diagonal” pattern
in LSCO with $x \leq 5\%$

Magnetic order ?

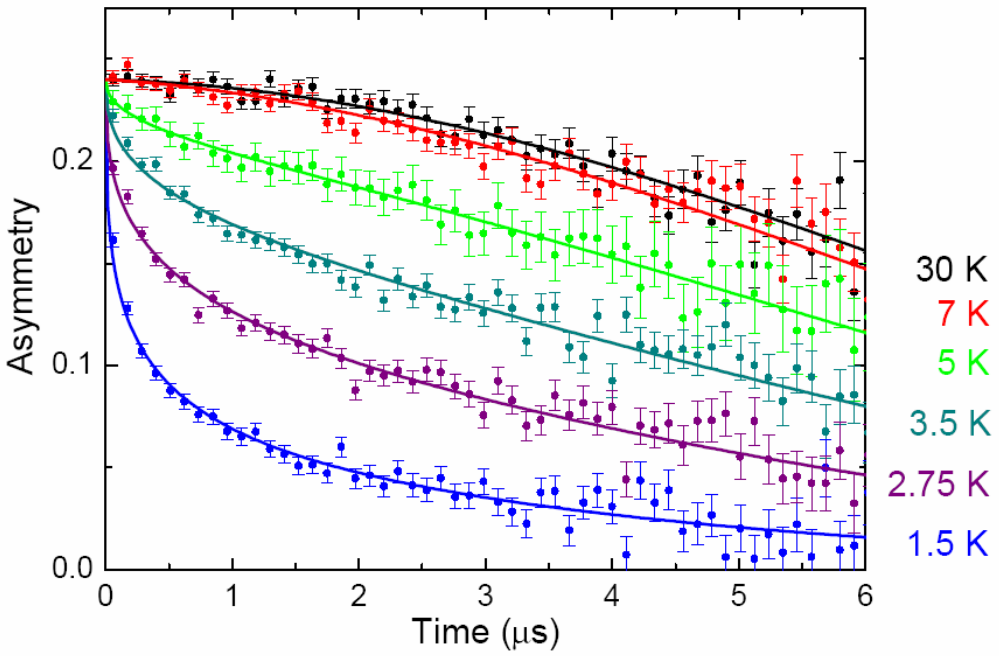


quasielastic neutron scattering

E ≤ 0.2 meV

significant signal for T ≤ 30 K

same geometry as inelastic signal



muon spin relaxation

E ~ 1 μeV

slow electronic spin relaxation for T ≤ 10 K

static magnetic order for T ≤ 2 K

generally consistent with

spin freezing phenomenology

in spin-glass regime of LSCO

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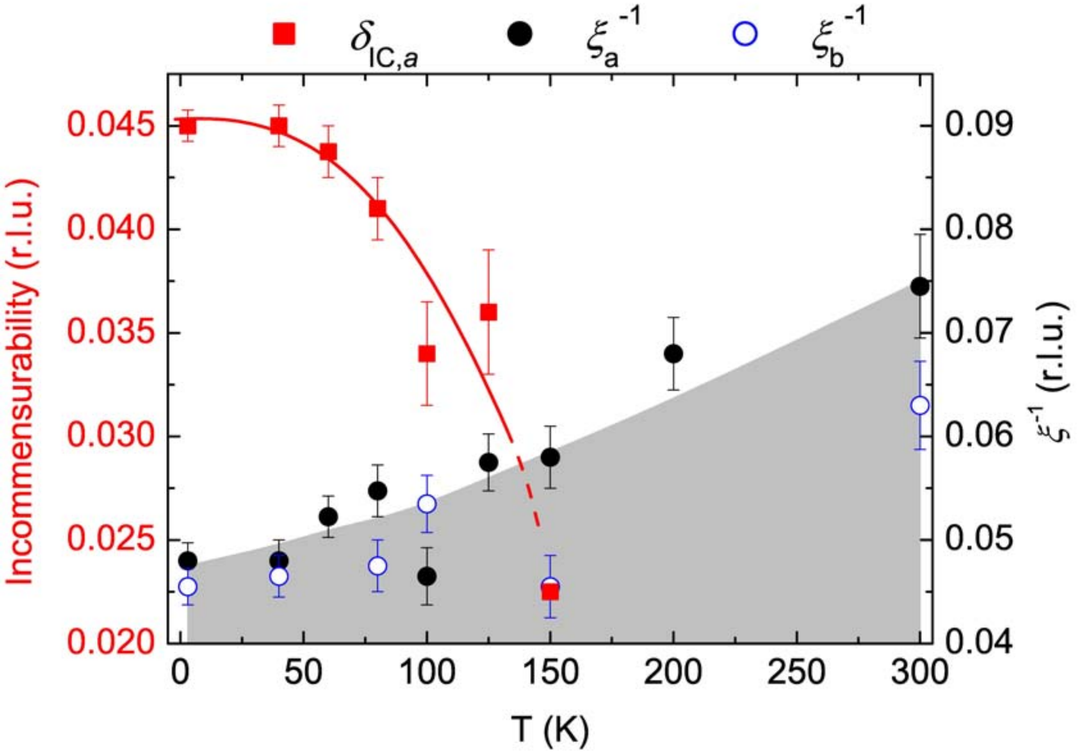
Nematic order ?



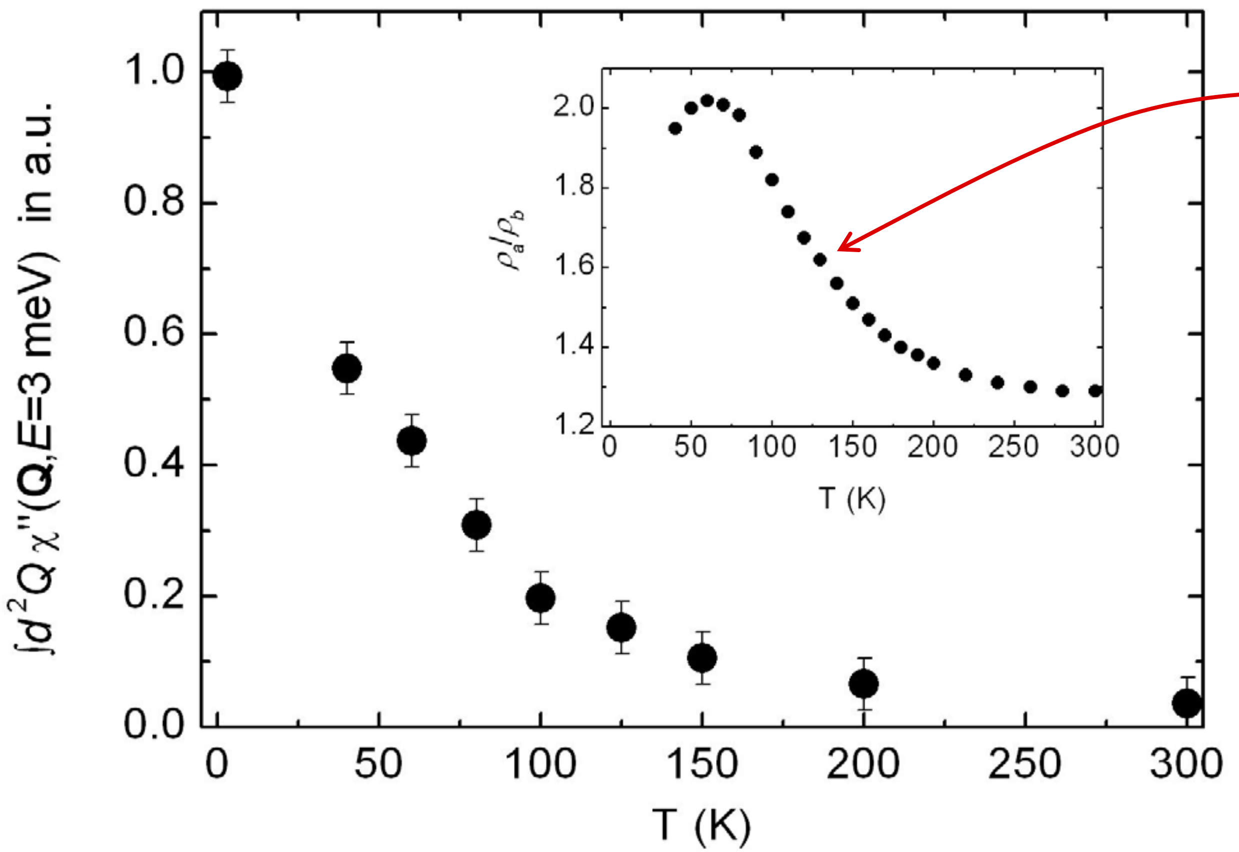
phase transition at T_{IC} ~ 150 K

spin system spontaneously develops 1D incommensurate modulation

weak structural in-plane anisotropy selects unique incommensurate domain

T_{IC} **two orders-of-magnitude higher** than onset of static magnetic order

Nematic order ?



