Univ. of Virginia, December, 2007

The Deep Puzzle of High-Temperature Superconductivity

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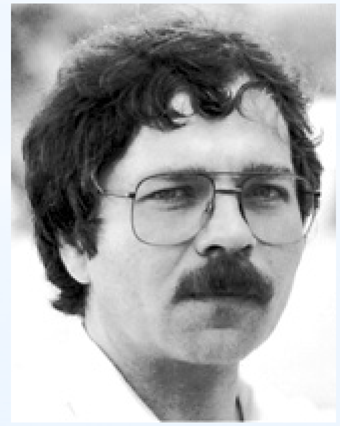
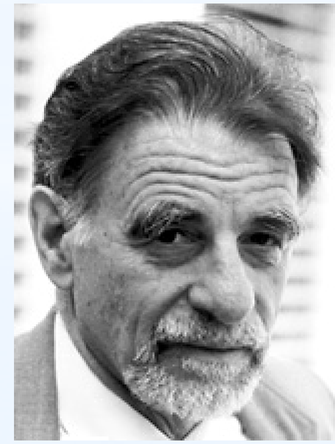
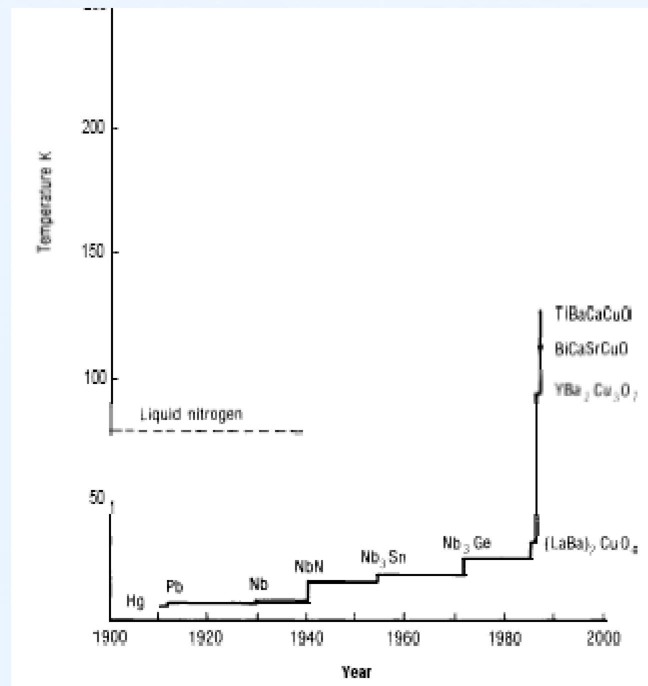
High-Temperature Superconductivity

- Discovered in 1986 by G. Bednorz and K. A. Müller (Nobel Prize in 1987).
- T_C saturated at 134K for 15 years.
- BCS theory with phonon does not work: T_C is too high, charge density is too low.
- Initial enthusiasm and slow progress since.





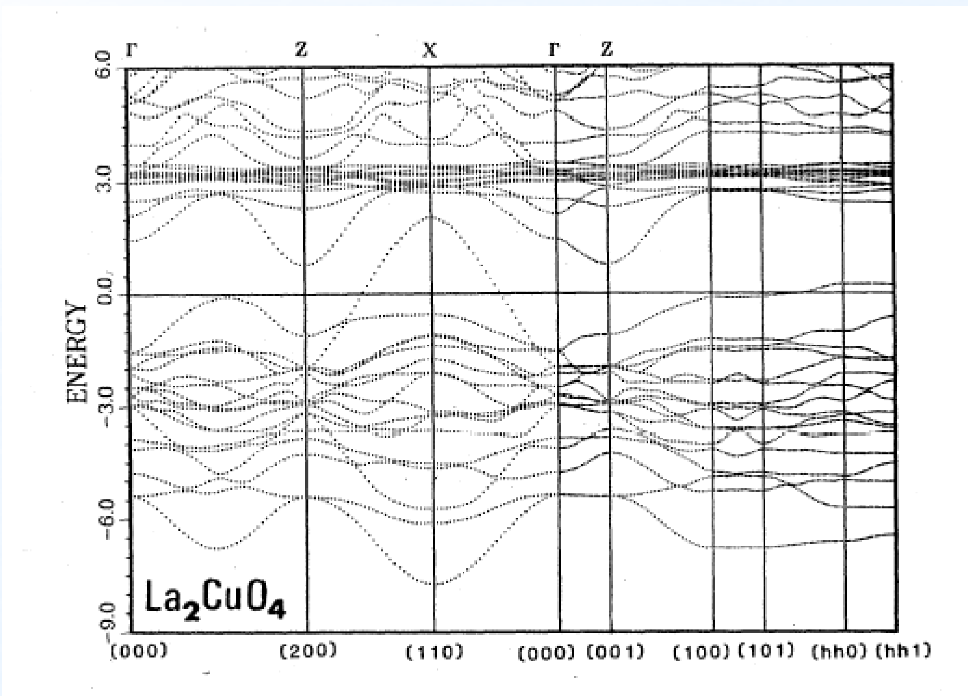


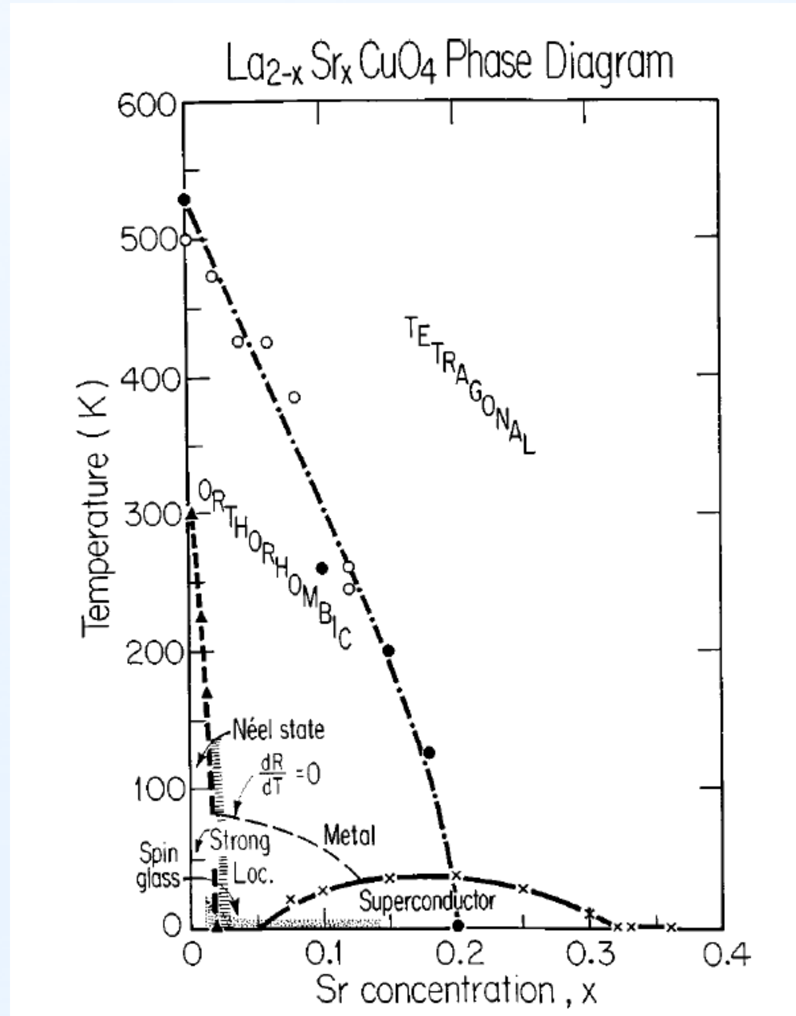
Outline

- The origin of high-temperature superconductivity (HTSC): A history of regression.
- What is the Mott-physics?
- The nature of the Mott transition and electronic nano-scale phase separation.
- Recent data with neutron scattering and Dark Matter in the cuprate physics.
- The possibility of intermediate order and a scenario of the spin-lattice synergy in the HTSC.

Spin Mechanism

- AFM phase near-by.
- The parent phase is a Mott insulator (charge transfer insulator).

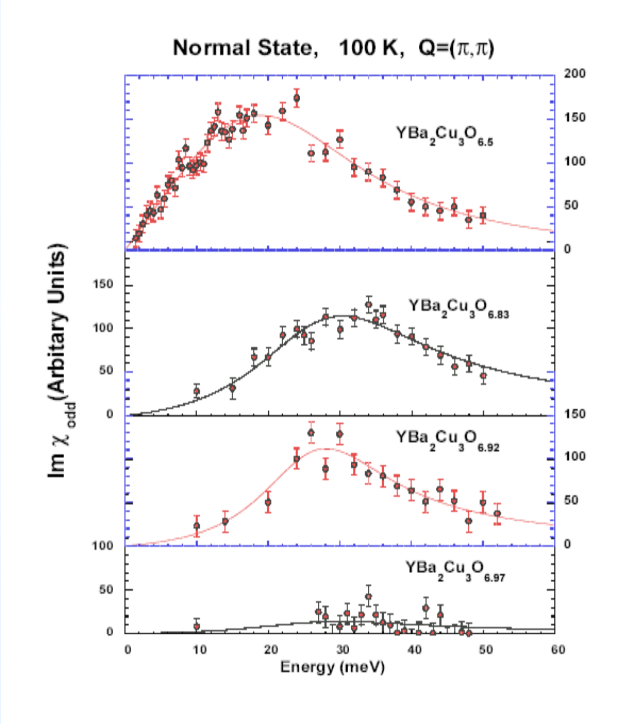




W. E. Pickett, *Rev. Mod. Phys.* **61,** 433 (1989)

Spin Mechanism

- **Spin fluctuation theory (Pines, Moriya,……).**
- **Exotic theories:**
  - **RVB (Anderson)**
  - **Flux phase (Varma)**
  - **Stripes (Kivelson,…..)**



Physica Scripta. T102, 10–12, 2002

Superconductivity in High Tc Cuprates: The Cause is No Longer A Mystery

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Total citation: 4

We Agree….

- A pair of electrons (holes) in the singlet state.
- The gap symmetry is **mostly** *d*.
- Coherence length is short.
- Not suppressed much by disorder.
- A doped single CuO_2 plane is enough.
- But, not much beyond. Experimentalists no longer listen to theorists…………

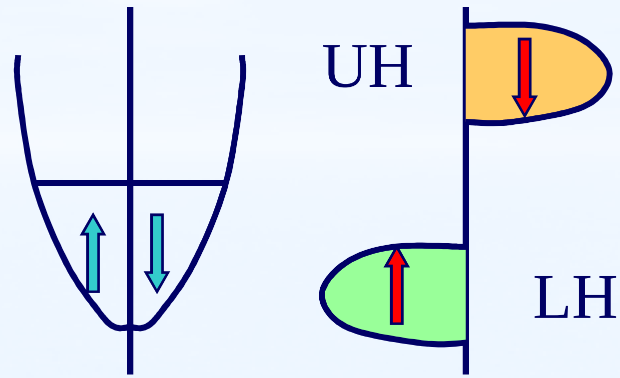
Why Theory and Experiment are so Far Apart?

- Experiment: Complex Reality
  - Chemical disorder, multiple degrees of freedom, inhomogeneity…….
- Theory: Simplicity
  - Cannot solve even toy models.
  - Long-range Coulomb interaction usually neglected.

“High-Energy” Physics

- Hubbard *U*. and Mott insulator

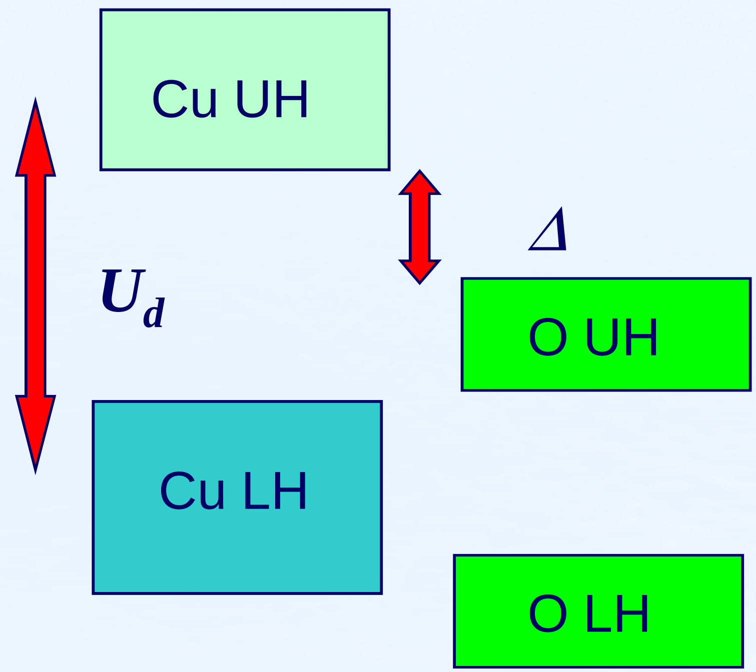
$$H = \sum_{i,j,\sigma} t_{ij}\left(c_{i\sigma}^{+}c_{j\sigma} + c_{j\sigma}^{+}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



- Charge transfer gap for multi-band Hubbard.

$$U_d = 8, \quad U_p = 4, \quad t_{pd} = 1$$

$$\Delta = 2$$

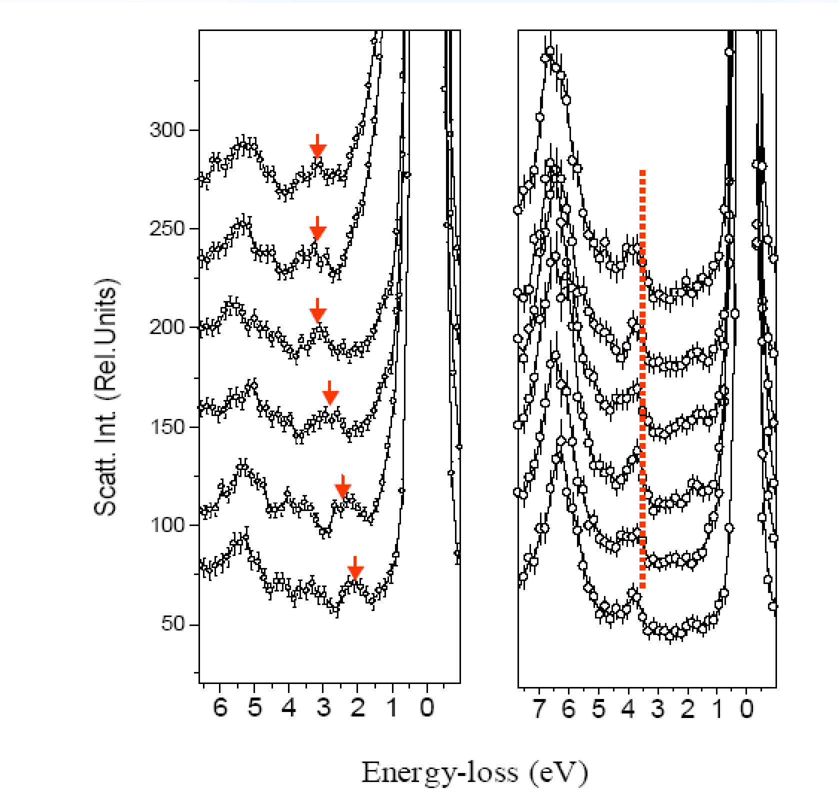


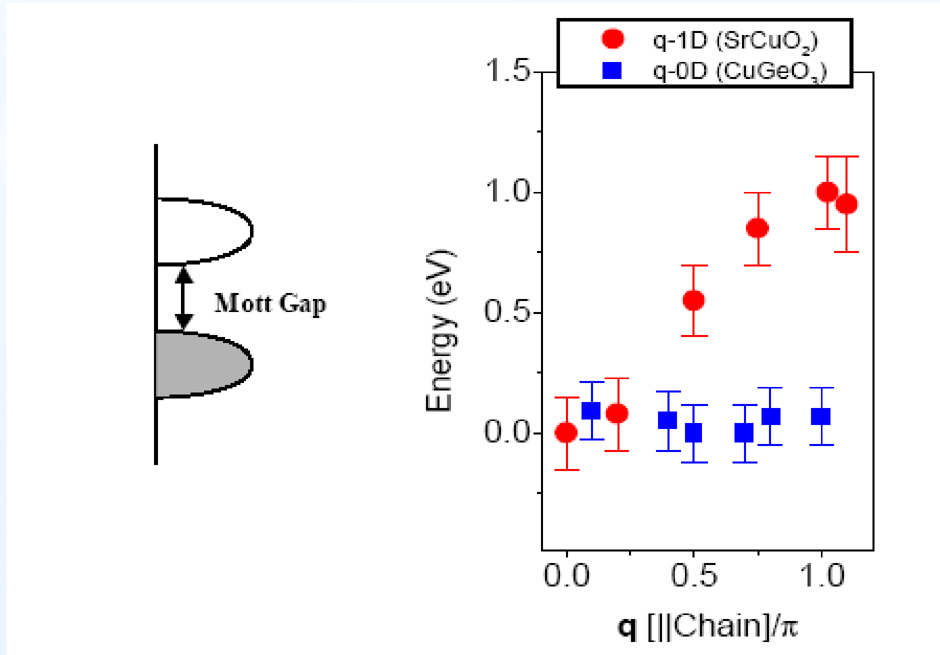
- *t-J* model.
  - Start with the *U* = ∞ state, expand by *t/U*.