at T_{IC}, pronounced increase of

- intensity of low-energy incommensurate spin fluctuations
- resistivity anisotropy $\rightarrow$ **isotropic-nematic transition**

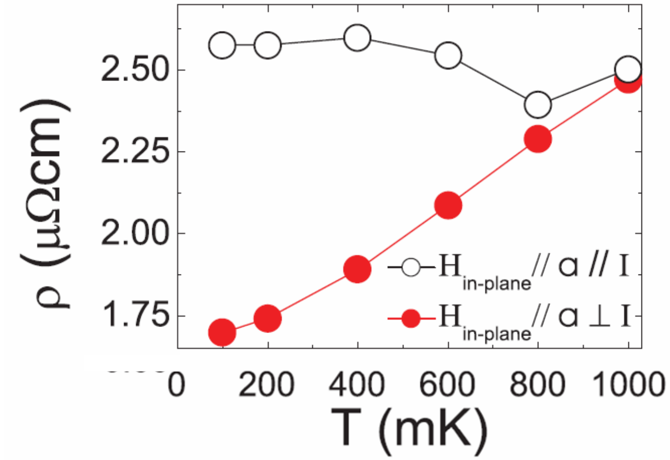
broadened by disorder, finite energy, finite field

NB: in $YBCO_{6.6}$ both quantities strongly reduced

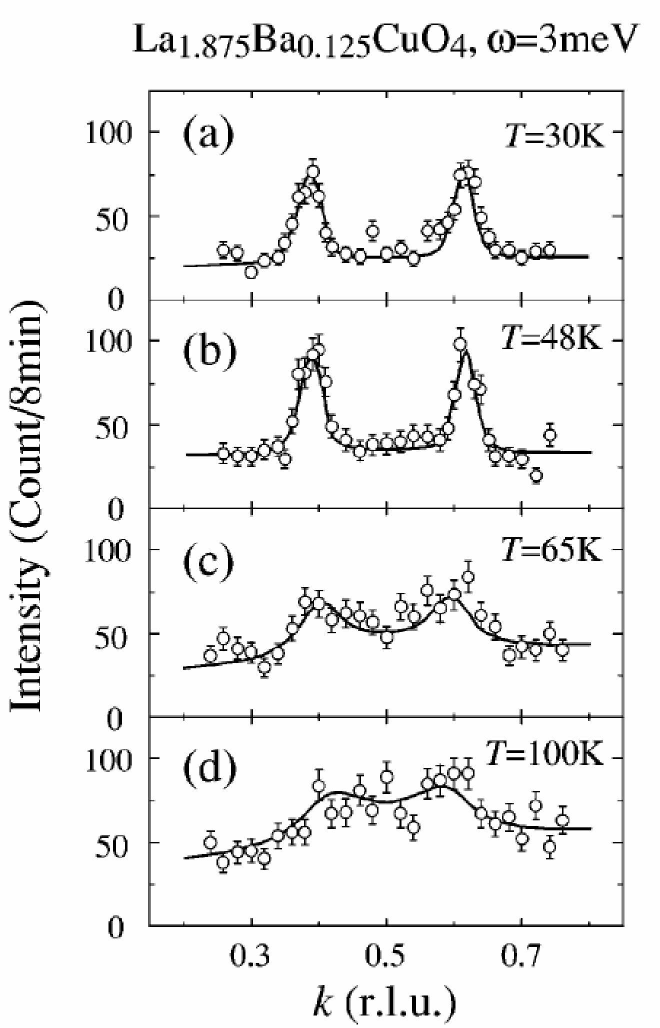
Analogies

1. nematic liquid-crystal in weak electric field

2. **“electronic nematic phase”** in $Sr_3Ru_2O_7$



Borzi et al., Science 2007



3. **“fluctuating stripes”** in $La_{15/8}Ba_{1/8}CuO_4$

   twinned crystal → 1D pattern not seen with neutrons

   other differences:

   - much sharper peaks
   - incommensurability larger, weakly T-dependent
   - static spin and charge order for T ≤ 50 K

Fujita et al., PRB 2004

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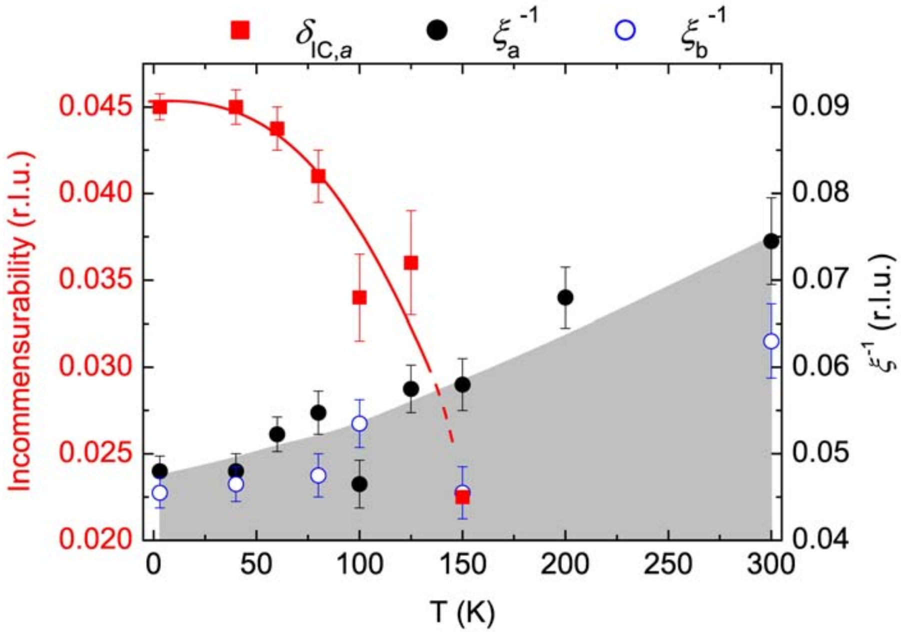
Fluctuating stripes ?



correlation length almost isotropic

→ almost isotropic exchange interactions

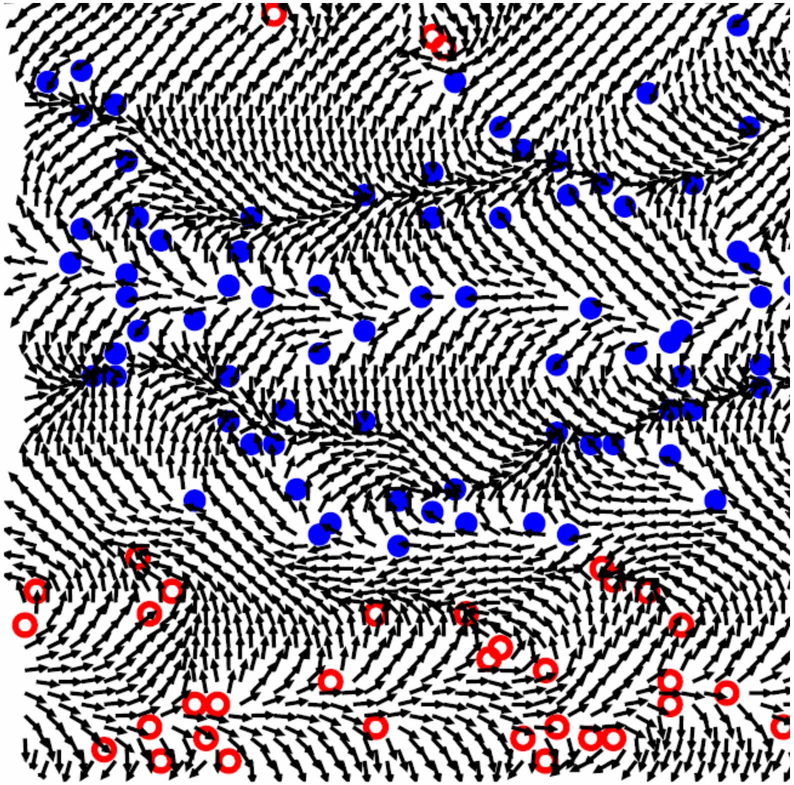
→ at most weak longitudinal spin modulation