$$H_{t-J} = \sum_{i,j,\sigma} t_{ij}\left(c_{i\sigma}^{+}c_{j\sigma} + c_{j\sigma}^{+}c_{i\sigma}\right) + J\sum_{i,j} \mathbf{S_i}\cdot\mathbf{S_j},$$

$$J = \frac{4t^2}{U}$$

Mott-Hubbard Gap by Inelastic X-ray Scattering

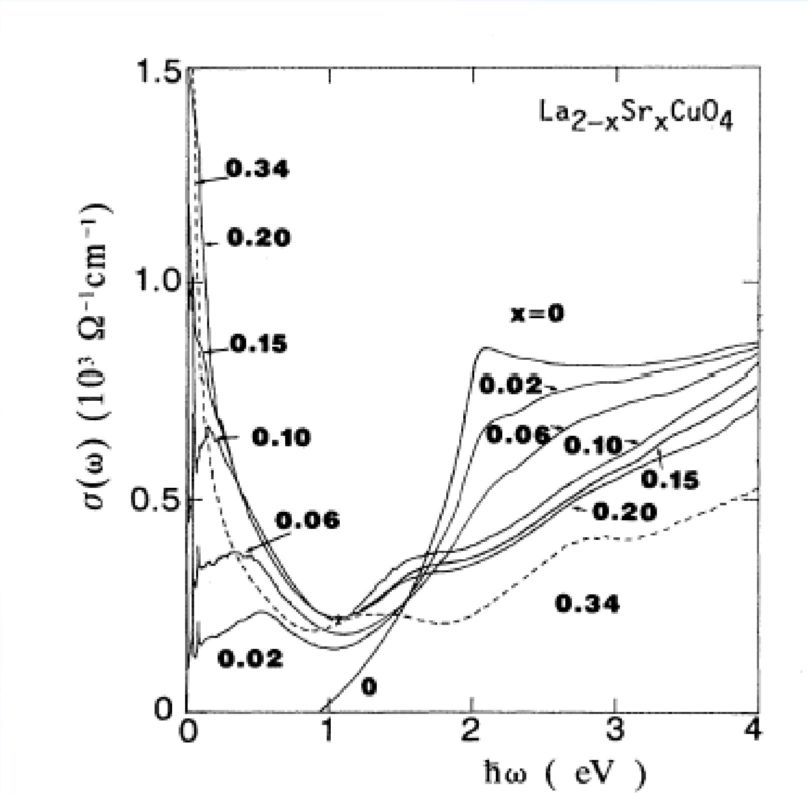




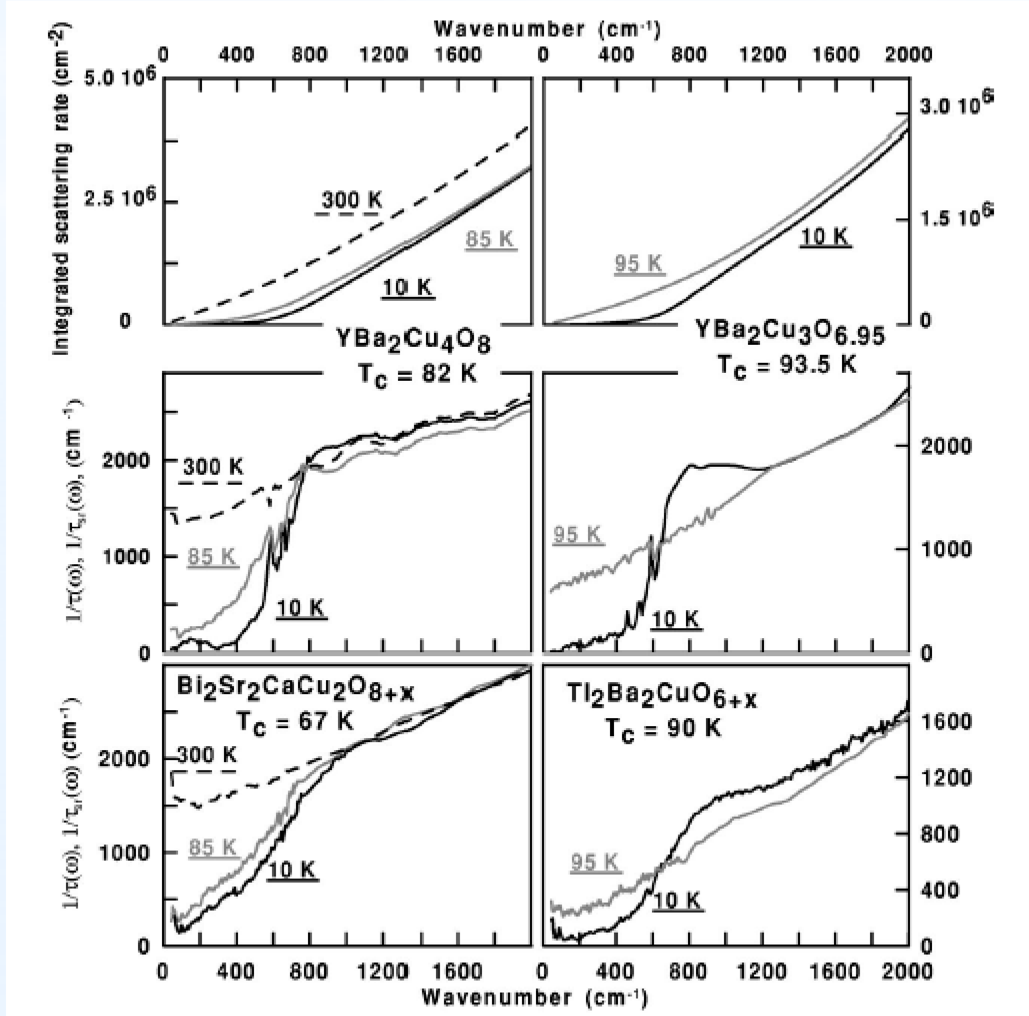
M. Z. Hasan, *et al.*, *Int. J. Mod. Phys. B* **17**, 3513; 3519 (2003); *Phys. Rev. Lett.* **88**, 177403 (2003).

- IXS: ΔE ~ 2 meV (non-resonant), ~ 100 meV (resonant).
- Dispersion in the Mott-Hubbard excitation. Stronger for the 2-d system ($SrCuO_2$) than 1-d system ($CuGeO_3$).

Optical Conductivity



S. Uchida, et al., PRB 43, 7942 (1991).

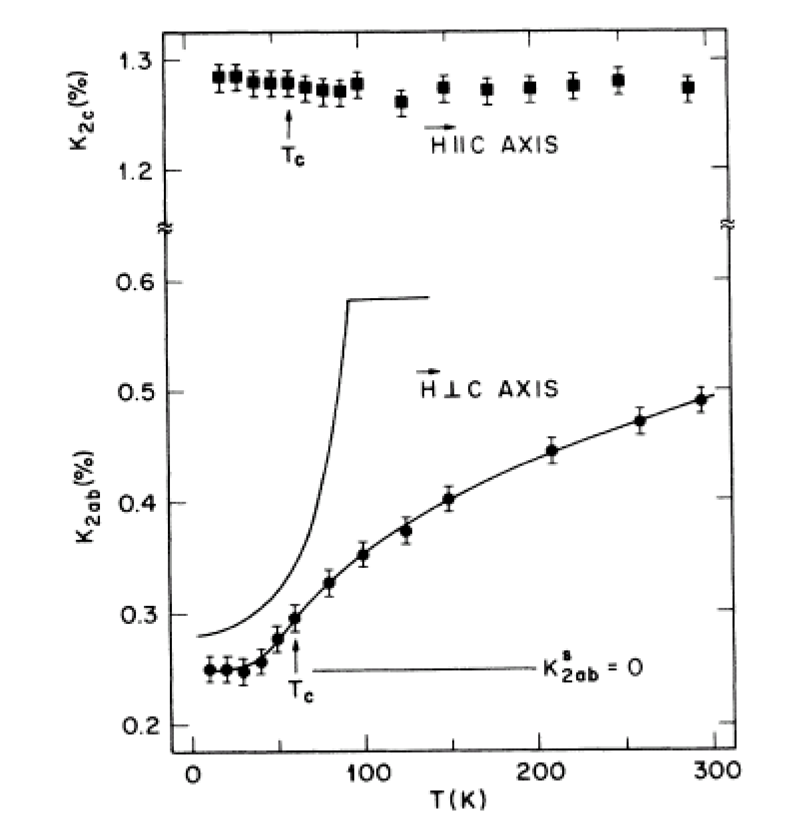


D. N. Basov, E. J. Singley and S. V. Dordevic, *Phys. Rev. B* **65**, 054516 (2002)

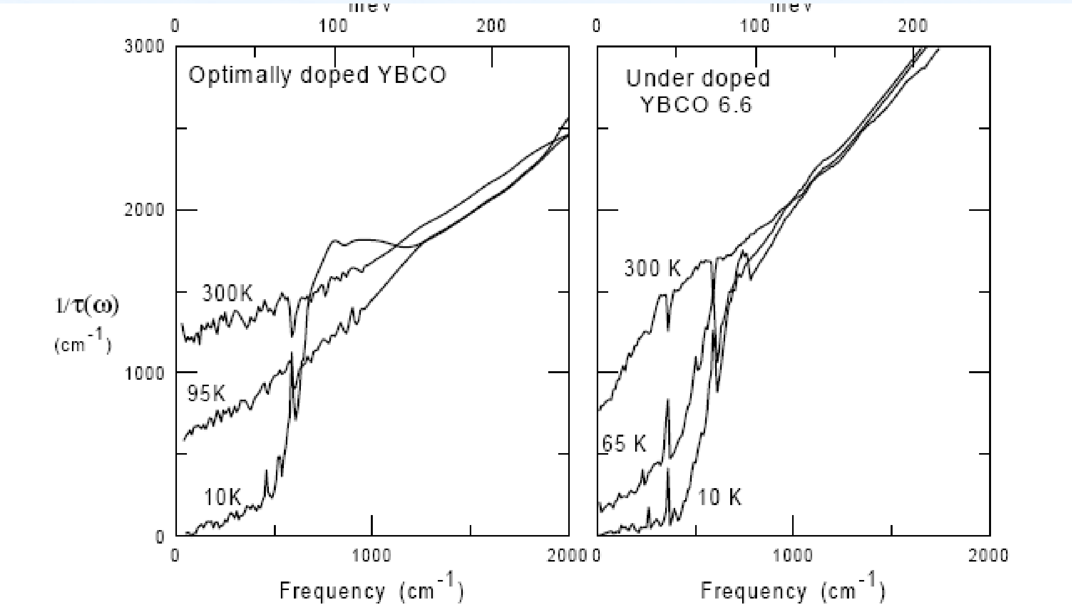
- "High-energy physics" reflected in low energy physics in more than one way through spin.

Pseudo-Gap

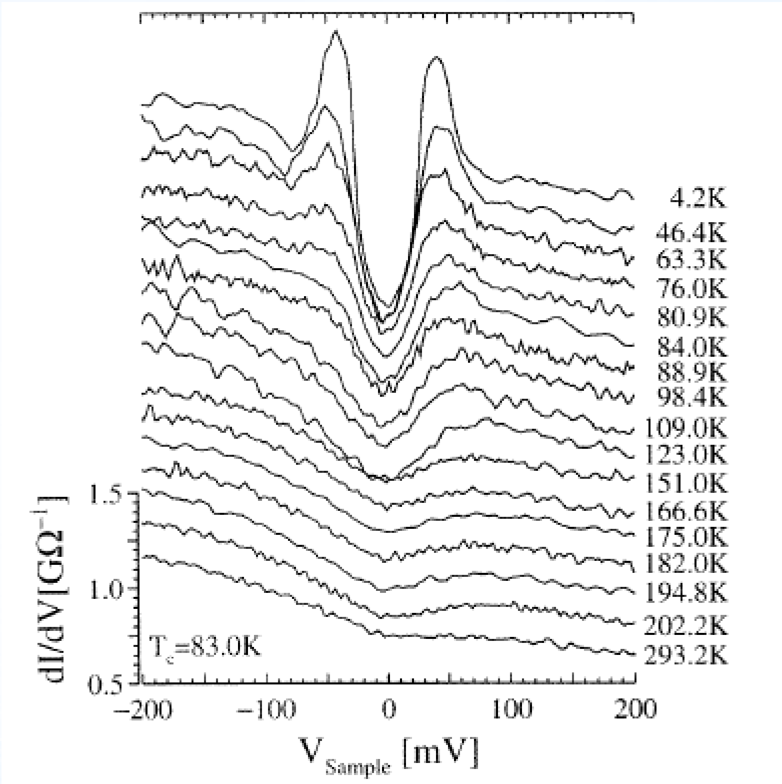
- Observed first by NMR.
- Clearly seen by IR, ARPES and tunneling probes including STS.
- Indirectly seen by resistivity, Hall effect, thermal conductivity.

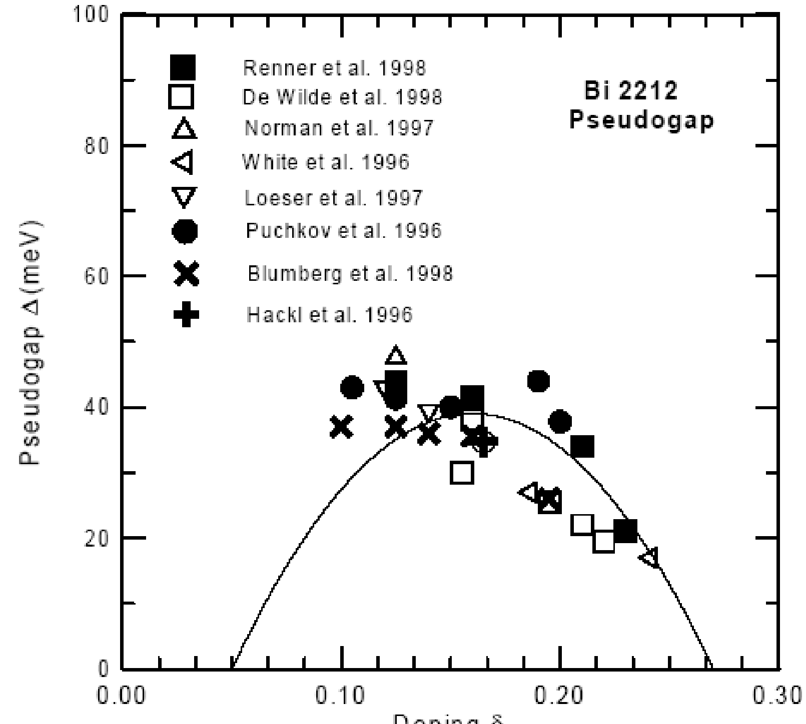


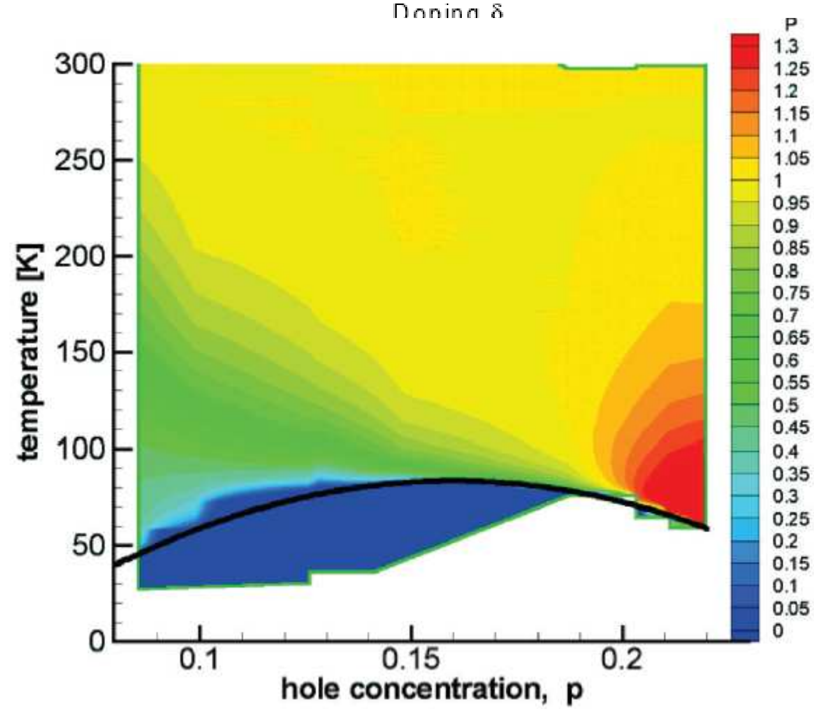
R. E. Walstedt et al., *Phys. Rev. B* **41**, 9574 (1990).



T. Timusk and B. Statt, *Rep. Prog. Phys*. **62**, 61 (1999).





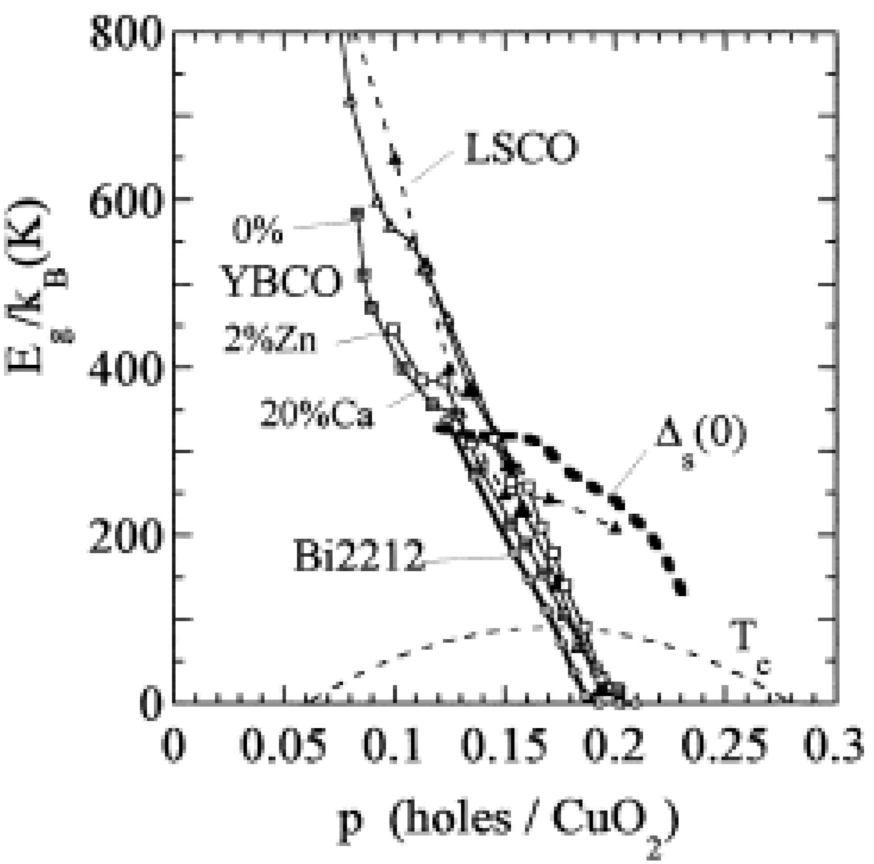


- SC gap for local pairing?
- Energy gap due to a competing order parameter?

T vs. $\rho(T)/(\rho_0 + \alpha T)$ for $Y_{0.7}Ca_{0.3}Cu_3O_{7-\delta}$, Tallon, Lorum

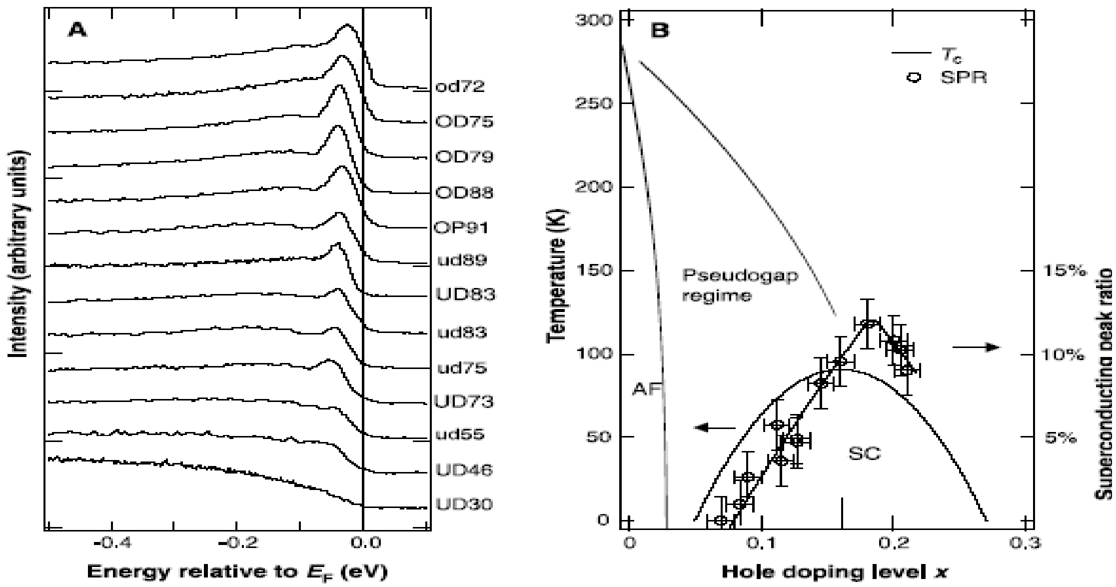
Quantum Criticality

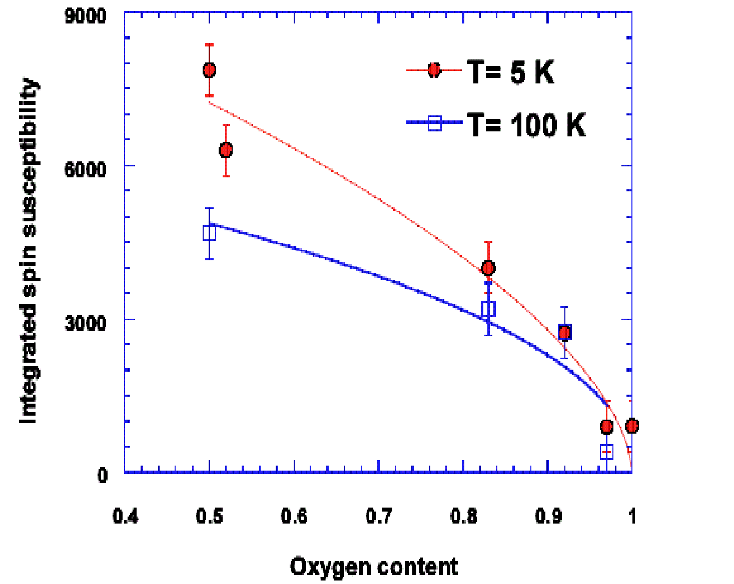
- Strong quantum fluctuations near the quantum critical point (QCP) promotes SC.
- The nature of the QCP is critical.



J. W. Loram, et al., *J. Phys. Chem Solids,* **62,** 59 (2001)

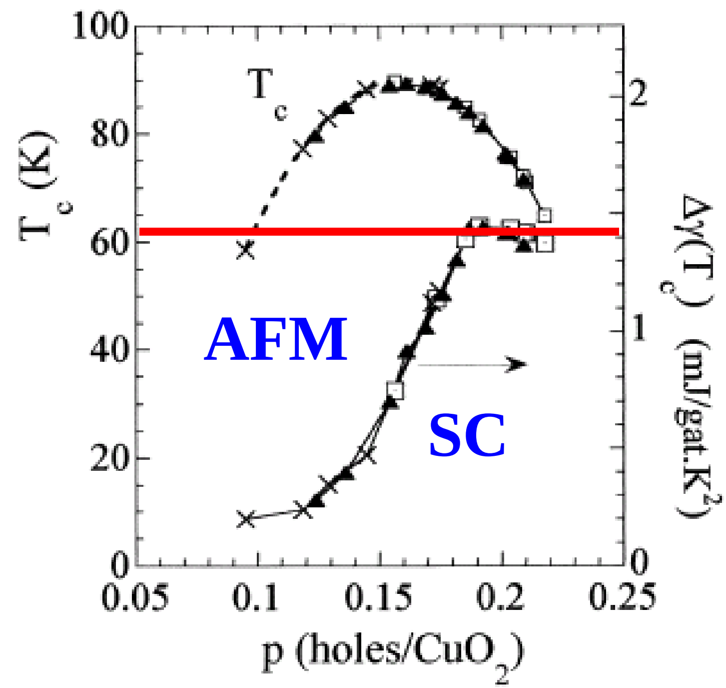
Superfluid Density from ARPES





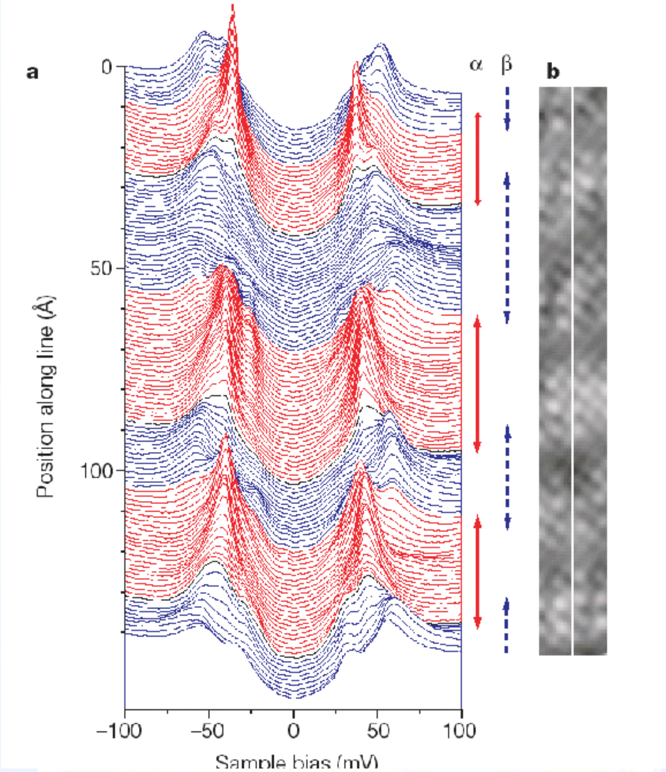
D. L. Feng, *et al, Science* **289**, 277 (2000).

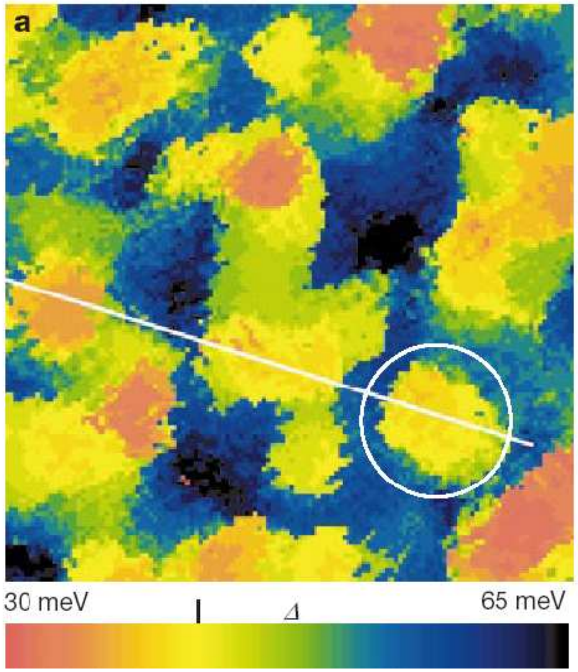
- Superconductivity competing against local AFM spin correlation.
- Sign of electronic phase separation (Moreo, Dagotto).
- PG phase mixture of SC and AFM phase.
- T_C is low because of phase coherence is low.



Spatial Electronic Inhomogeneity

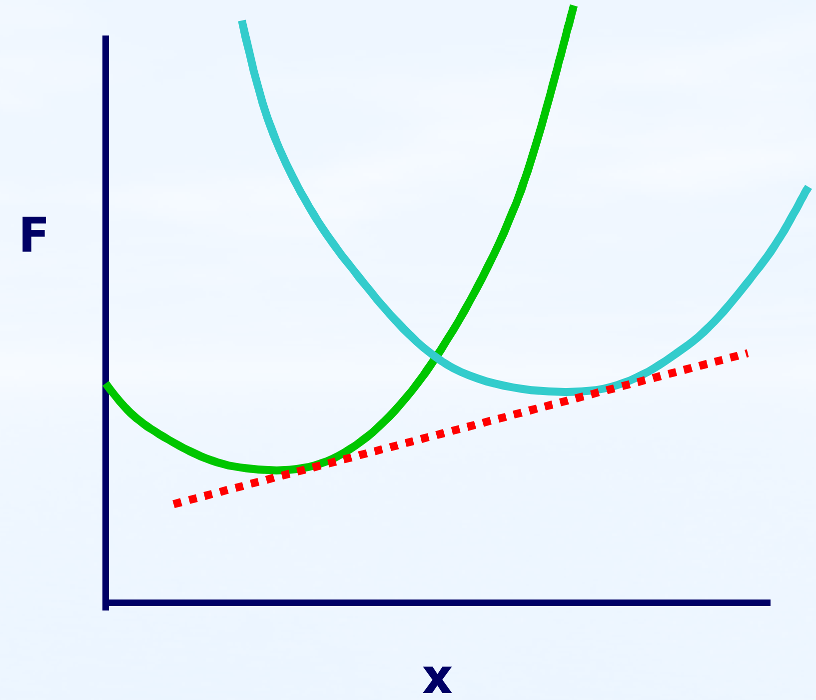
- Predicted by Gor'kov (1987), and studied by many (K. A. Muller).
- STM/STS studies by the group of Seamus Davis reveal electronic inhomogeneity in the underdoped cuprates.
- The size of the domains is comparable to ξ.
- The nature of the variation unclear.

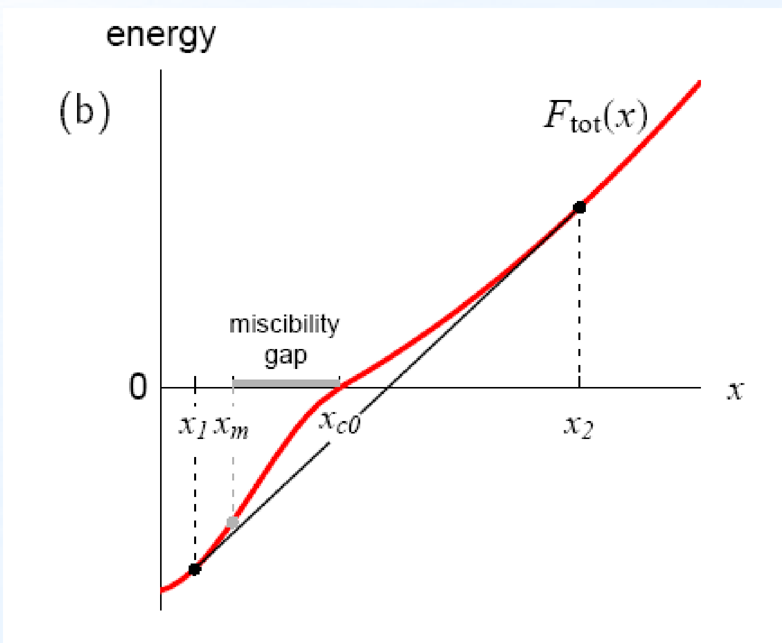


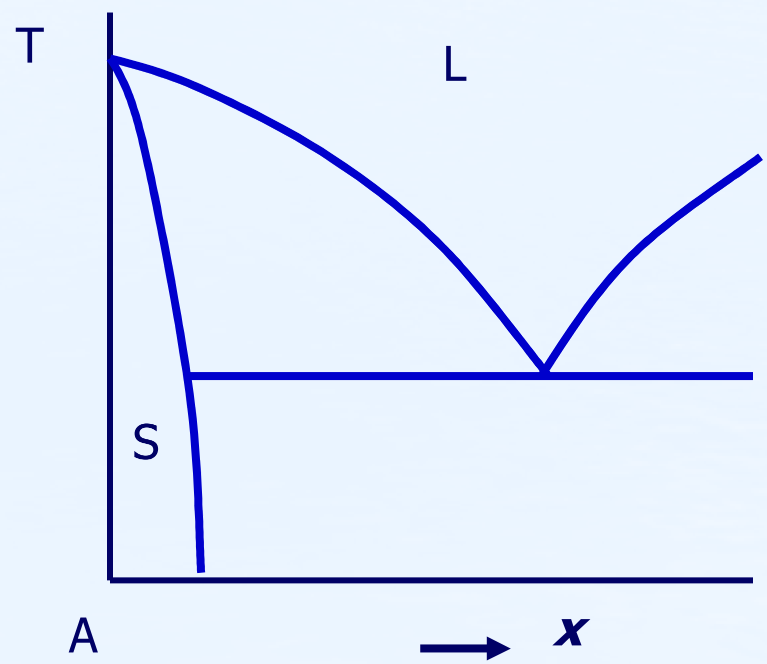


Phase Transition and Phase Separation

- Phase transition is a recipe for phase separation; water and ice.
- Similar argument for the second order transition.



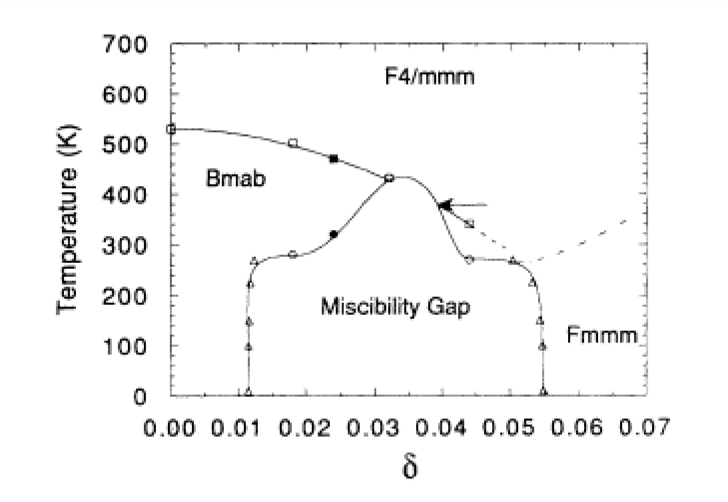




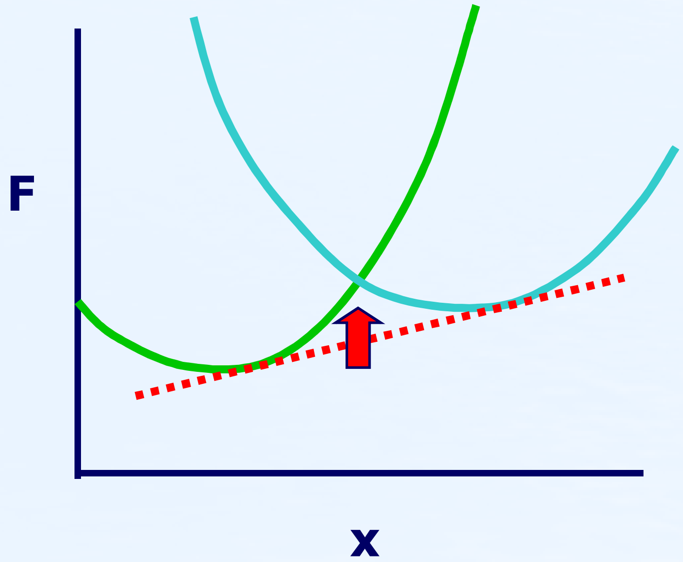
Electronic Phase Separation

- Macroscopic phase separation occurs if atoms are mobile.
- If electronic mobility is high but atomic mobility is absent, **electronic phase separation with charge** occurs (V. Emery and S. Kivelson, E. Dagotto, et al.).
- Long-range Coulomb attraction and short range repulsion for phase separation creates the medium-range order (A. R. Bishop).

$La_2CuO_{4+\delta}$

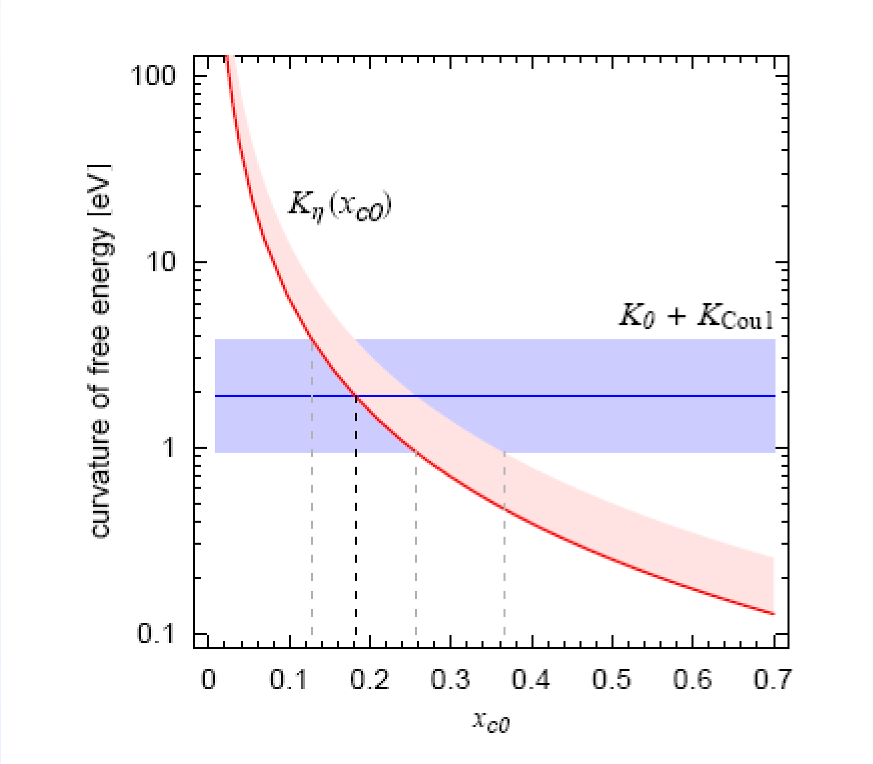


P. G. Radaelli, et al., *Phys. Rev. B* **49,** 6239 (1994).



Electronic Phase Separation in the Cuprates

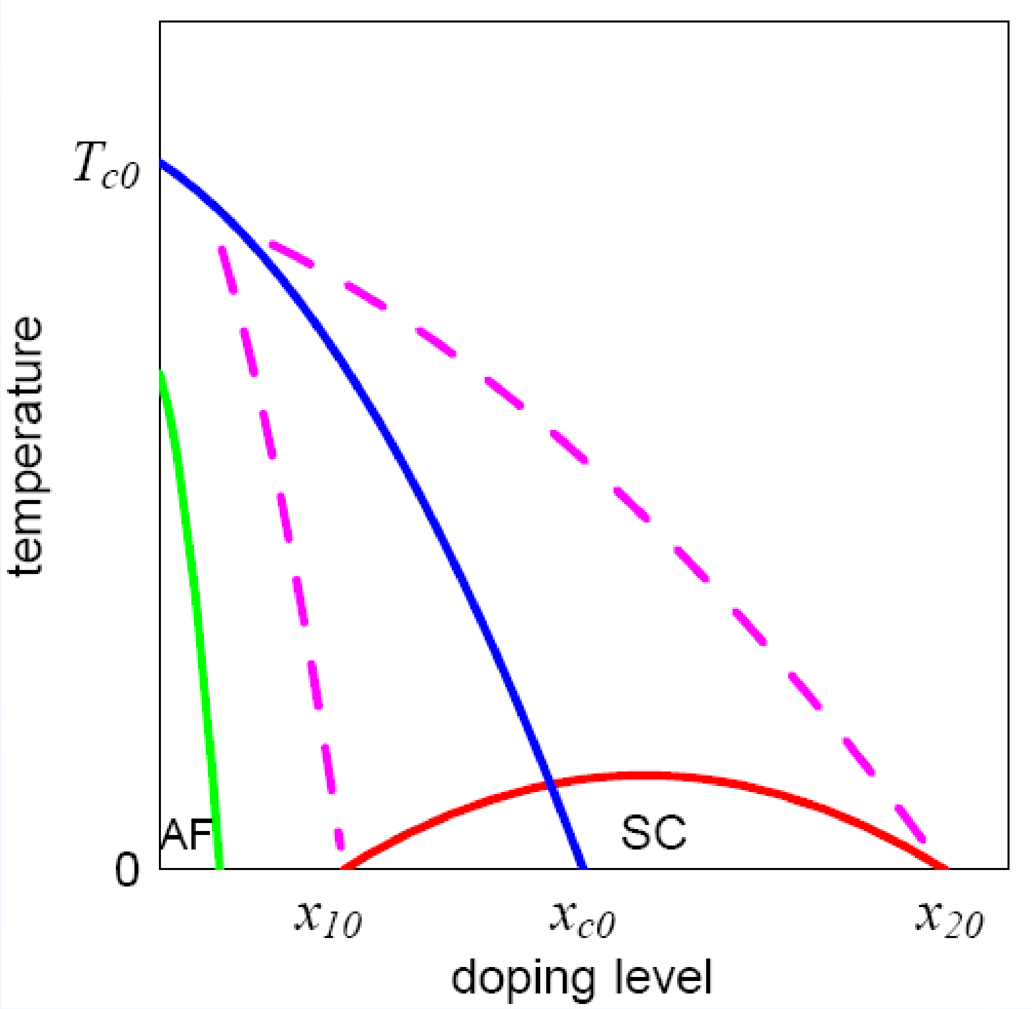
- Realistic model calculation including long-range Coulomb interaction.
- LR Coulomb interaction suppresses AFM.
- Phase separation likely.
- Self-organization into nano-scale phases, including the "lasagna" model (pasta model in cosmology), and other 2-D intermediate phases.