alternative: transverse spin modulation

disordered spiral pattern

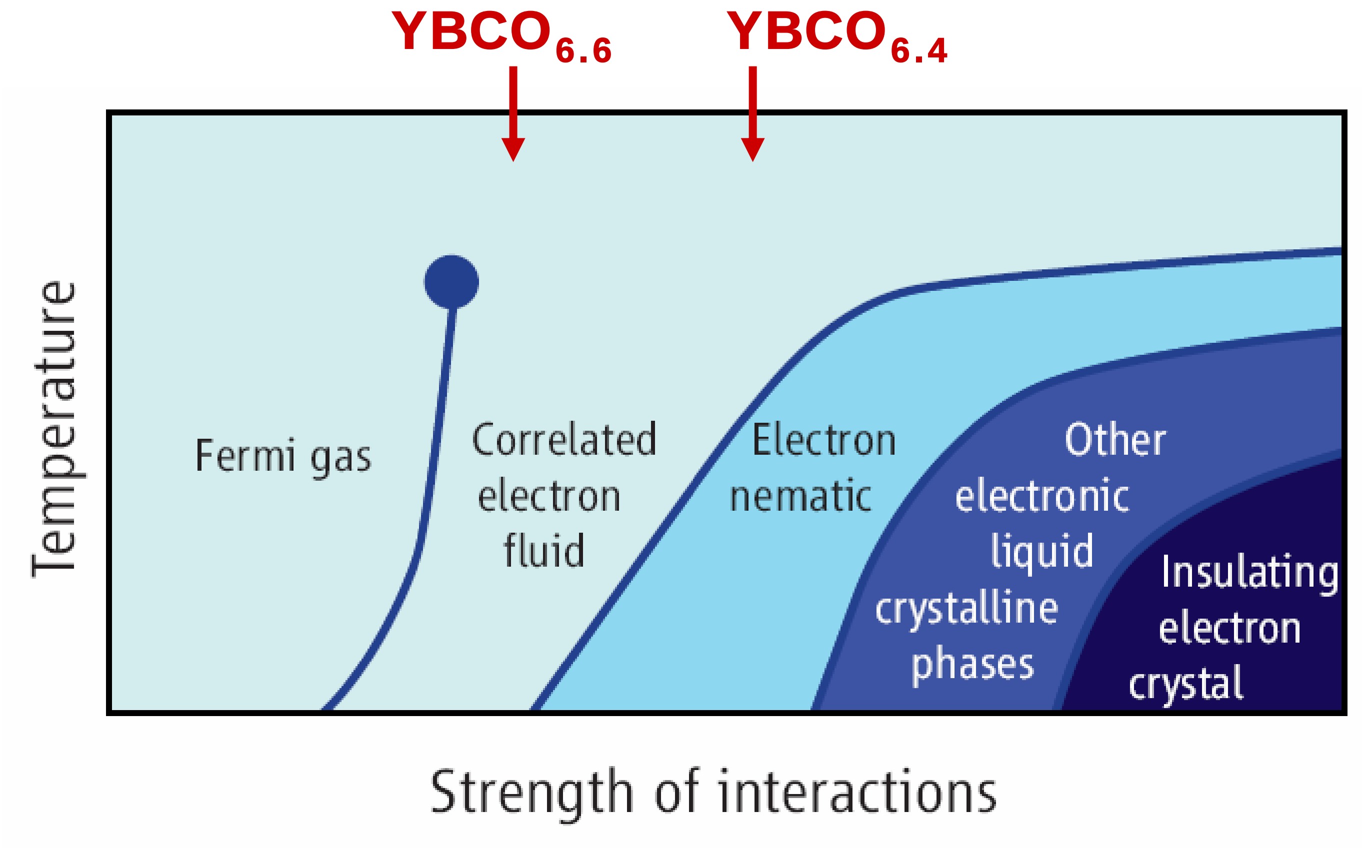
proposed for $La_{2-x}Sr_xCuO_4$ for $x \leq 0.05$

Luscher et al., PRL 2007



$YBCO_{6.4}$ summary

- **robust electronic liquid-crystal phase** in weak aligning field



Kivelson et al. Nature 1998

- dynamical spin correlation functions determined
- some similarity to gapped “vertical dispersion” in pseudogap state of $YBCO_{6.6}$
- open question: longitudinal or transverse spin modulation ?

Collaborators: Superlattices

neutron scattering	
J. Chakhalian	MPI Stuttgart → Univ. of Arkansas
J. Stahn, C. Niedermayer	PSI Villigen
T. Charlton, R. Dalgliesh	ISIS
x-ray spectroscopy	
J. Chakhalian	MPI Stuttgart → Univ. of Arkansas
J. Freeland	Argonne National Lab.
J. Cesar	ESRF
IR spectroscopy	
A. Boris	MPI Stuttgart
C. Bernhard	MPI Stuttgart → Univ. of Fribourg
theory	
G. Khaliullin	MPI Stuttgart
M. van Veenendaal	Argonne National Lab.
samples	
H.U. Habermeier, G. Cristiani	MPI Stuttgart

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YBCO-LCMO superlattices

LCMO = $La_{0.7}Ca_{0.3}MnO_3$

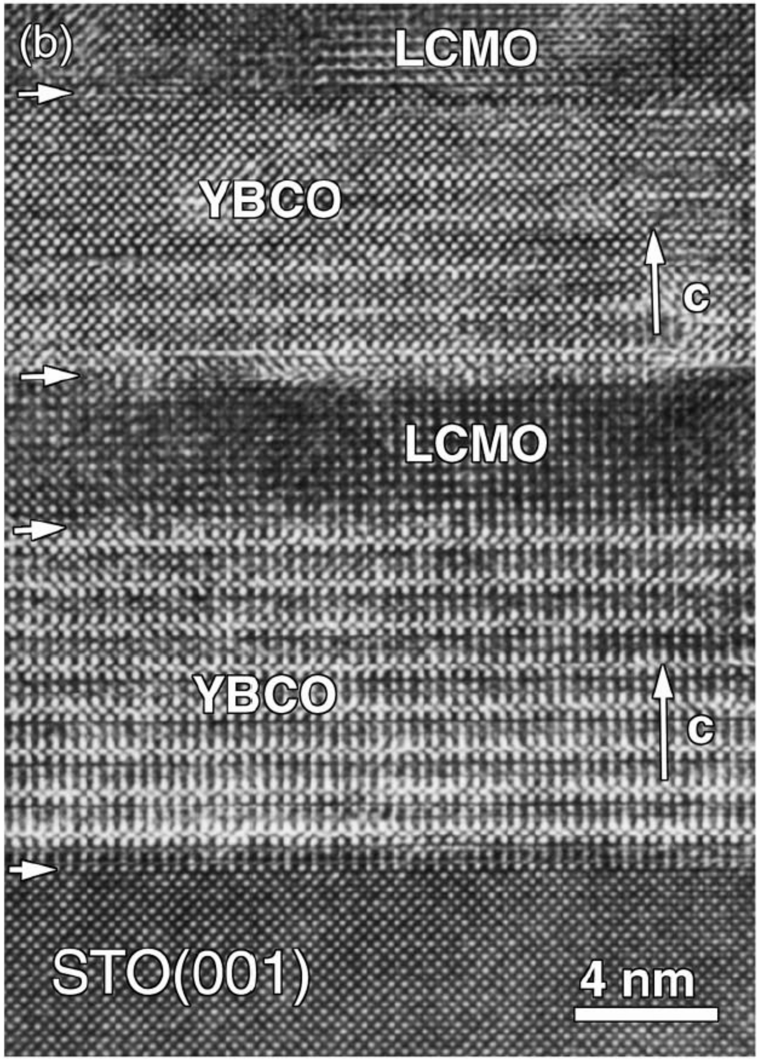
metallic ferromagnet, T_C = 160 K

lattice constants almost indentical to YBCO

superb interface quality

- TEM: atomic-scale epitaxy

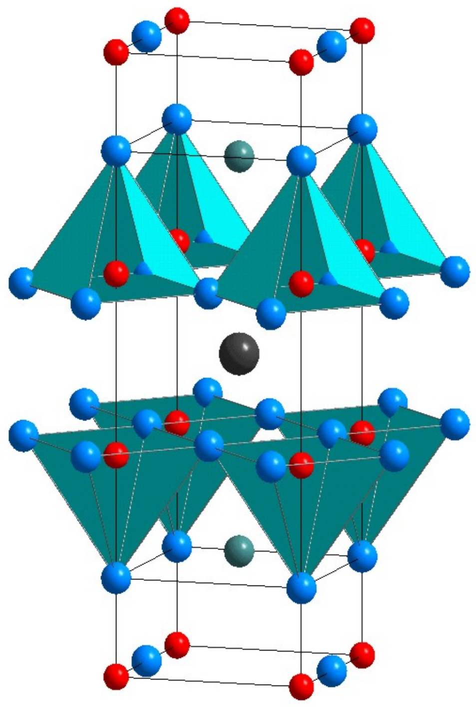
- neutron reflectivity of 1×1 cm^2 sample:
  average roughness ~ 5 Å



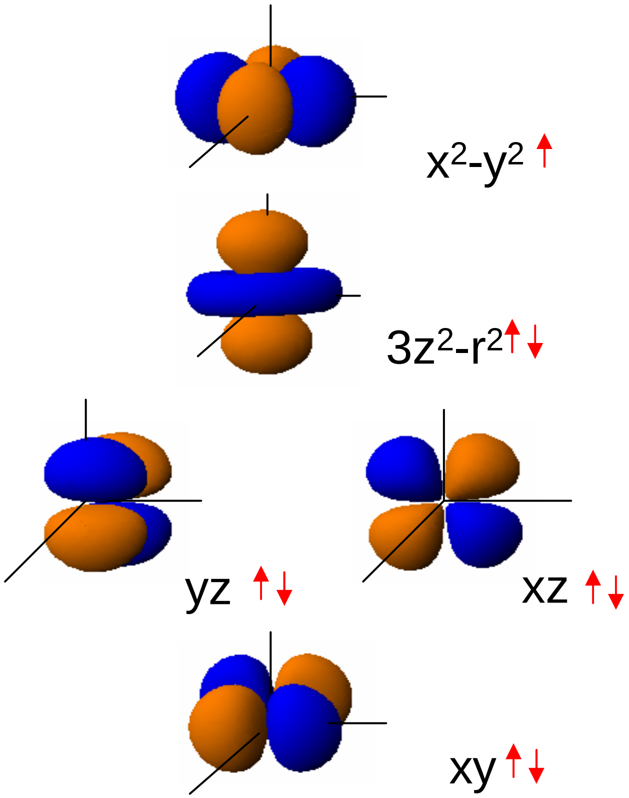
Holden et al., PRB 2004

$YBa_2Cu_3O_{6+x}$

lattice structure



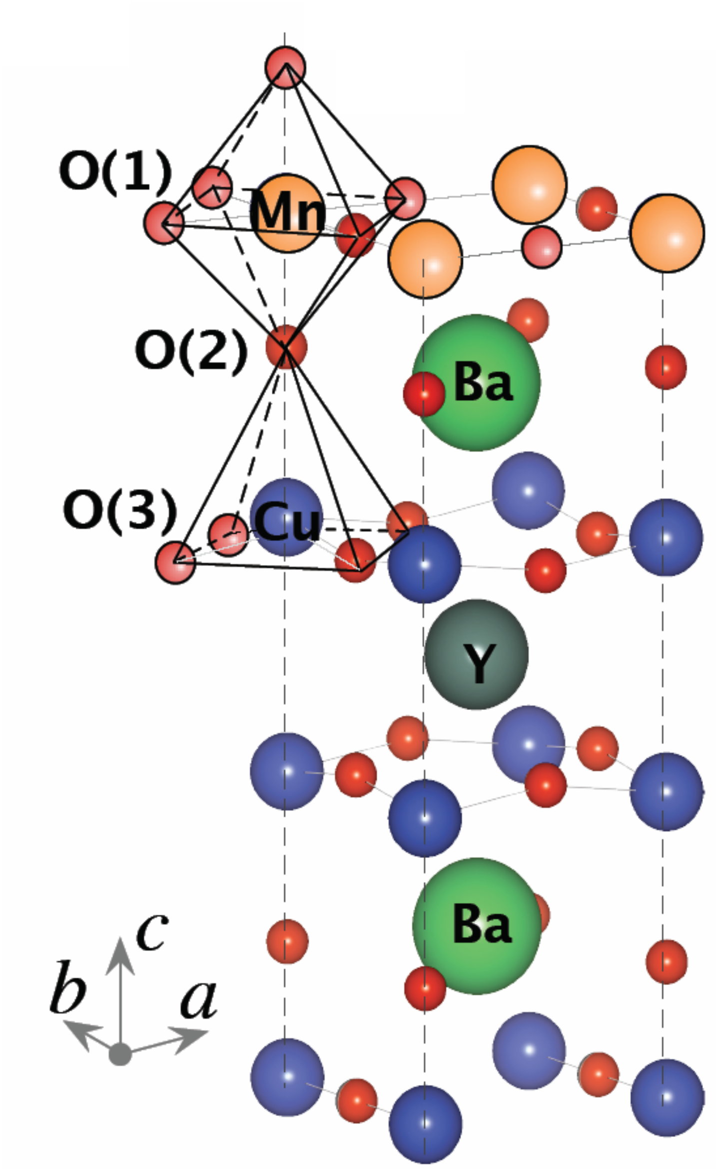
electronic structure



strong superexchange of electrons in Cu x^2-y^2 orbital

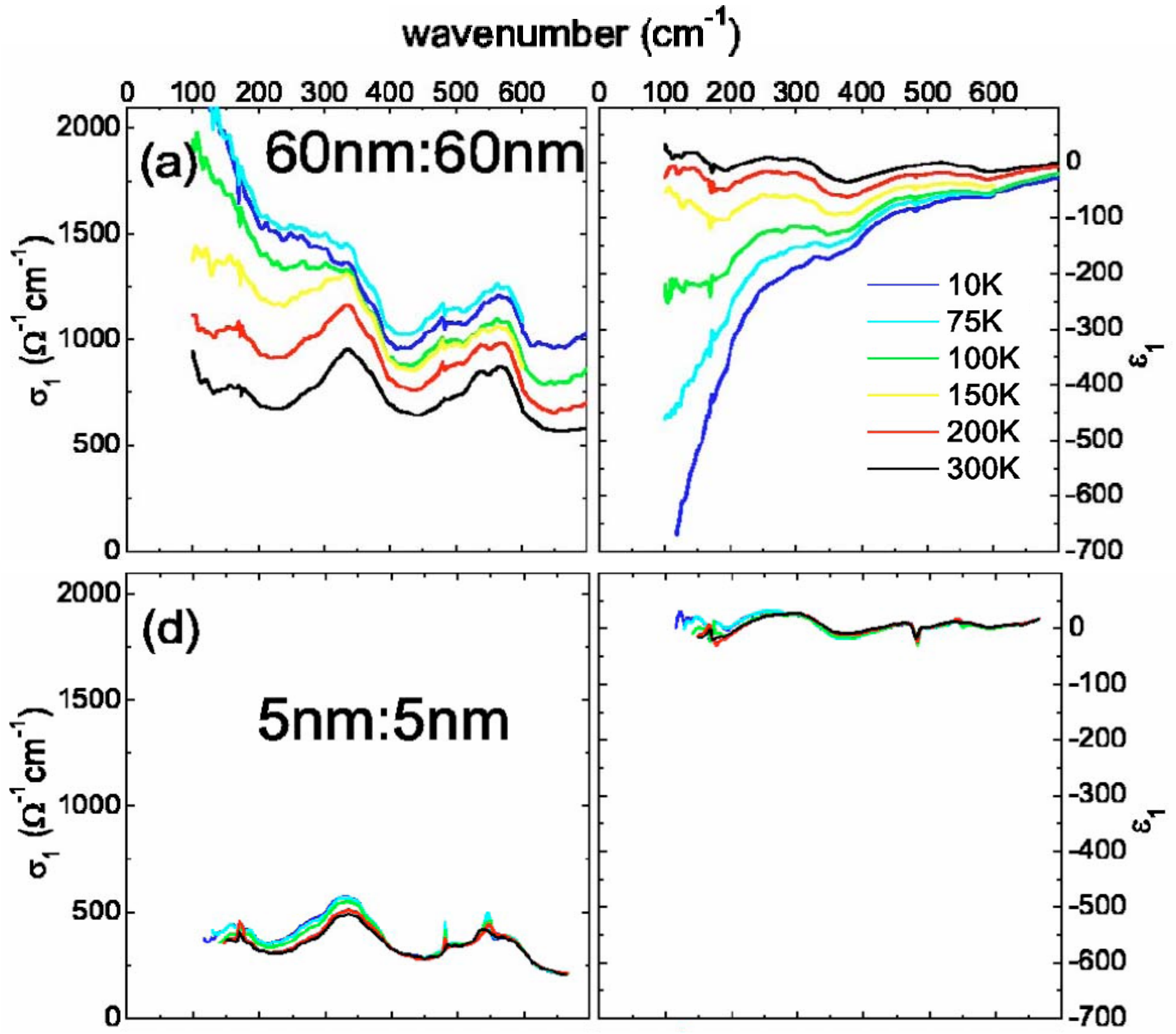
nearly antiferromagnetic spin fluctuations throughout phase diagram