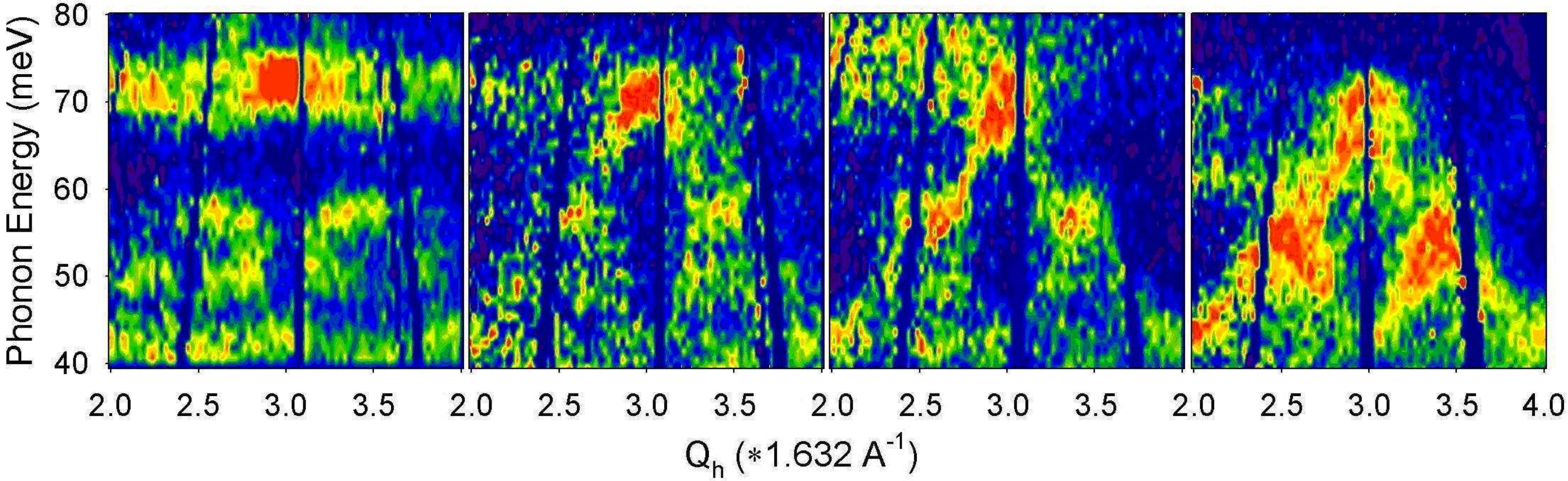
B. Fine and T. Egami, arXiv/0707.3994, PRB in press.

A New Phase Diagram

- x_{c0} (~ 0.12) is the QCT.
- x_{c0} close to the MIT point under filed.
- The upper limit line defines T_{PG}.



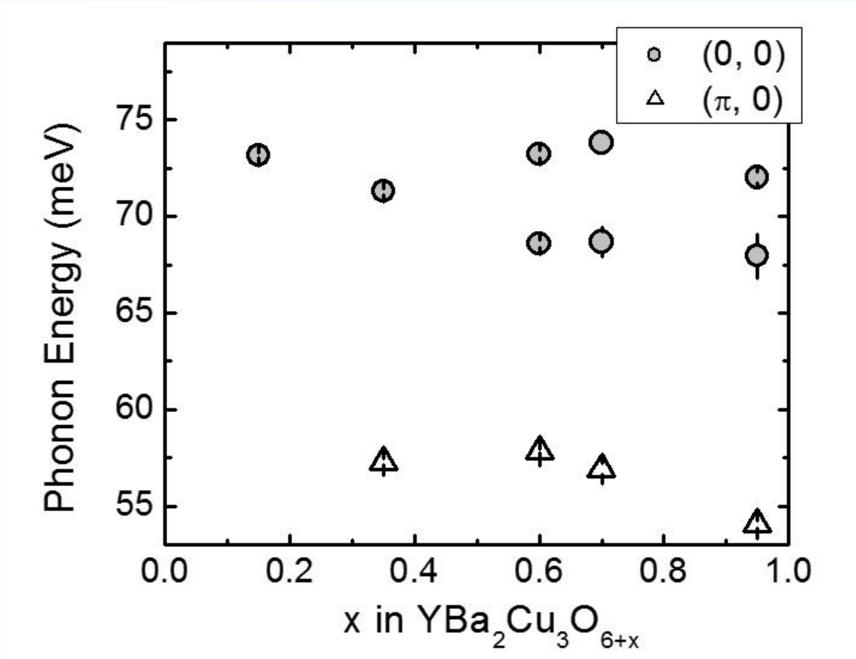
Cu-O Bond-Stretching Phonon in $YBa_2Cu_3O_x$

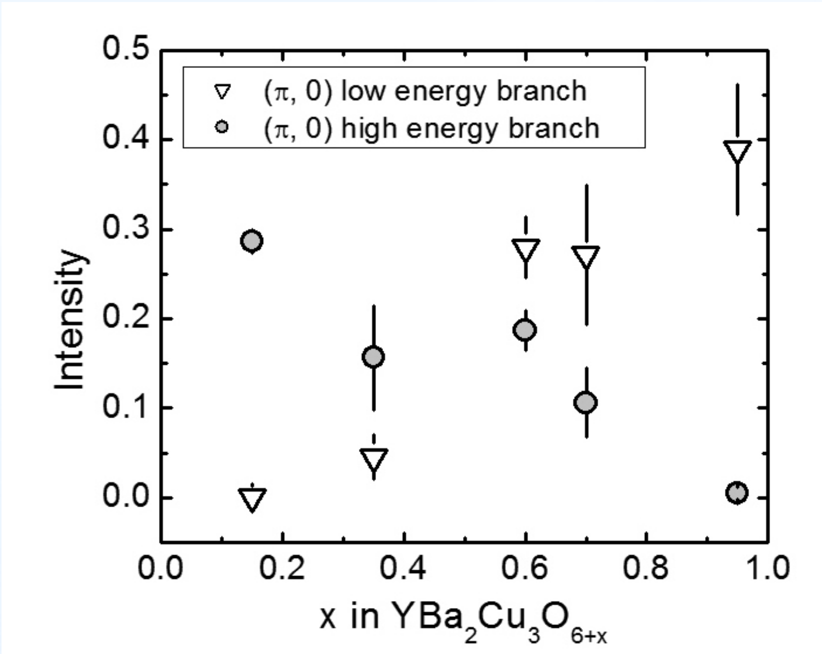


6.15 **6.35** **6.6** **6.95**

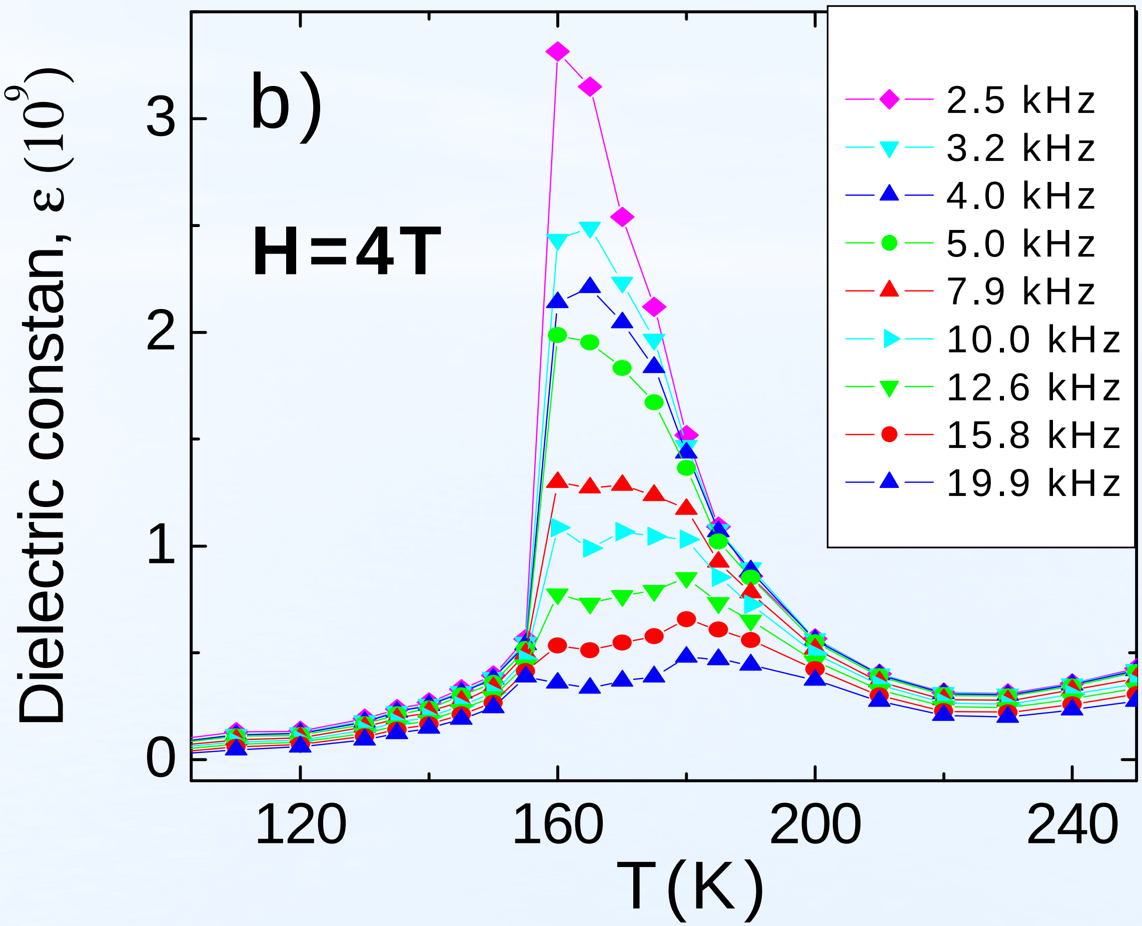
- No dispersion for YBCO x = 6.15.
- Not much difference in dispersion from 6.35 to 6.95.
- Intensity at zone-boundary changes.
- Since 6.35 is tetragonal this is not the consequence of anisotropy.

T. Egami, *Physica C*, **460-462,** 267 (2007)





- The magnitude of softening is independent of *x*, but the intensity of the softened branch increases with increasing *x*.
- At $x = 6.15$ the intensity is due to the apical mode.
- The increase has to be due to the local modes.
- Softened (SC) and unsoftened (AFM) domains?



- Maxwell-Wagner effect in $La_{0.875}Sr_{0.125}MnO_3$.

R. Mamin, T. Egami, Z. Marton and S. A. Migachev, *PRB* **75,** 115129 (2007).

Nature of the Phase-Separation

- Competing order simply reduces T_C in the underdoped samples.
  - AFM order disrupts SC phase coherence.
- Necessary for the mechanism.
  - Stripes: AFM phase provides spin fluctuations.
  - Intermediate order and two-component scenario: Magnetic phase supports local bipolarons.
  - **Increases the energy of the normal state, and promotes SC (Zaanen): A glass half-full or half-empty.**

Neutron Scattering from YBCO6.6 Single Crystal

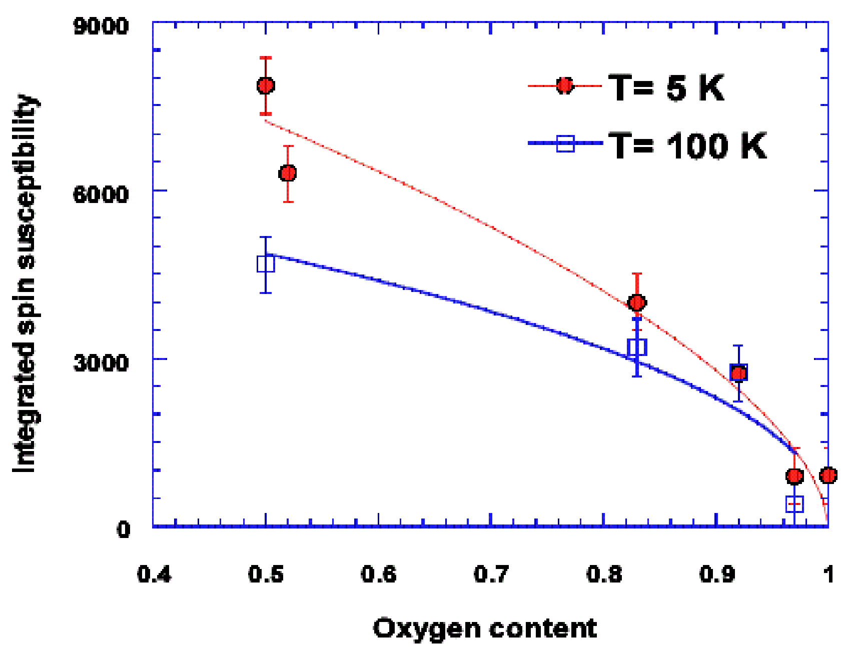
- $YBa_2Cu_3O_{6.6}$ single crystal (25g). T_C = 60 K.
- Neutron elastic scattering, spin unpolarized.
- SPINS, NIST; HB1-A, HFIR, ORNL.
- Temperature dependent scattering.
- Green phase (Y_2BaCuO_5) ~ 10%, T_N = 16K.
- Close to $Q = 0$, almost no effect of phonons.

Spectral Weight

- Fluctuation-dissipation theorem:

$$\langle S(t)S(0)\rangle = \frac{kT}{\pi}\int_0^\infty \frac{\chi_{im}}{\omega}\cos(\omega t)\,d\omega$$

$$\frac{kT}{\pi}\int_0^\infty \frac{\chi_{im}}{\omega}\,d\omega = \langle S(0)^2\rangle = S(S+1)$$



Philippe Bourges, in “neutron Scattering In Novel Materials”, ed. A. Furrer (World Scientific, 2000); cond-mat/0009373

Localized spin $\rightarrow$ Itinerant spin

Energy scale changing from *J* to *t*.

Dark Matter?

- Does total intensity satisfy the sum-rule; Dark Matter?

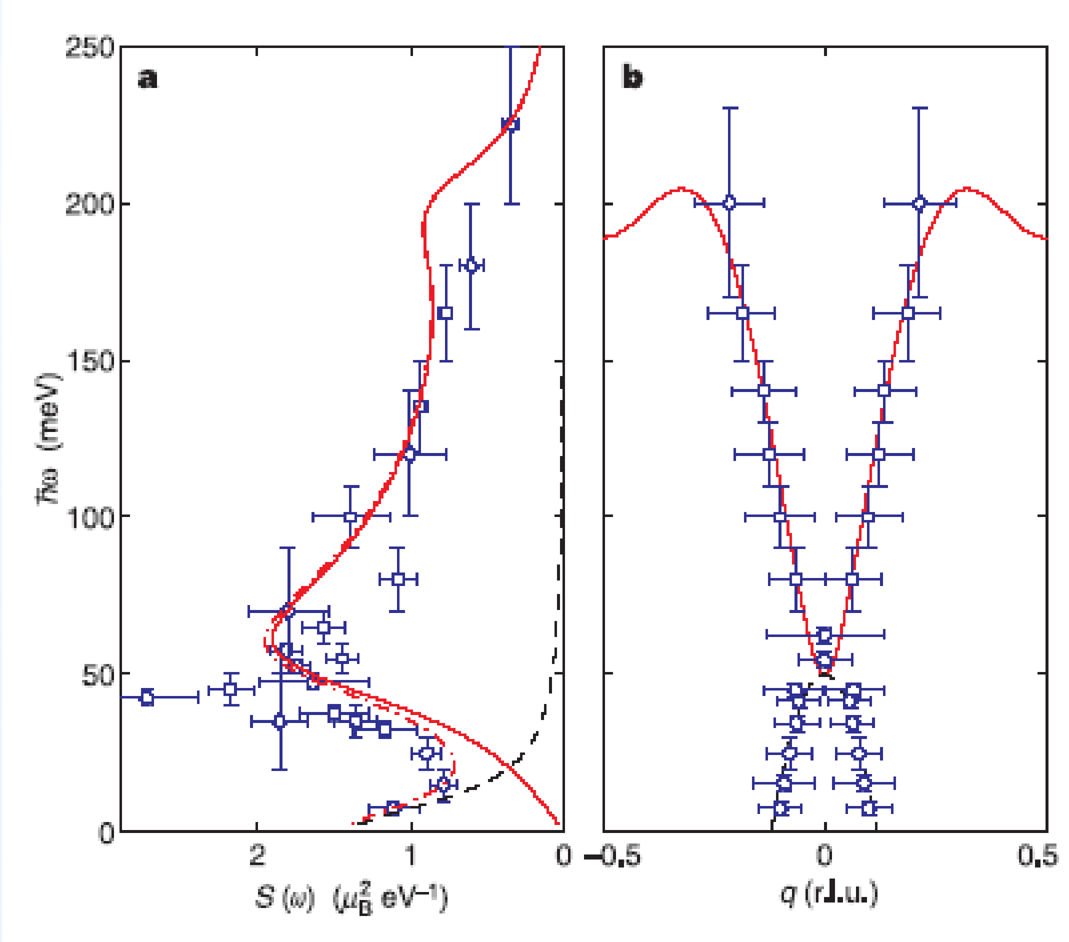
- Integrated value of $\langle\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle\rangle$:

	Inelastic	Elastic
6.15	0.4 μ_B^2	The rest
6.6	0.38 μ_B^2	?
6.95	0.18 μ_B^2	?

H. Woo, et al., *Nature Physics* **2,** 600 (2006).

More Mysteries

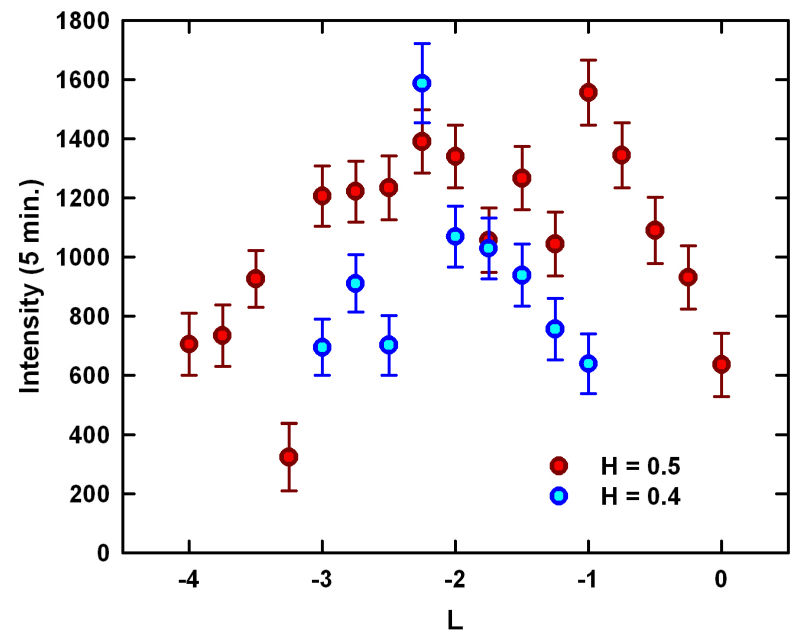
- Long correlation length (~50 Å) of spin excitations, but the spin correlation never directly seen.
- Similarity in the spectrum is the basis for dynamic (nematic) stripe state. But no one has seen dynamic stripes…….