YBCO-LCMO interface



- different magnetic environment
- different crystal field
- different covalent bonding ?

YBCO-LCMO superlattices



suppression of metallicity

for layers thinner than ~ 5 nm

Holden et al., PRB 2004

YBCO-SRO, YBCO-LNO superlattices

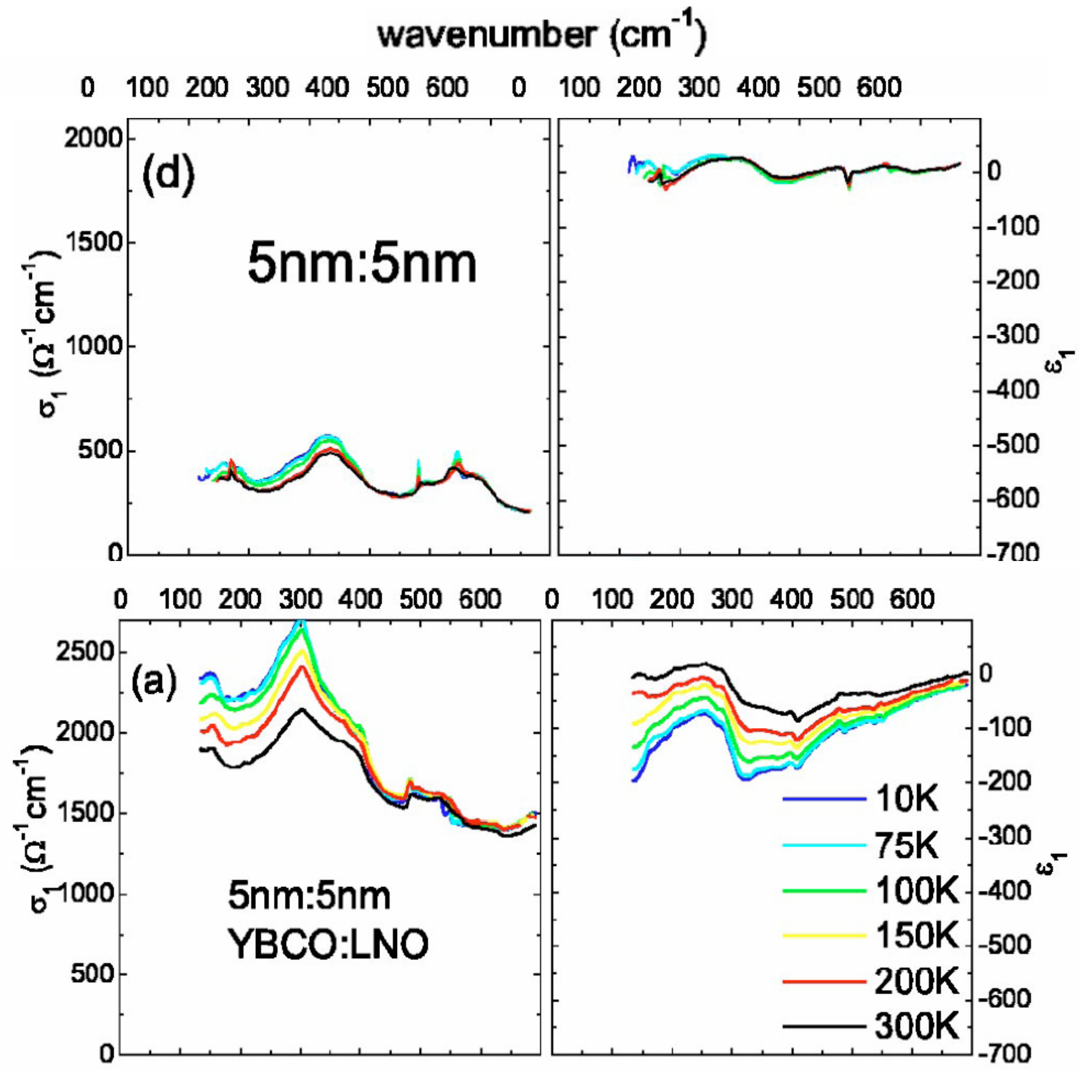
similar behavior in
$YBa_2Ca_3O_7$ / $SrRuO_3$ SL
(ferromag. metal)

much weaker effect in
$YBa_2Ca_3O_7$ / $LaNiO_3$ SL
(paramag. metal)

→ **significant role of magnetism**

surprising because
- robust AF spin correlations
- short spin diffusion length

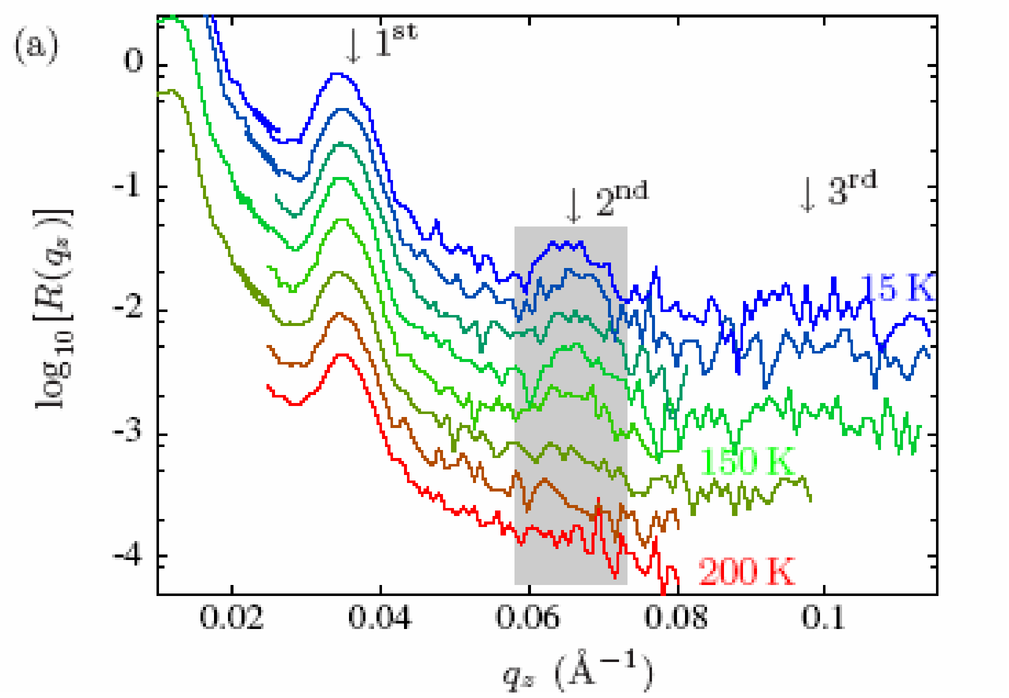
expected in YBCO



YBCO-LCMO superlattices

neutron reflectivity

→ Bragg reflections due to structural and magnetic periodicity

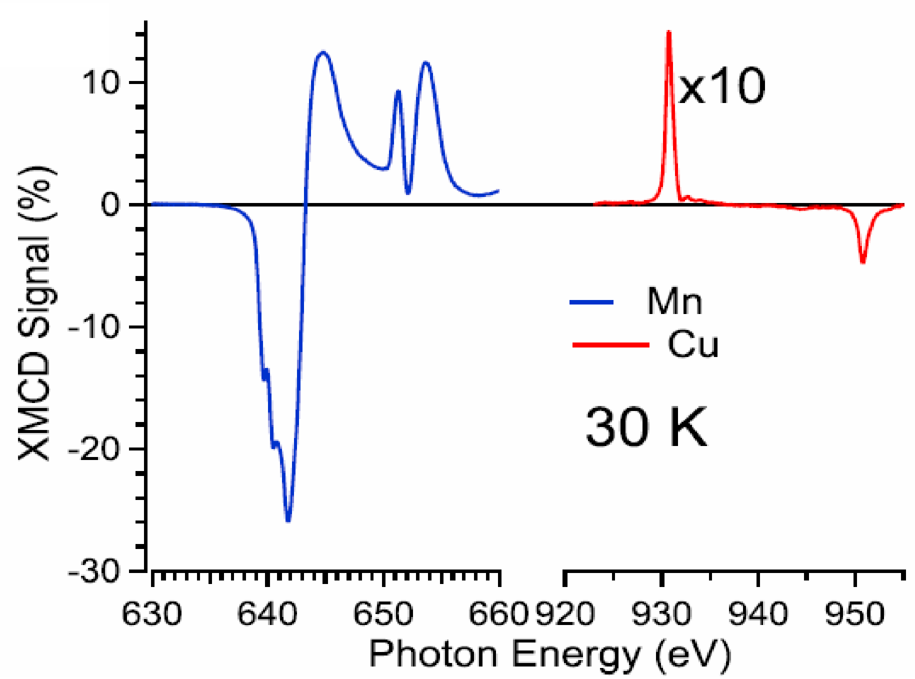


Stahn et al., PRB 2005

magnetic circular dichroism

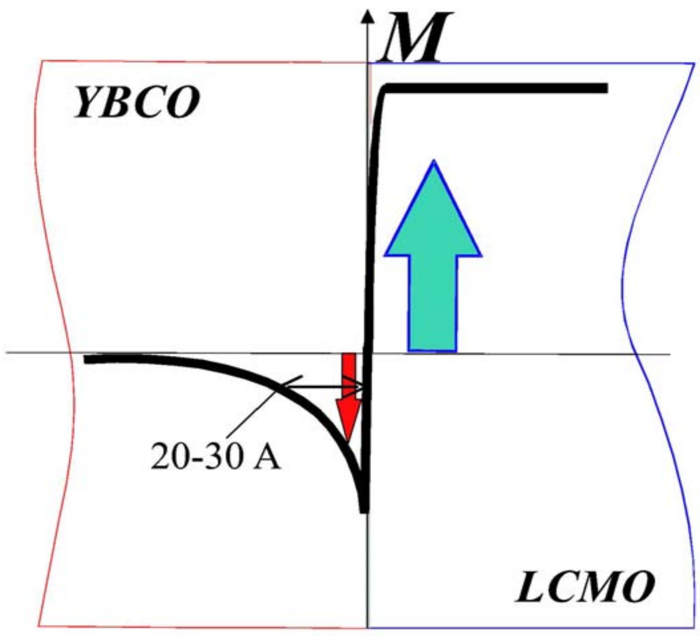
at L- absorption edges

→ element-specific magnetization

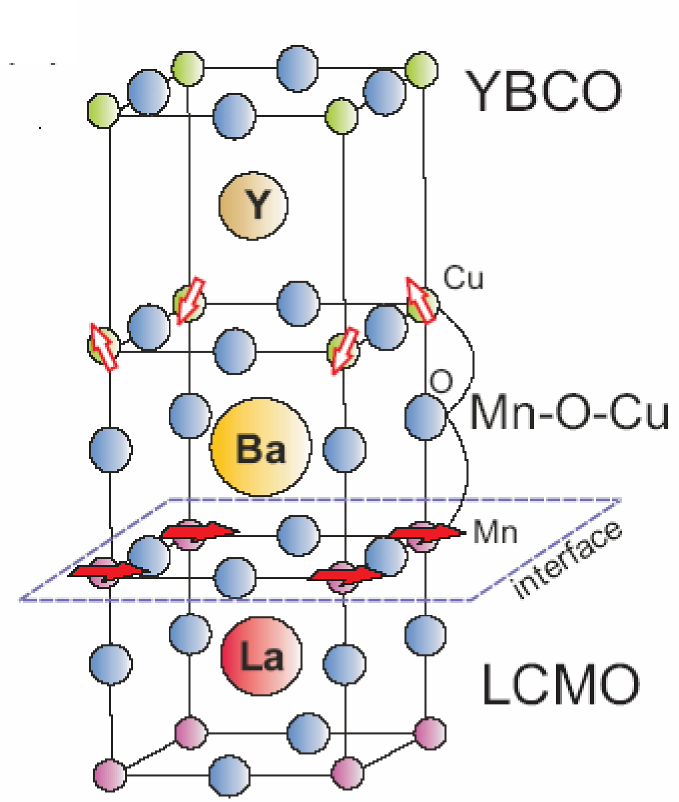


- ferromagnetic polarization of Cu in YBCO
- direction antiparallel to Mn

Spin polarization at interface



magnetization profile

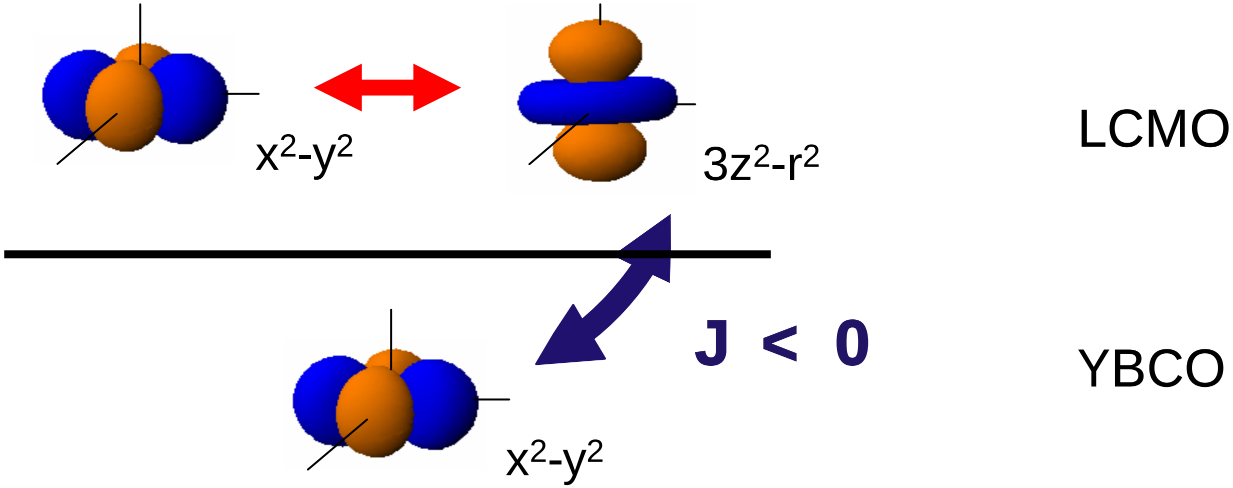


superexchange across interface

Chakhalian et al., Nature Phys. 2006

Exchange coupling across interface

assume bulk orbital occupancy is maintained at interface



→ **weak ferromagnetic exchange** across interface
expected from Goodenough-Kanamori rules