J. M. Tranquada, et al., *Nature,* **429,** 534 (2006).

CuO_2 Bilayer

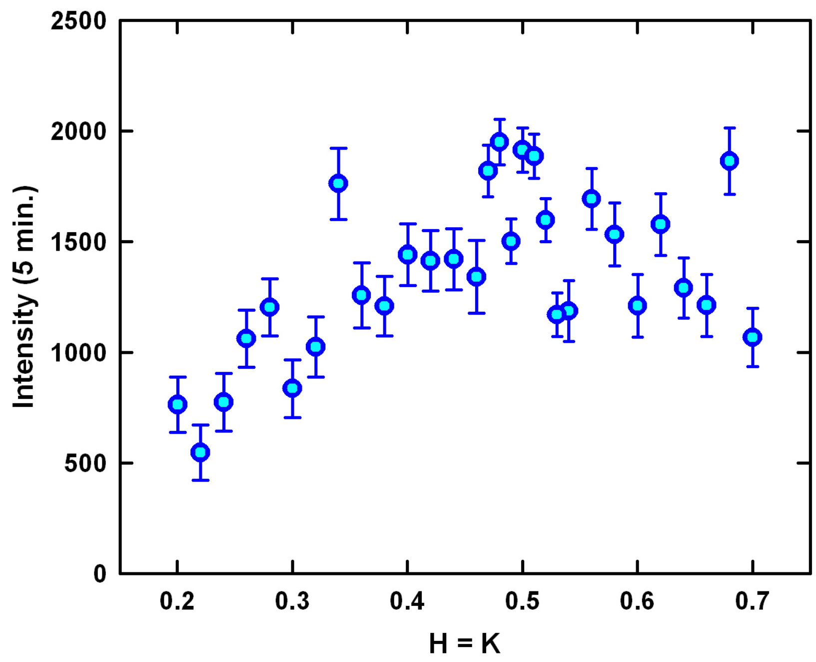
- CuO_2 bilayer with the separation of 3.2 Å, corresponding to L = 3.6.
- A peak at L = 1.8 most likely due to AFM spin correlation in the bilayer.
- Similar peak seen for the neutron resonance peak.



I(20K) – I(270K) for (H, H, L) scan. A peak at L = -2 most likely due to bilayer AFM correlation.

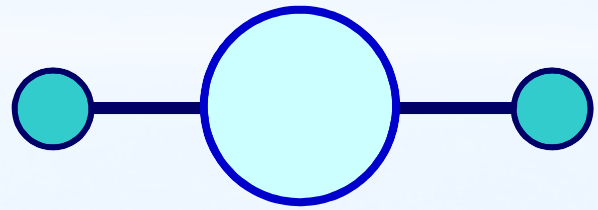
Spin-Glass-Like Behavior

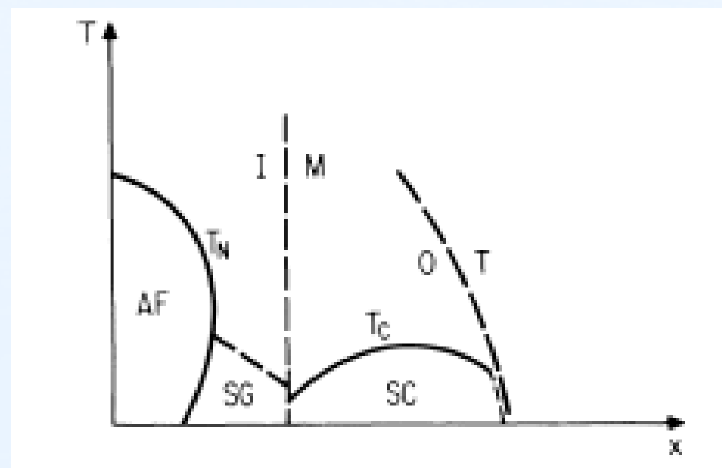
- Broad in H.
- If cluster AFM, the temperature dependence should be super-paramagnetic 1/T behavior.
- Likely to involve positive *J* as well.
- **Poster P24**, Watanabe, et al. by μSR.



Spin-Glass and Variation in J

- The presence of spin-glass state implies that some *J*'s are positive.
- Amnon Aharony and Vick Emery predicted it, when hole resides on oxygen, not in the Z-R singlet state.
- In manganites double-exchange results in positive *J*.
- *t-J* model is insufficient.
- Average *J* decreases with doping (**Yamada, yesterday**)
- The system is **STRONGLY FRUSTRATED**.

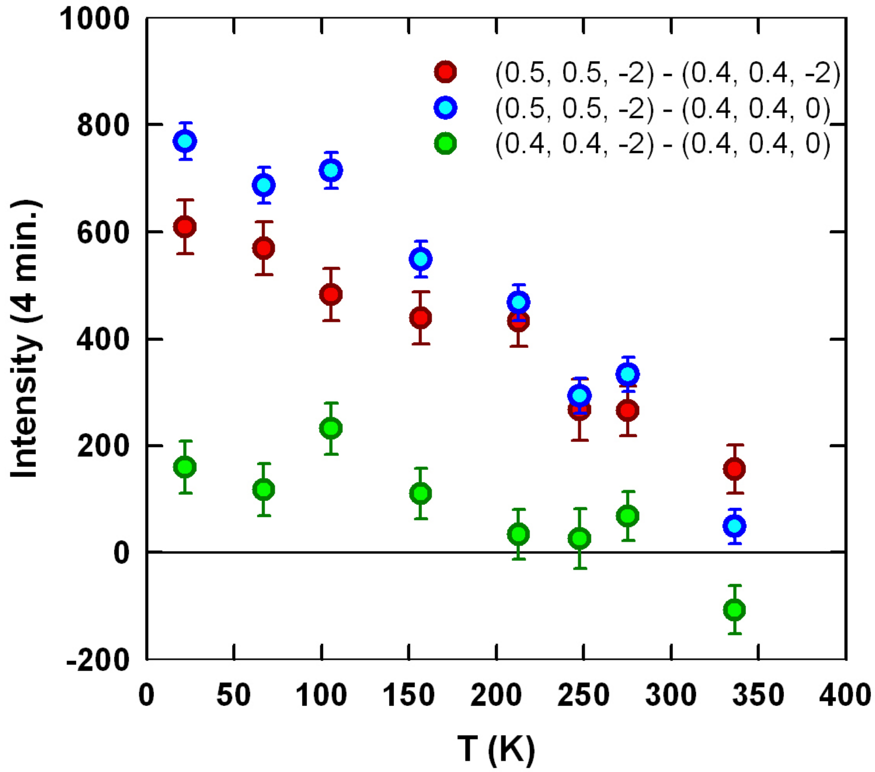




A. Aharony, et al., *PRL* **60,** 1330 (1988)

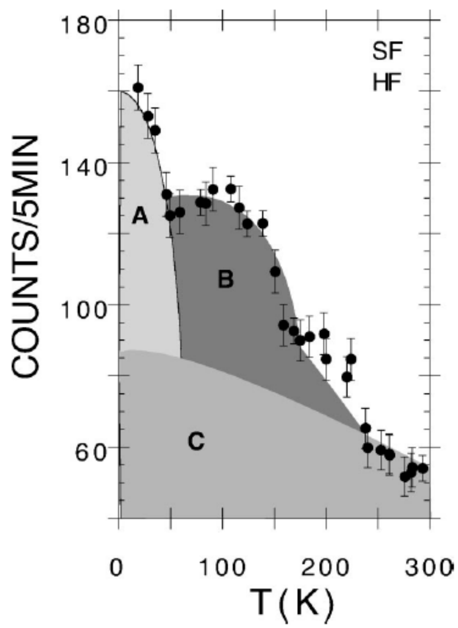
Temperature Dependence

- H = 0.5 feature up to T_{PG1} = 350 K.
- H = 0.4 feature up to T_{PG2} ~ 175 K.
- SG correlation with ξ ~ 20 Å up to T_{PG}.

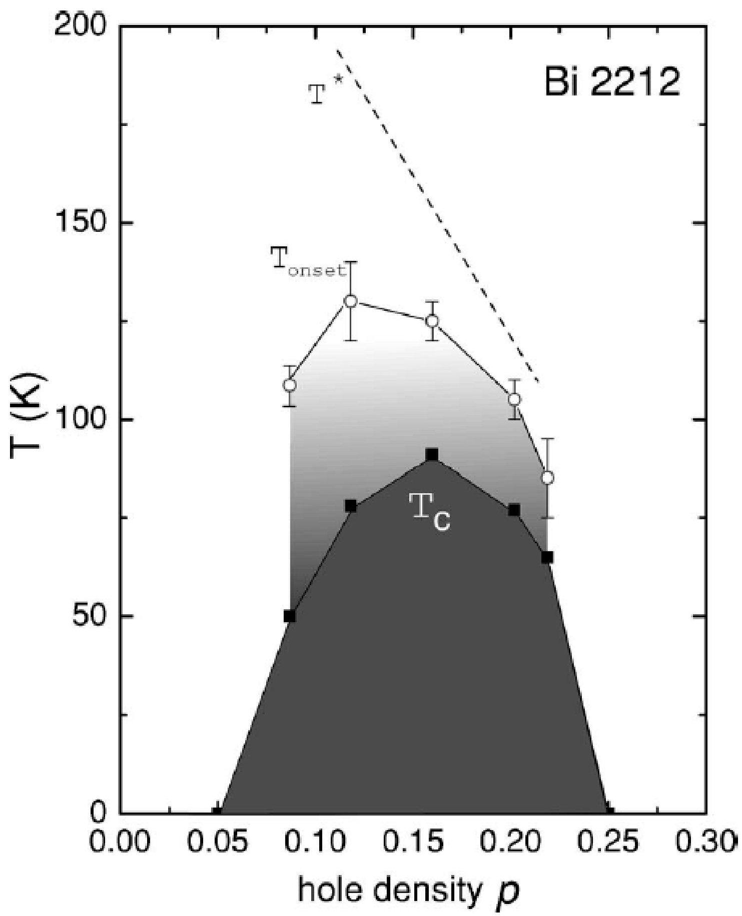


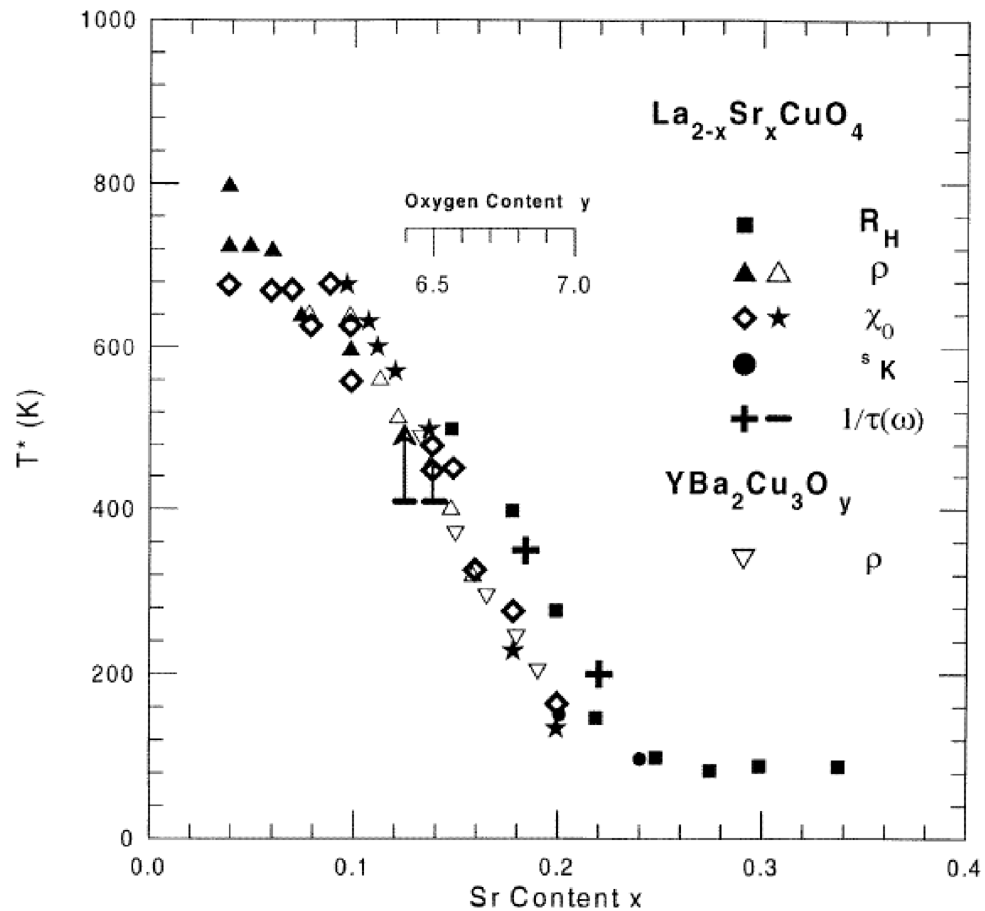
Peak at (0.5, 0.5, 0) in YBCO6.6.

H. A. Mook, *et al*, *PRB* **66,** 144513 (2002).



Pseudogap Temperature





N. P. Ong, *Phys. Rev. B* **73,** 024510 (2006)

T. Timusk and B. Statt, *Rep. Prog. Phys.* **62**, 61 (1999).

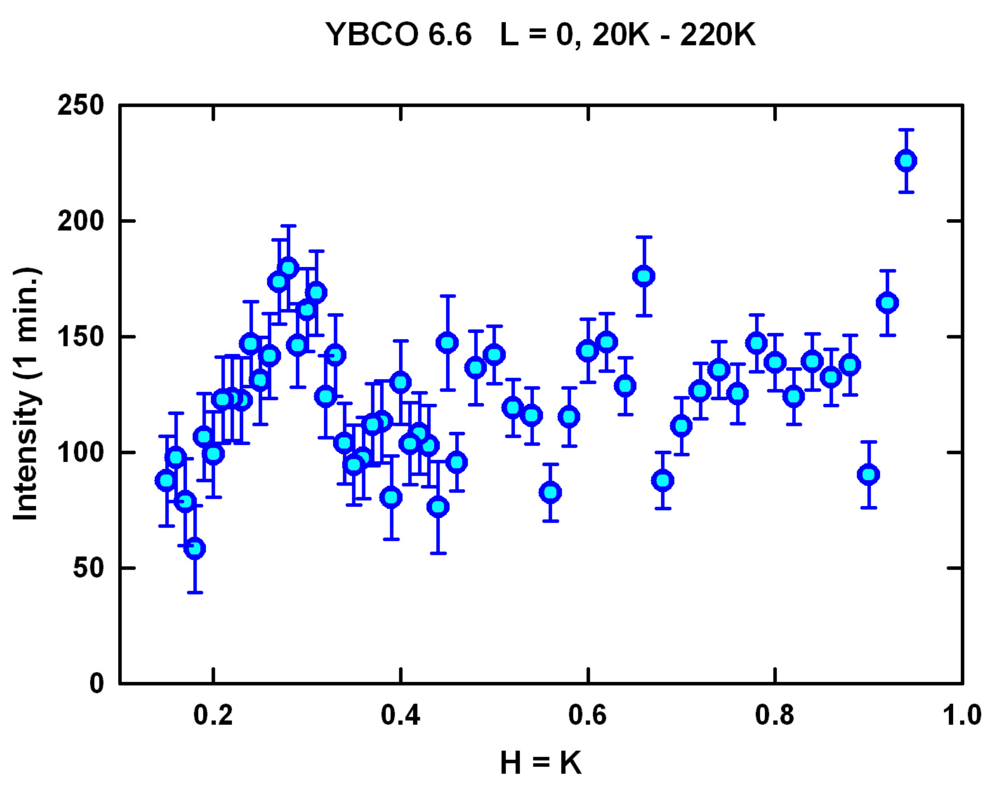
Nature of the PG State

- Competing order
  - Magnetic ordering (local)
  - Orbital magnetism (flux state, *d*-*d*-wave)
  - Charge ordering
- Pre-formed pair
  - Local BCS pairing
  - Bipolarons
- ***Our results***
  - ***T_{PG1}: Local SG order***
  - ***T_{PG2}: Local bipolarons??***

L = 0 Scan

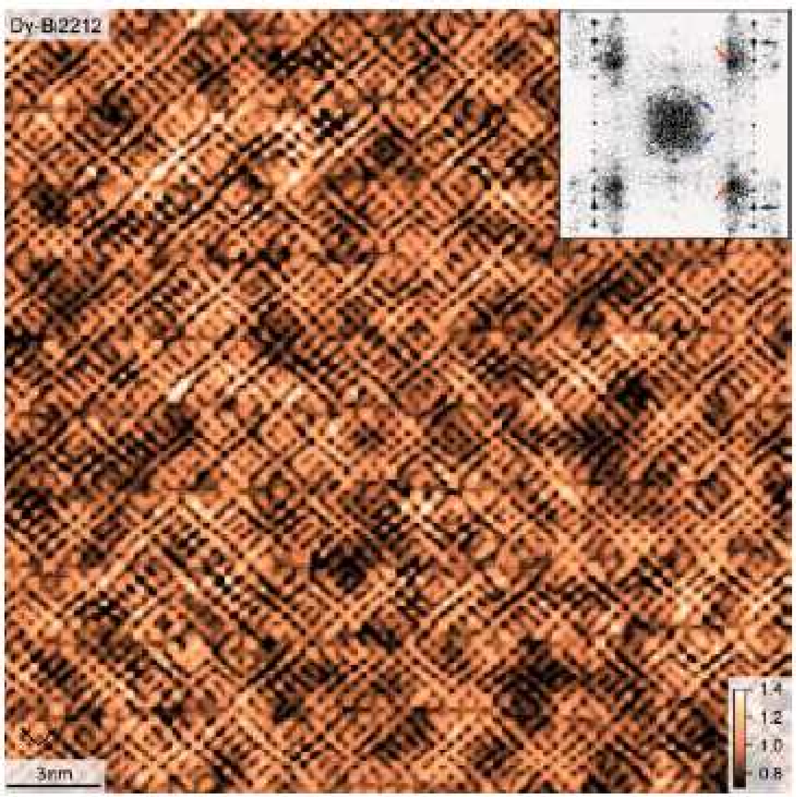
- Complex behavior with a peak around (0.28, 0.28, 0) ~ (1/4, 1/4, 0) could be related to the $2\sqrt{2}\times 2\sqrt{2}$ electronic medium-range order.

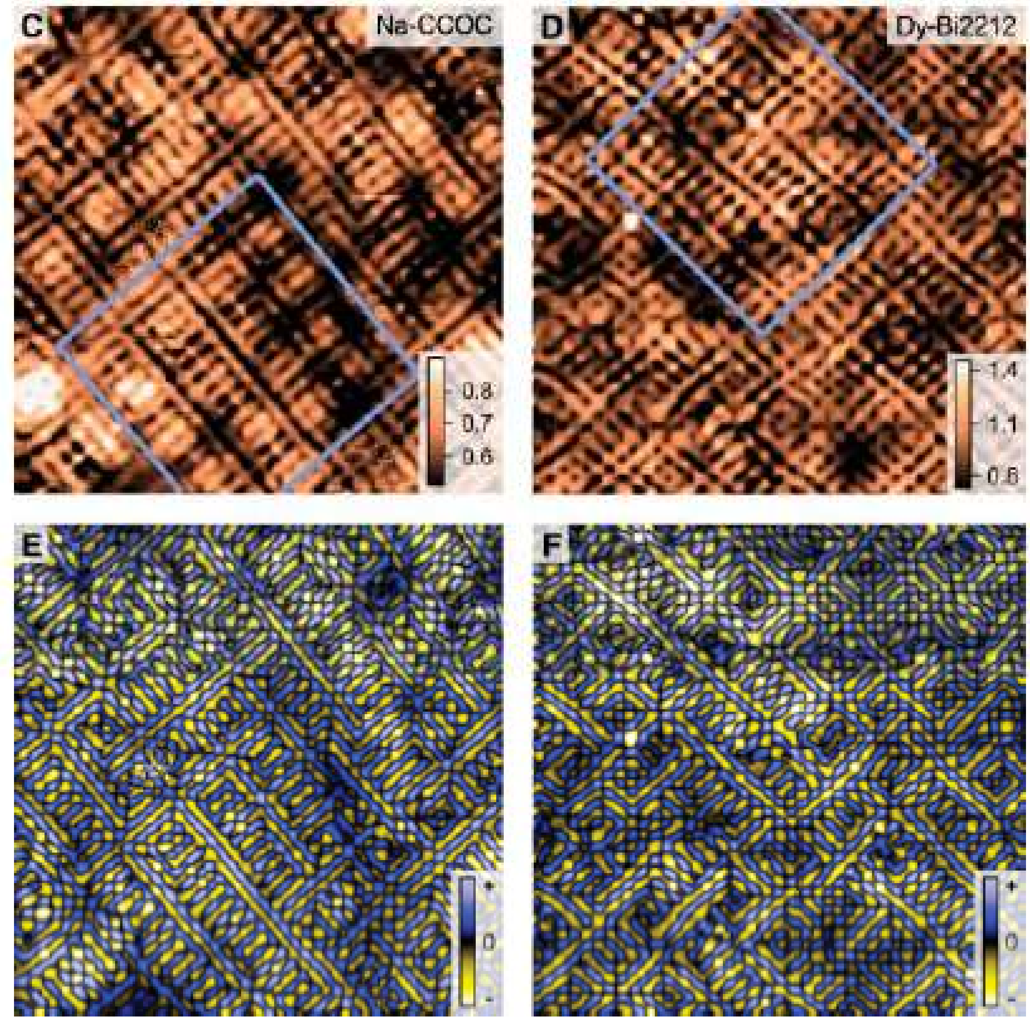
- Significant background; very small at low Q.