inconsistent with experiment → **orbital reconstruction ?**

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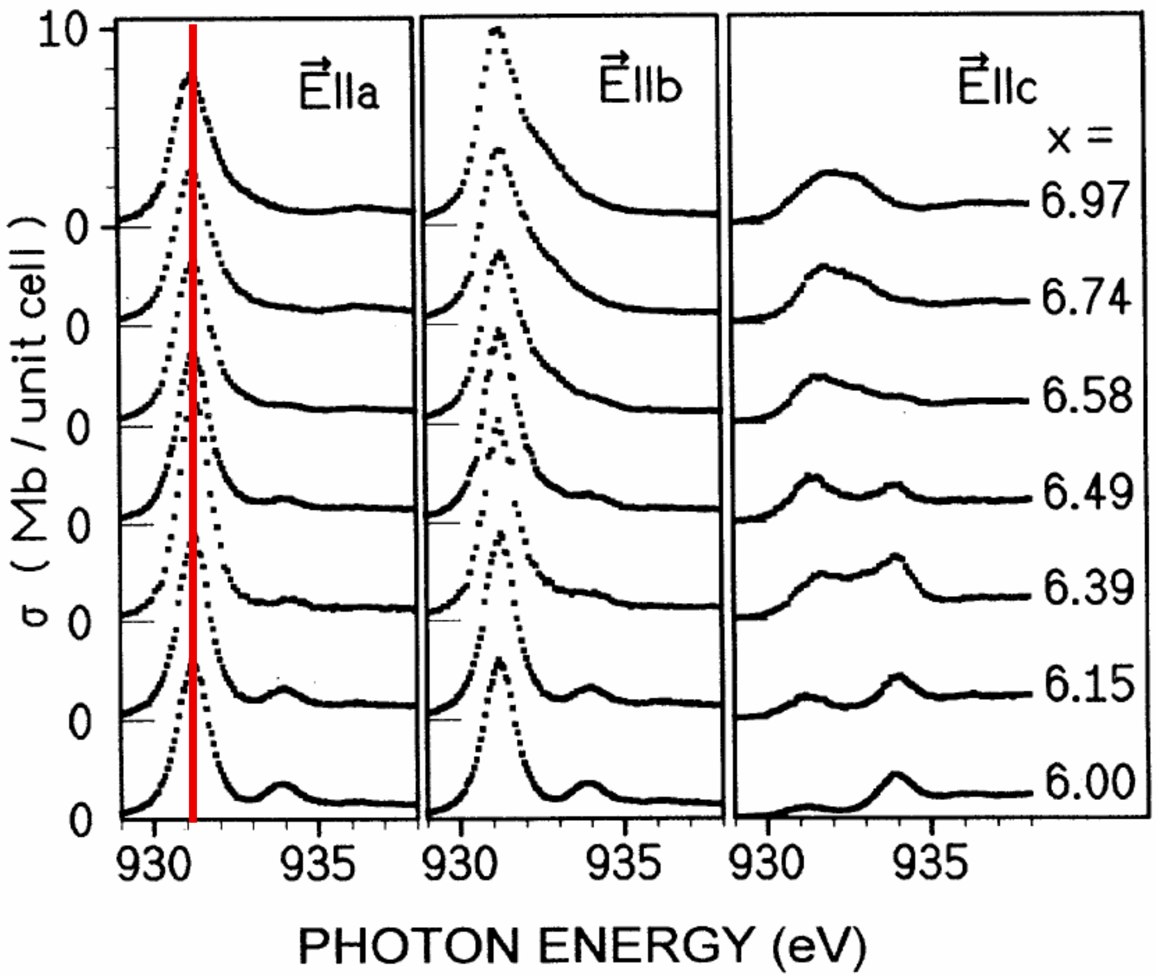
X-ray linear dichroism

bulk YBCO



- absorption cross section much greater for E || ab-plane → x^2-y^2 orbital partially occupied

- peak position independent of doping (Zhang-Rice singlet state)

Nücker et al., PRB 1995

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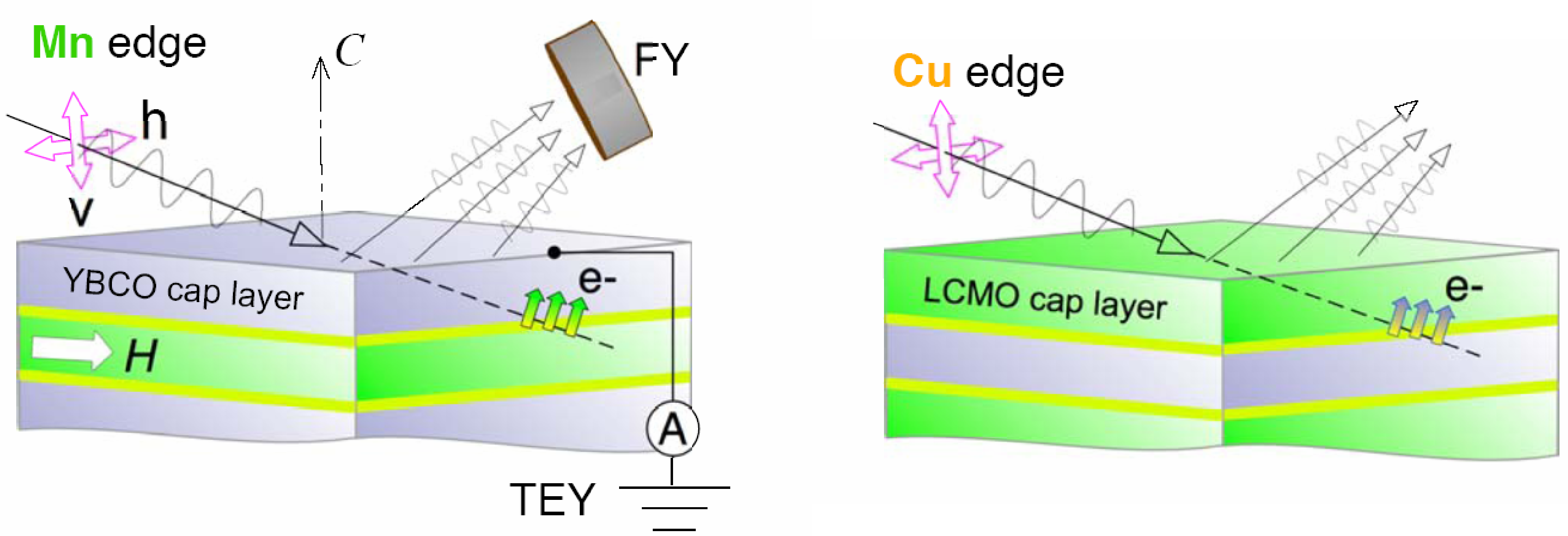
X-ray linear dichroism