Checkerboard

- Hole on oxygen, 4 x 4 structure…..

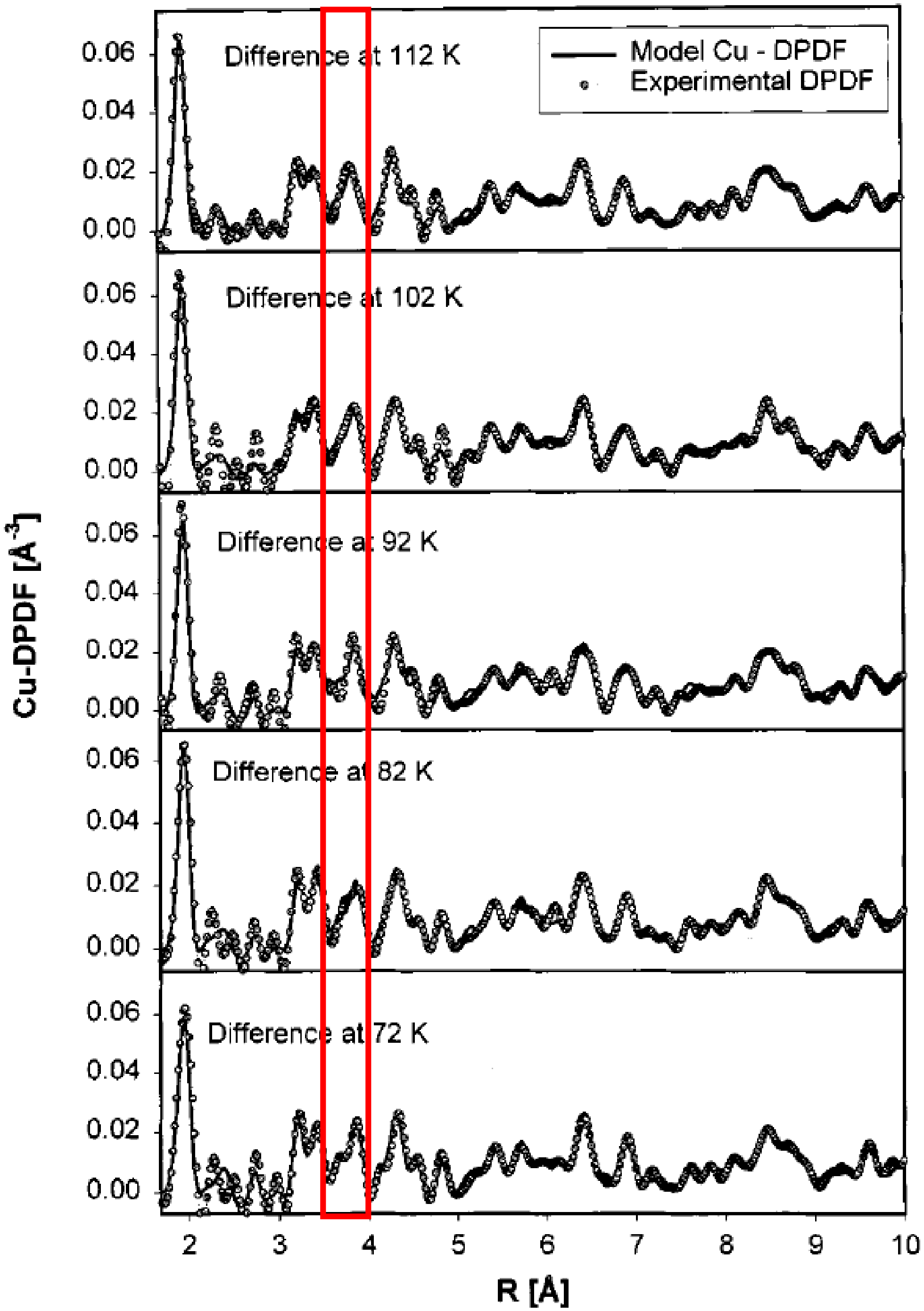




Y. Kohsaka, et al., *Science* **315,** 1380 (2007)

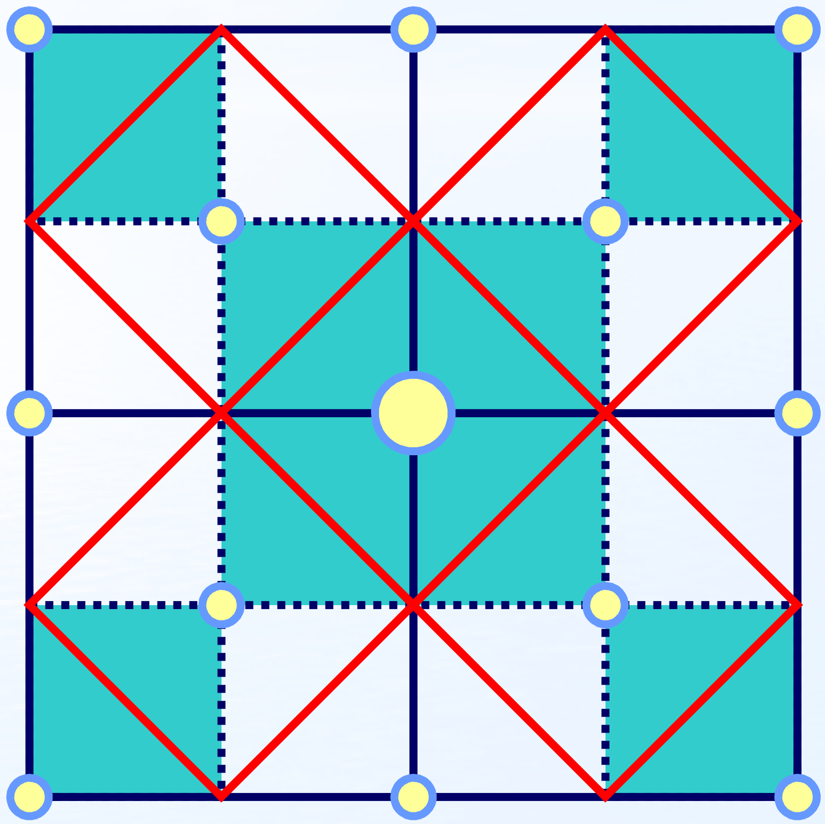
Cu-Cu Peak

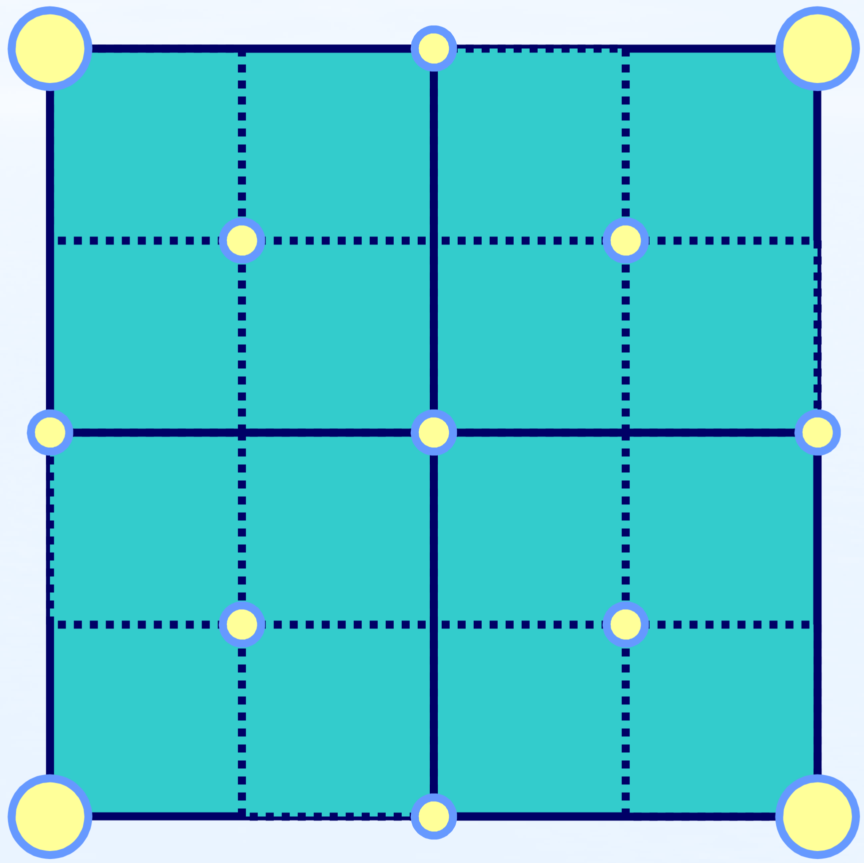
- Cu-partial PDF determined using pulsed neutron PDF with $^{63/65}Cu$ on YBCO6.93 [D. Louca *et al, PRB* **60**, 7558 (1999)] shows the Cu-Cu peak splits into two subpeaks below Tc.



Superlattice

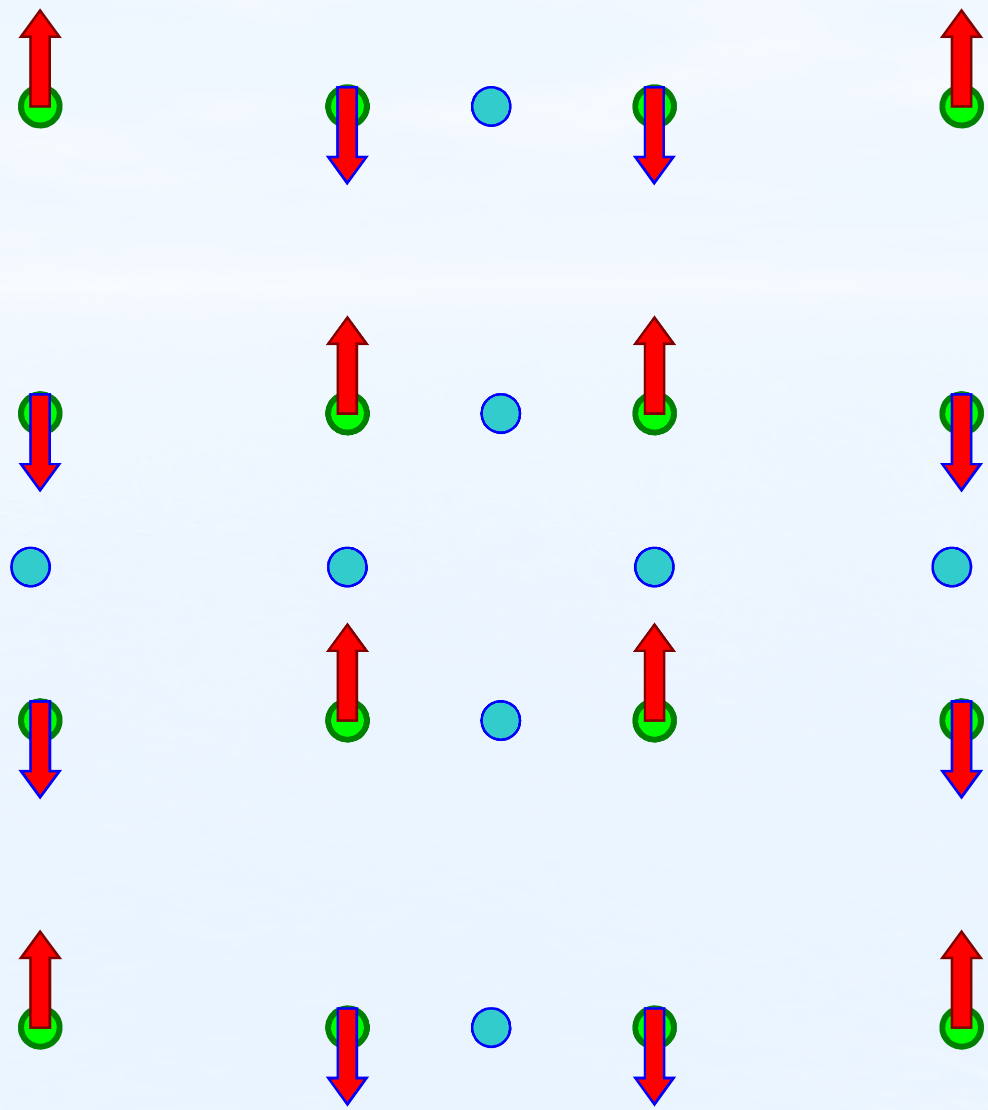
- (π/2, π/2) superlattice.

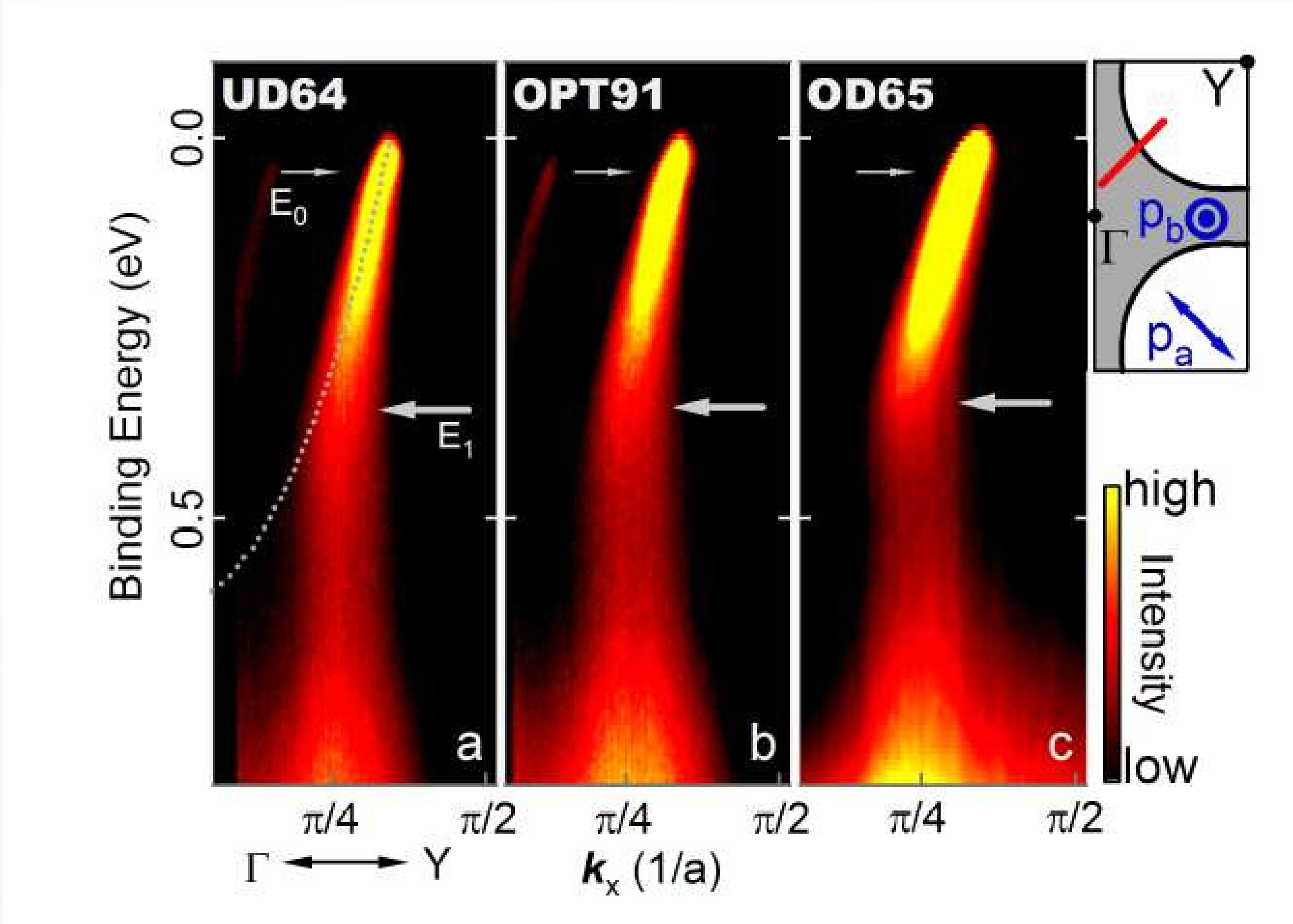




Superlattice

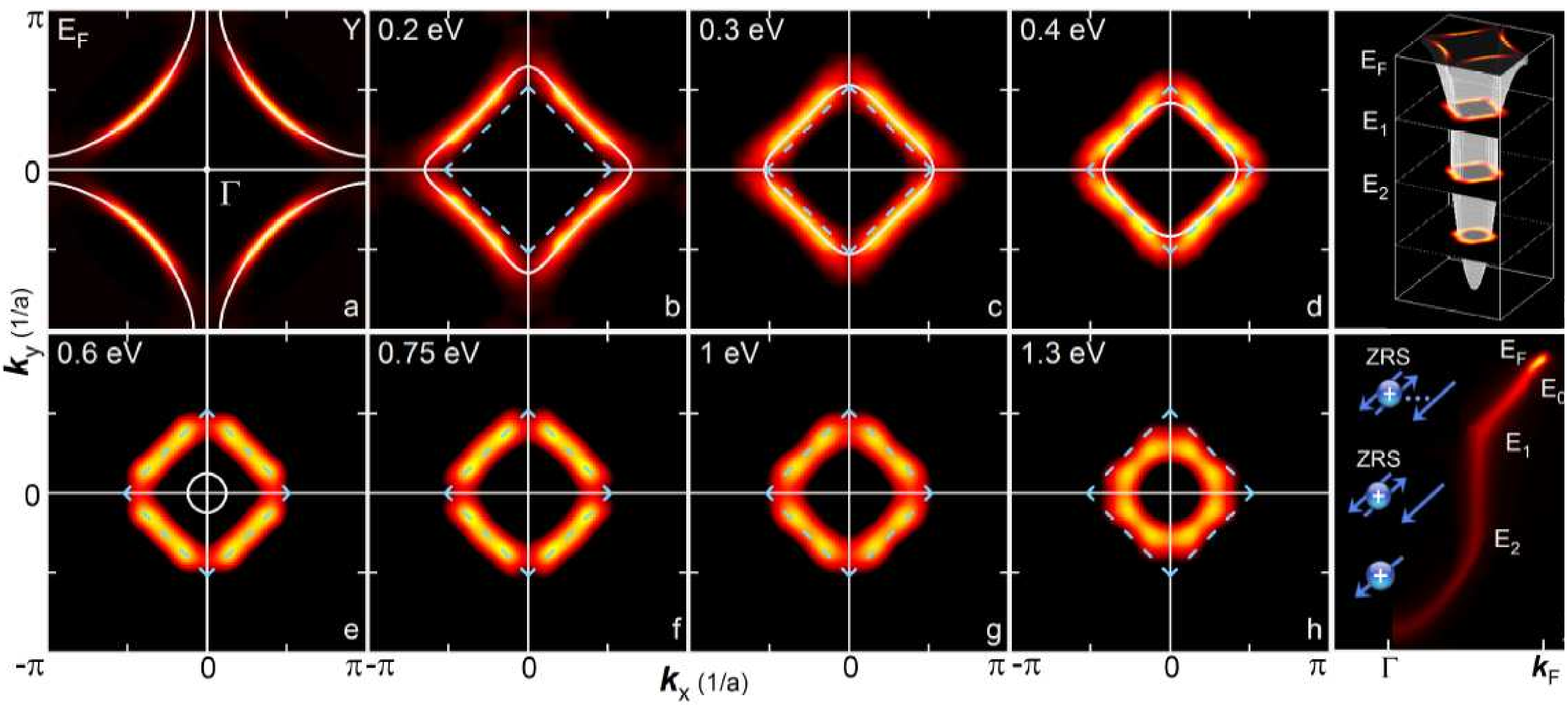
- J > 0 for oxygen with holes (●).
- (π/2, π/2) superlattice.





J. Graf, G.-H. Gweon, K. McElroy, S. Y. Zhou, C. Jozwiak, E. Rotenberg, *cond-mat/0607319*

- Gap-like feature from -0.4 to – 1 eV, regardless of doping.

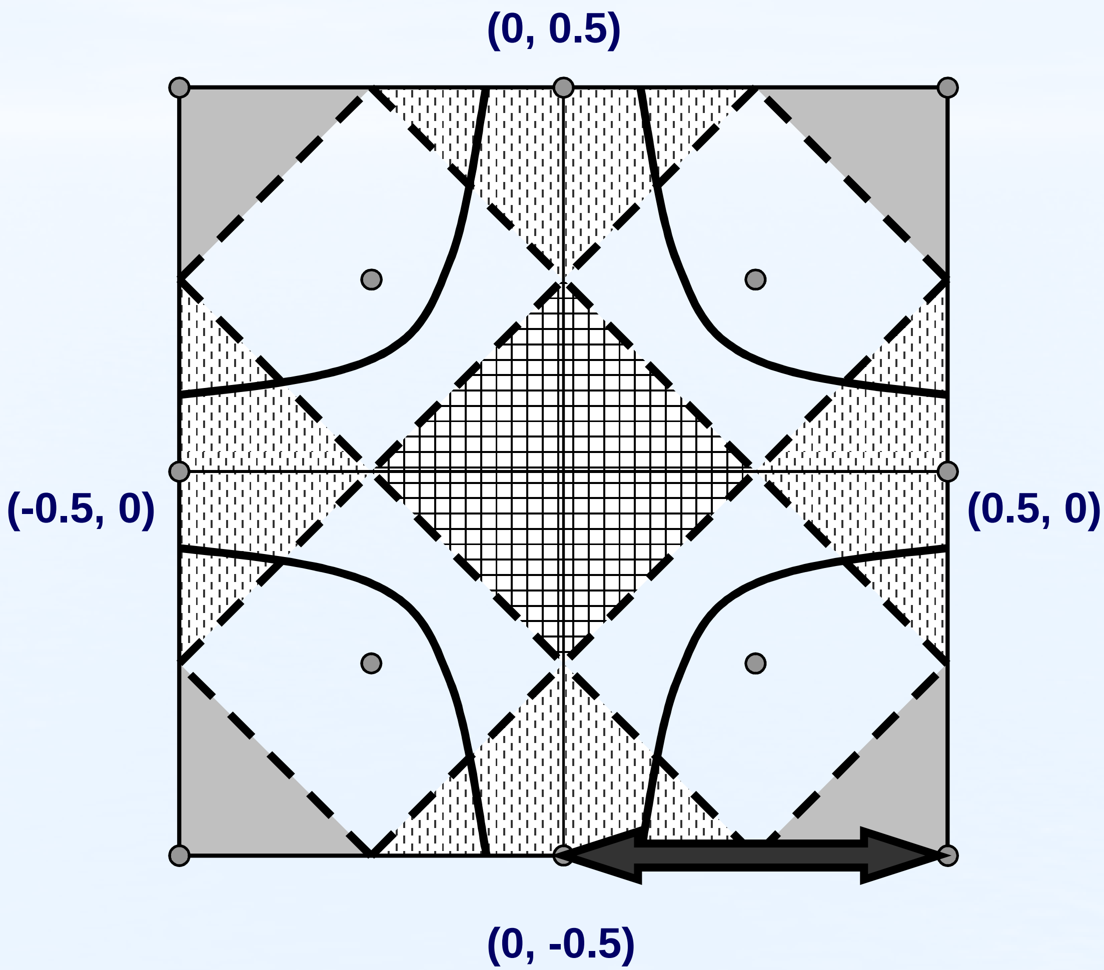


J. Graf, G.-H. Gweon, K. McElroy, S. Y. Zhou, C. Jozwiak, E. Rotenberg, *cond-mat/0607319*

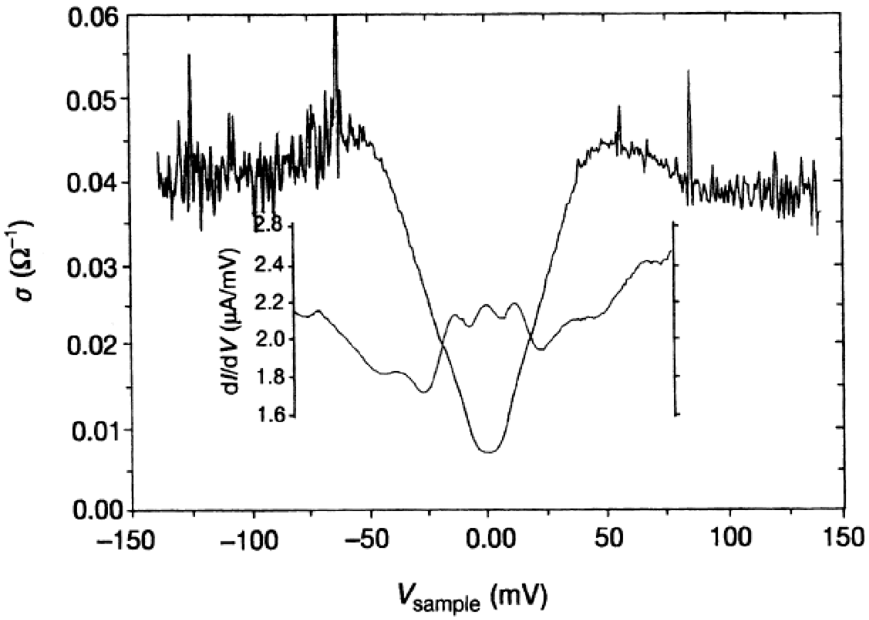
- Brillouin zone (?) by 8 fold ($2\sqrt{2}\times2\sqrt{2}$).

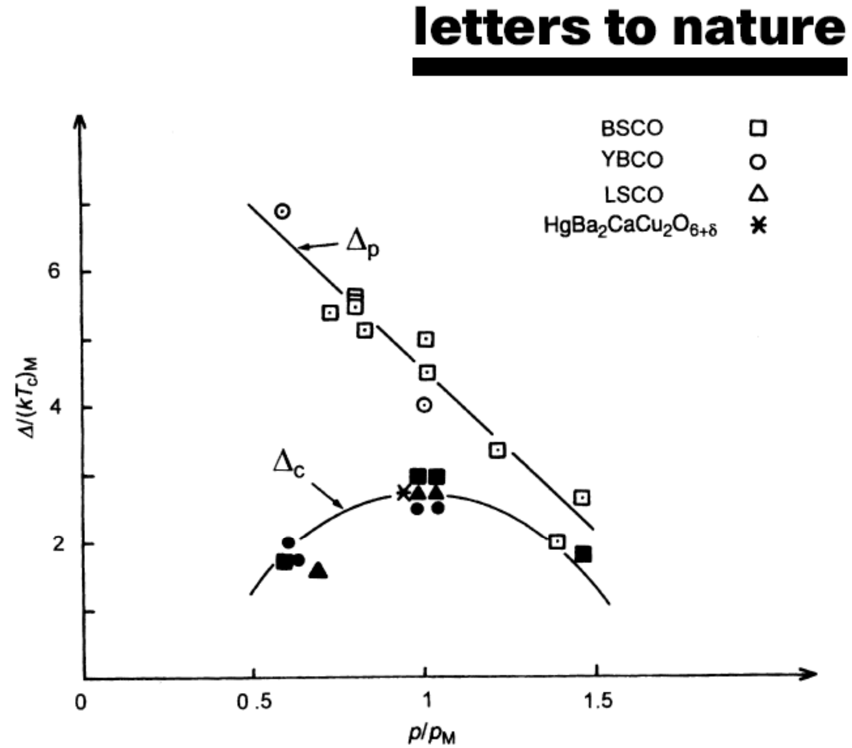
Sub-Brillouin Zones

- Nodal and anti-nodal particles in different sub-B. Z.
- Anti-nodal particles with more Cu character, and nodal particle with oxygen character.
- Anti-nodal states may be localized.



Two Gaps



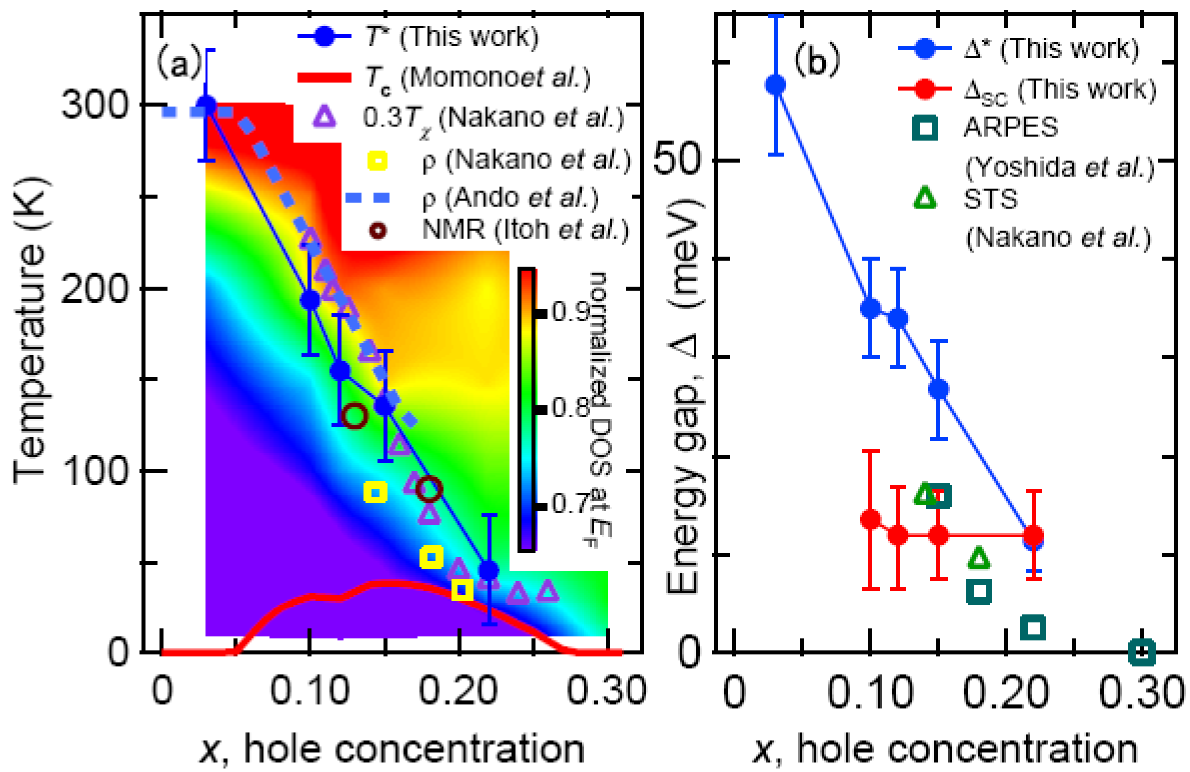


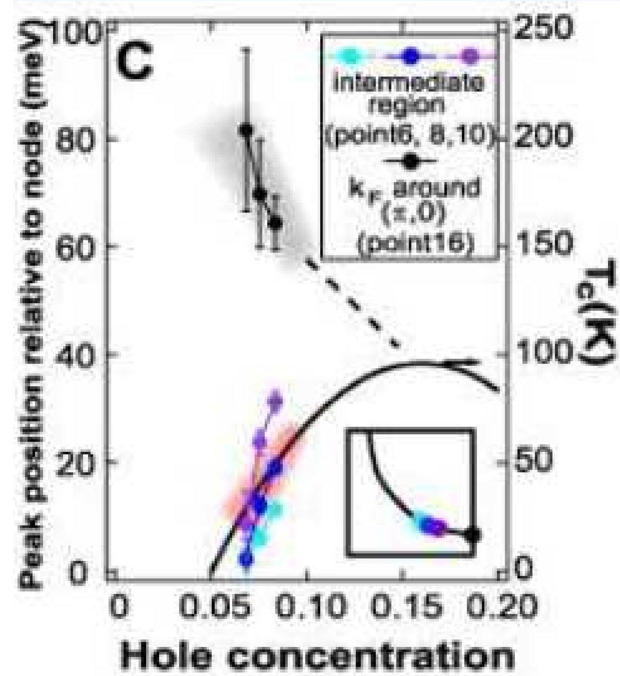
G. Deutscher, *Nature* **397,** 410 (1999)

- Coherence peak by Andreev reflection follows T_C, while the pseudogap follows T_{PG}.

$$\frac{2\Delta_{SC}}{kT_C} \approx \frac{2\Delta_{PG}}{kT_{PG}} \approx 4$$

Two Gaps



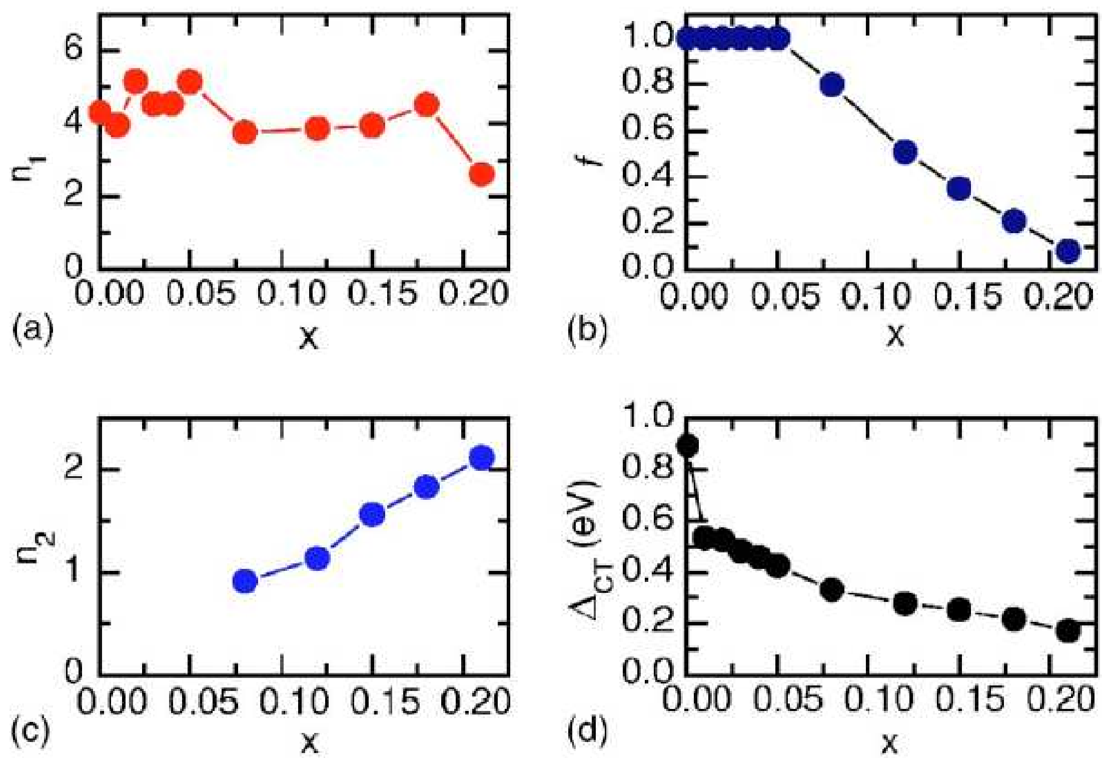


M. Hashimoto, T. Yoshida, K. Tanaka, A. Fujimori, M. Okusawa, S. Wakimoto, K. Yamada, T. Kakeshita, H. Eisaki and S. Uchida, *Phys. Rev. Lett.*, to be published

K. Tanaka, W. S. Lee, D. H. Lu, A. Fujimori, T. Fujii, Risdiana, I. Terasaki, J. D. Scalapino, T. P. Devereaux, Z. Hussain and Z.-X. Shen, *Science*, **314,** 1910 (2006).

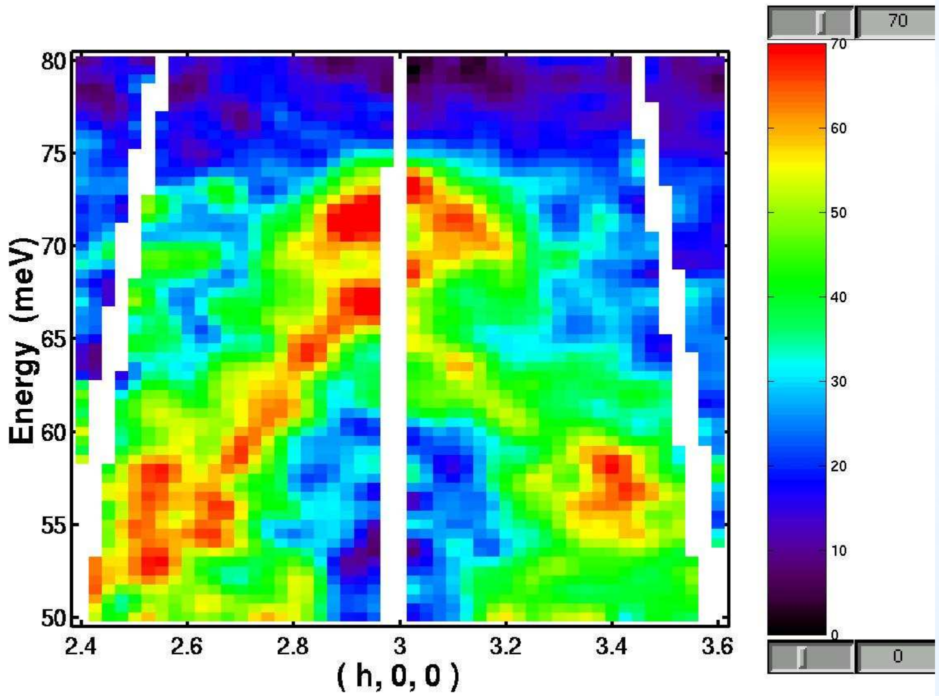
Charge Nature of the PG State

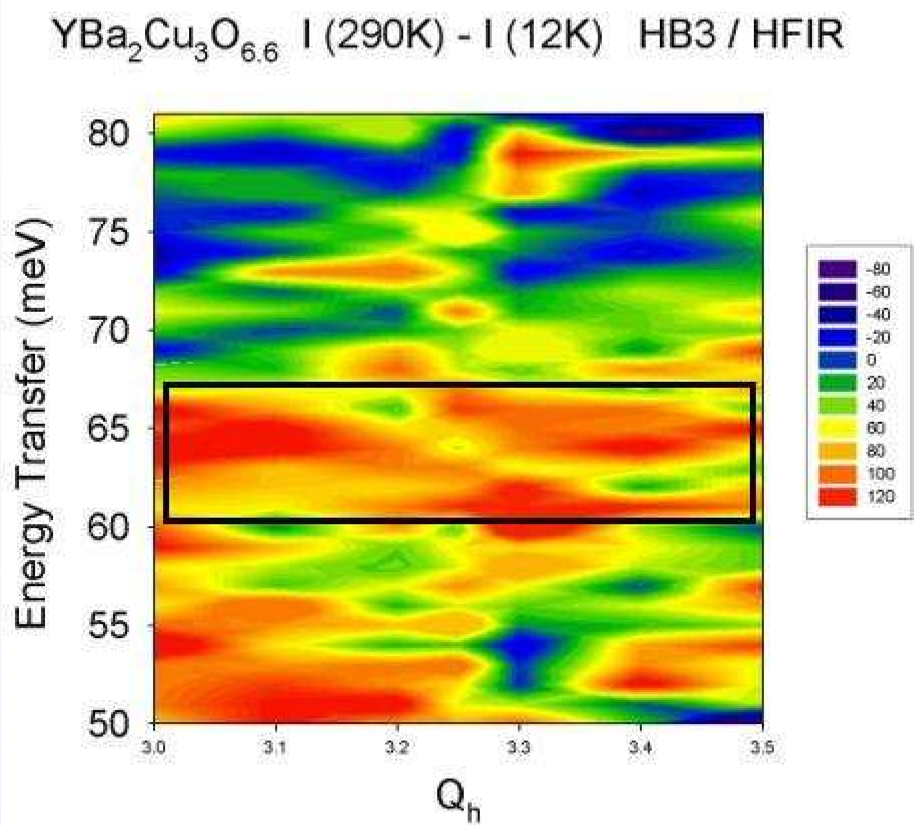
- Two kinds of carriers.
- The one associated with PG involves charge excitation gap.
- Agrees with the metal-insulator transition seen under high magnetic field.