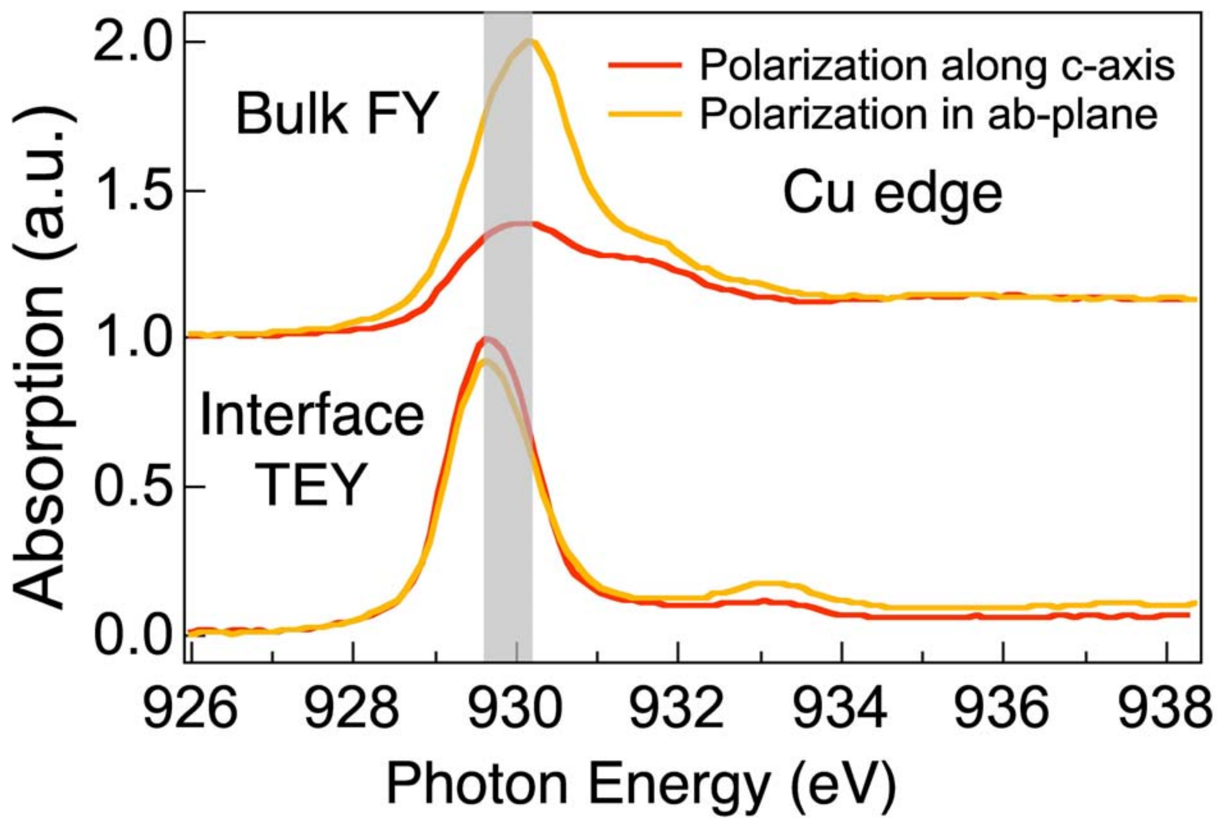
interface sensitivity through “cap layers”



FY bulk sensitive

TEY low electron escape depth $\rightarrow$ probes first interface

Orbitals at interface



Chakhalian et al.
submitted

FY matches data on bulk YBCO (Nücker et al.)

TEY shifted → ~ 0.2 electrons / Cu ion transferred across interface

not subject to Zhang-Rice singlet formation

almost isotropic → partial occupation of Cu $3z^2$-r^2 orbital

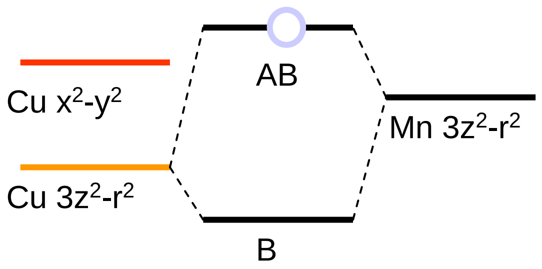
orbital reconstruction

für Festkörperforschung

Cluster calculations

possible origins

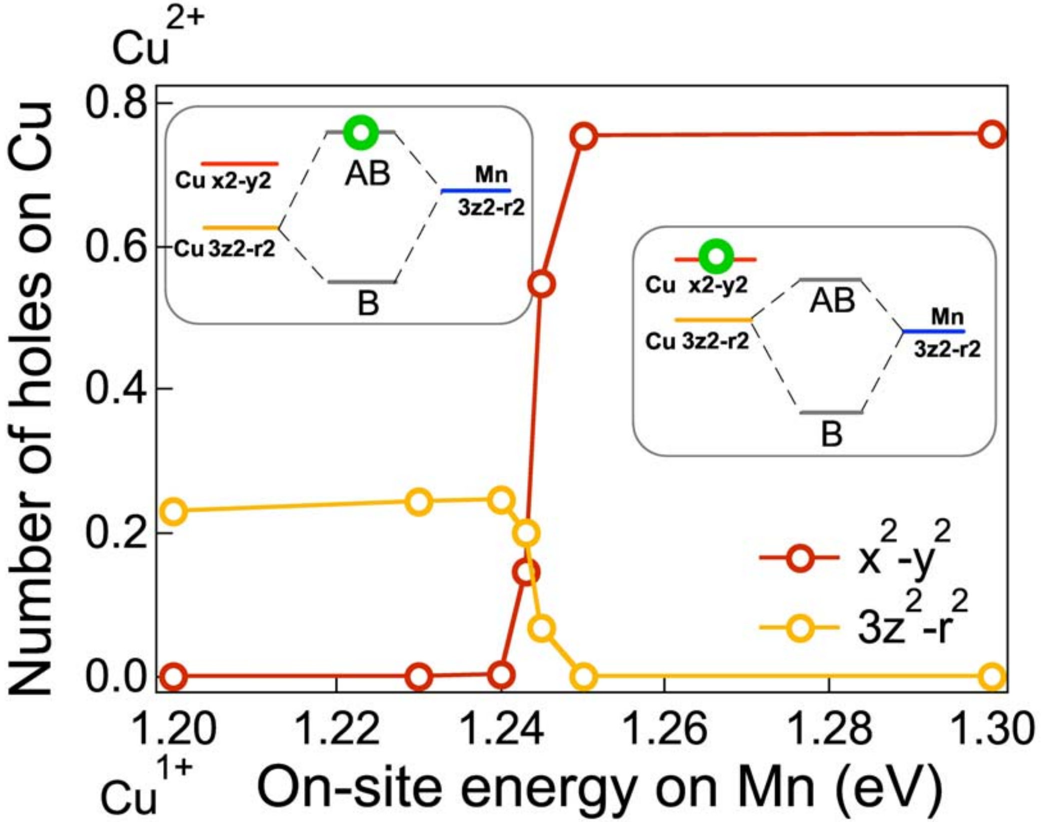
- different crystal fields at interface — unlikely
- covalent bonding ?



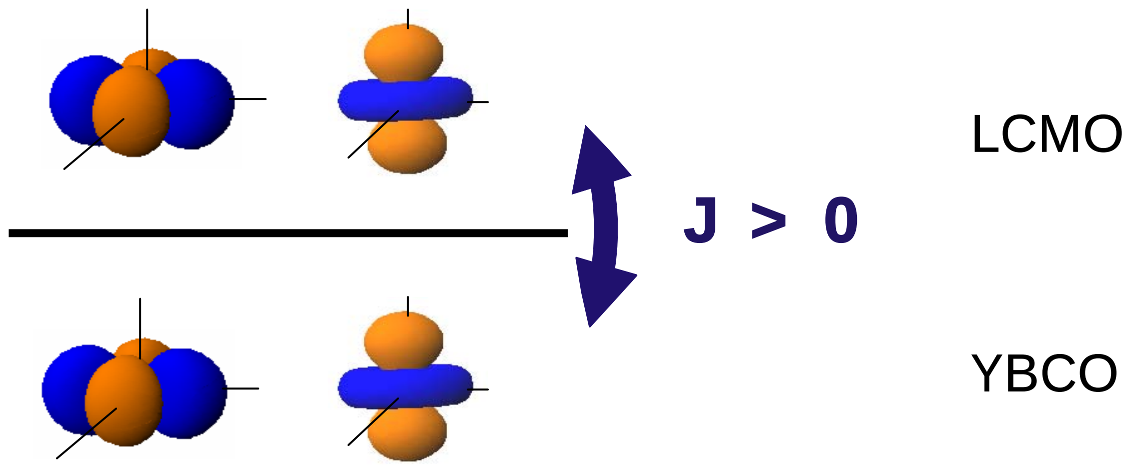
exact-diagonalization

calculations on small clusters

→ covalent bonding realistic



Exchange coupling across orbitally reconstructed interface



Cu $3z^2$-r^2 orbital partially occupied

→ **strong antiferromagnetic exchange across interface**

→ **reduced in-plane antiferromagnetic correlations**

combination may explain large ferromagnetic susceptibility, suppression of metallicity and superconductivity of YBCO near interface

Summary

bulk YBCO

nearly antiferromagnetic spin correlations

electronic nematic phase

YBCO- LCMO interface

ferromagnetic spin correlations

orbital reconstruction driven by covalent bonding