S. Ono, S. Komiya and Y. Ando, *PRB* **75,** 024515 (2007)

Cu-O Bond-stretching Mode

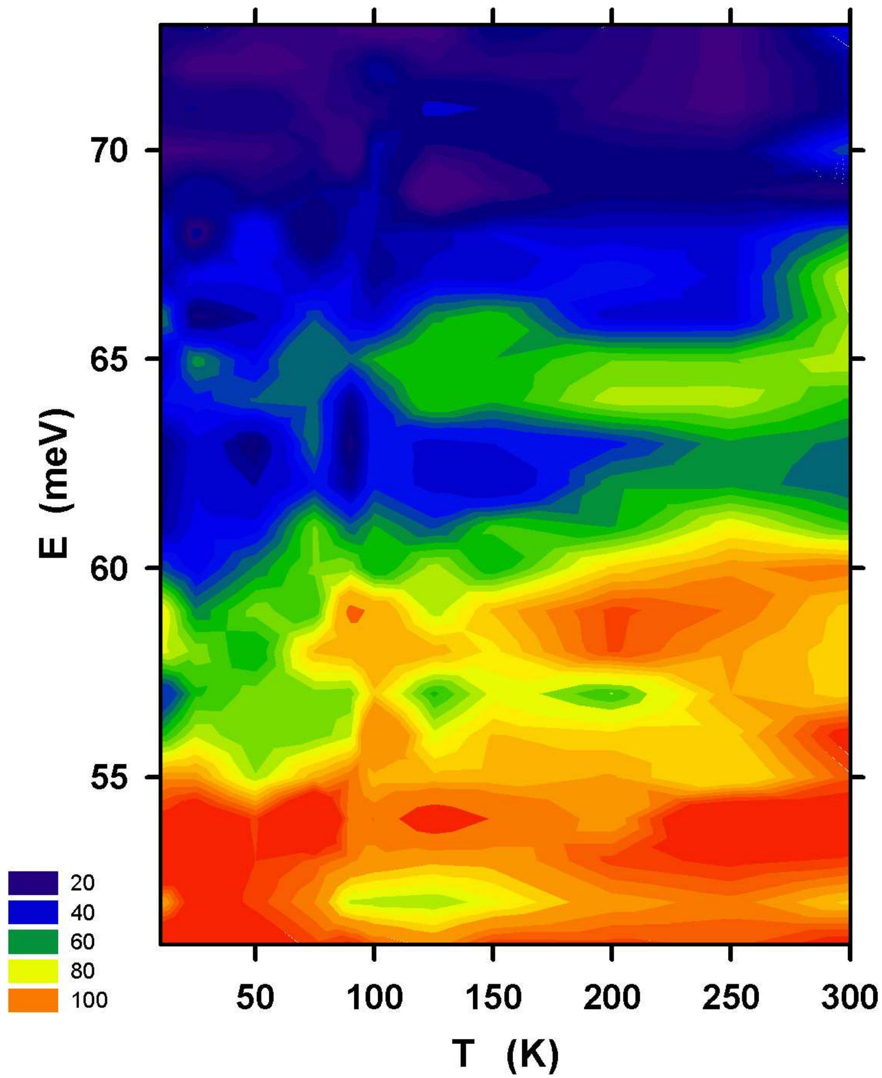




J.-H. Chung, et al, *Phys. Rev. B* **67**, 014517 (2003)

T. Egami, *Physica C*, **460-462,** 267 (2007)

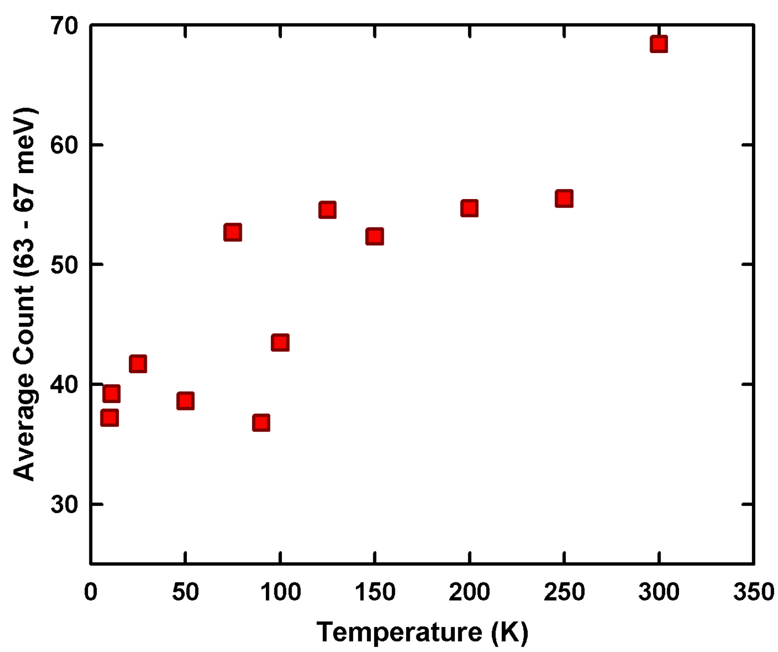
$YBa_2Cu_3O_{6.95}$ corrected for BE factor



Temperature scan at (3.25, 0)

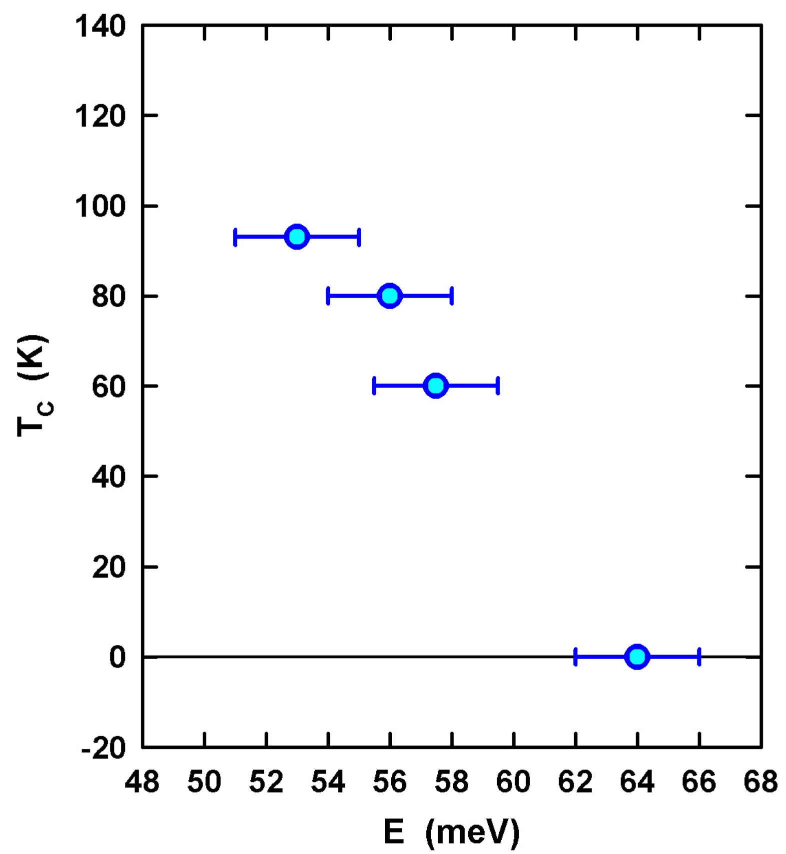
- The mode at 64 meV disappears below T_C (= 93 K).
- It softens to 53 meV below T_C.

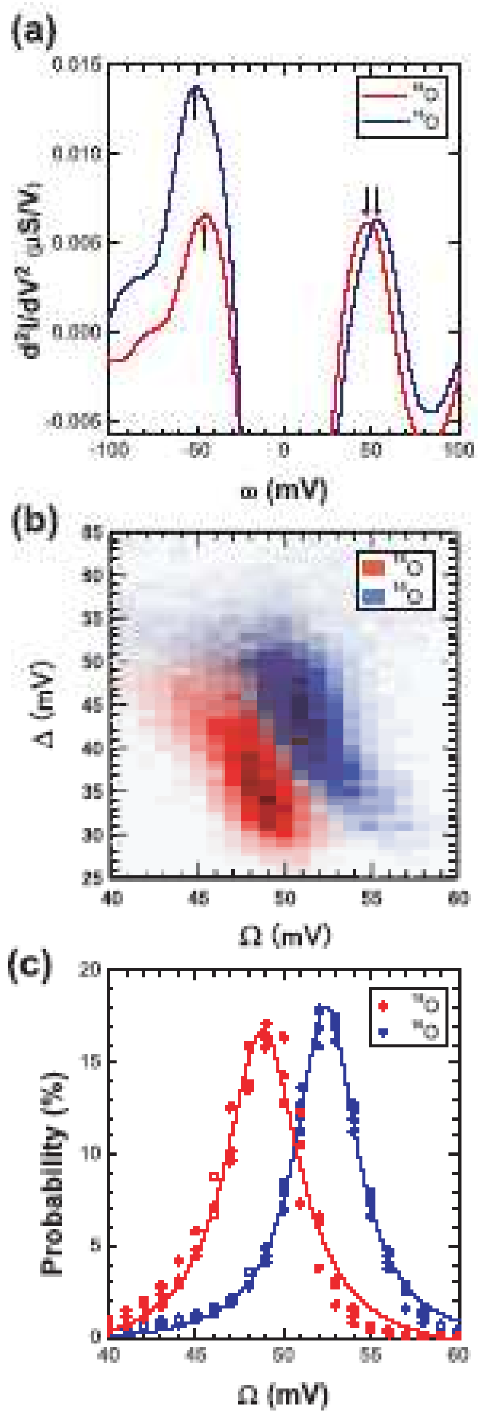
I(63 – 67 meV)

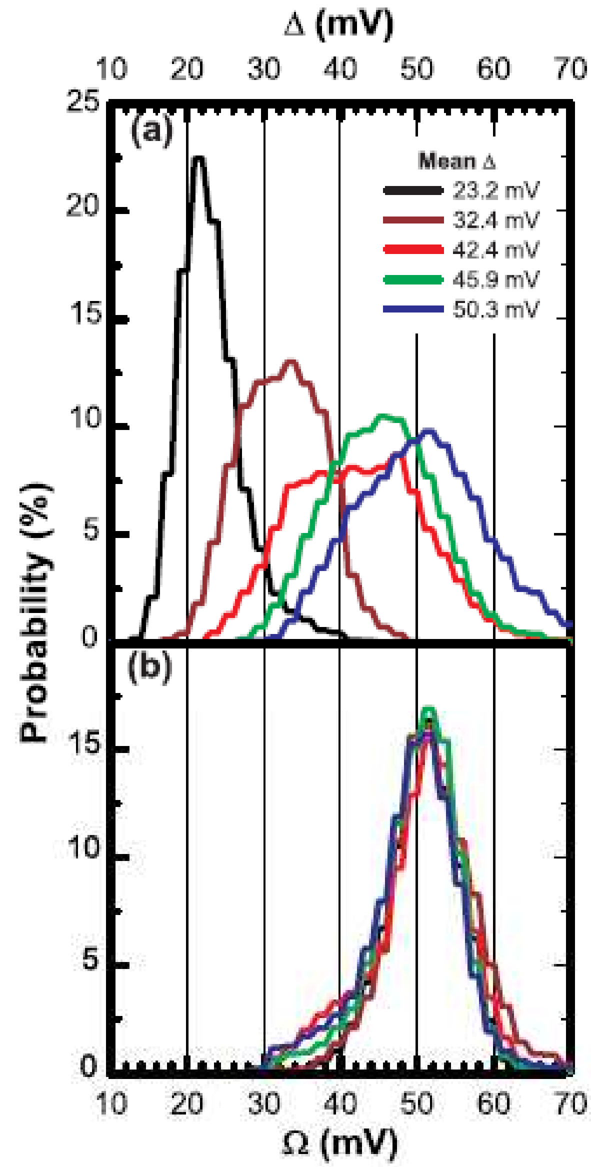


Phonon Softening

- E (T = 0K) decreases with increasing T_C.
- Phonon softening linearly related to T_C (Uemura plot?).
- The amount (20%) is anomalously large.



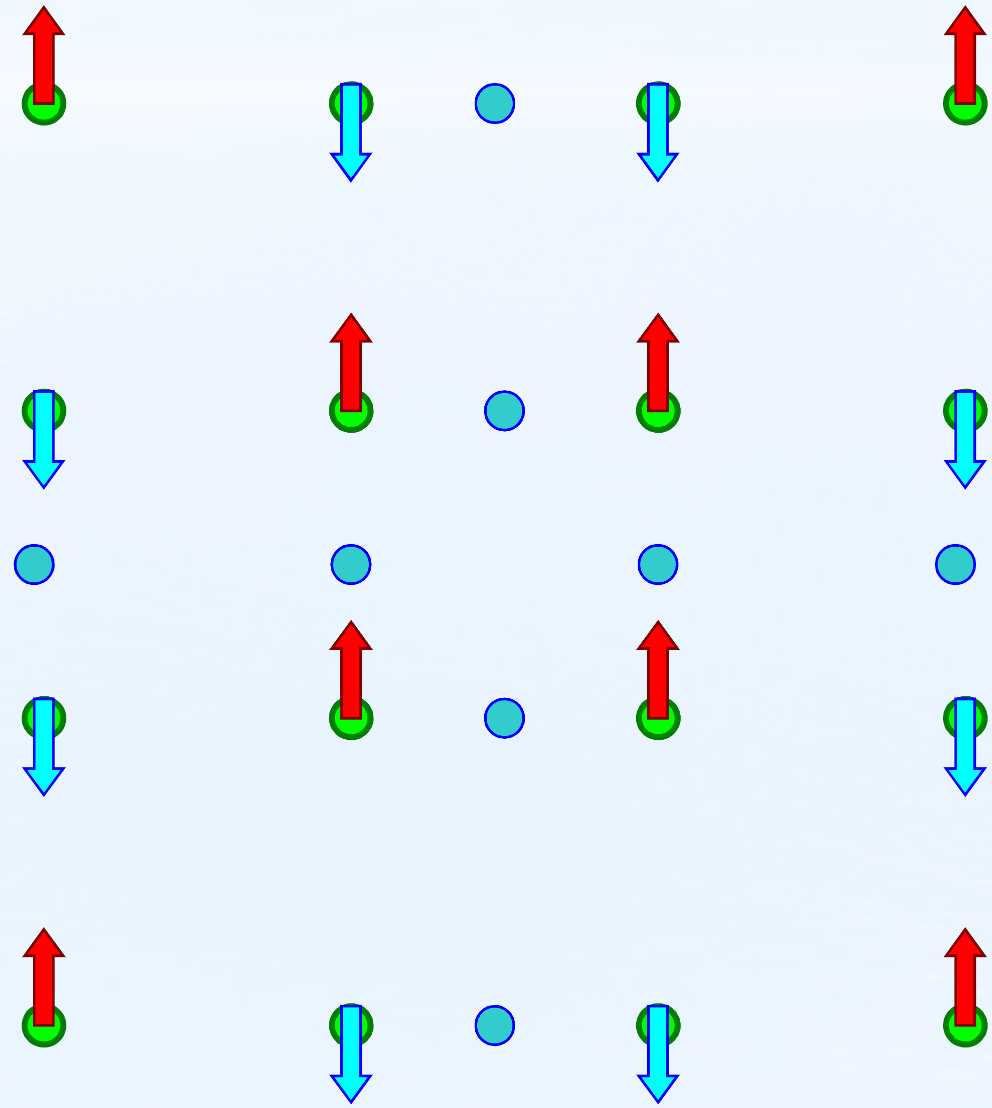




[Jinho Lee *et al Nature*, **442,** 546 (2006)]

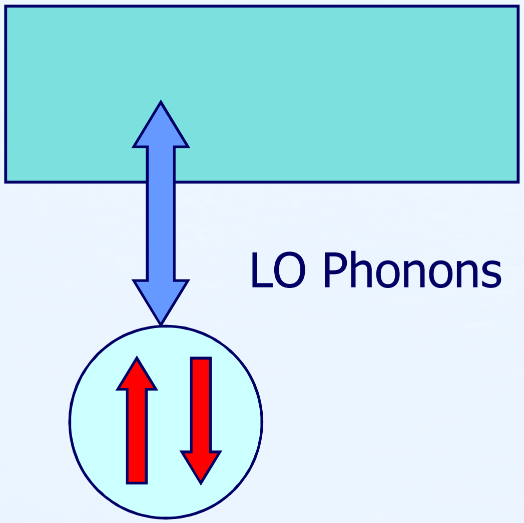
Spin Flustration

- Each spin has 2 up and 2 down neighbors.
- If holes move away they are completely frustrated!!
- Easy to set up local singlet states.



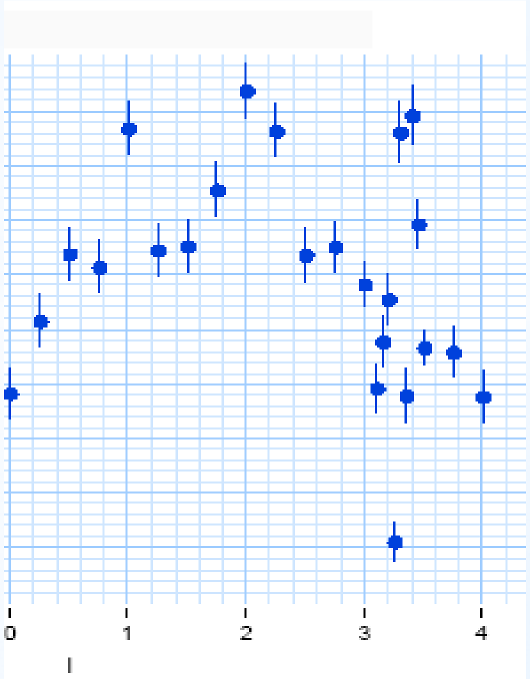
Two-Component Model

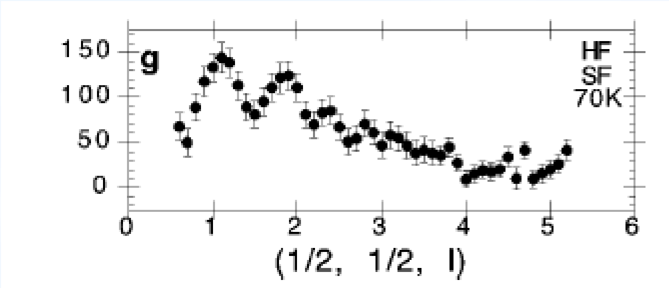
- Below T_{PG1} AFM with the intermediate local order develops.
- Charges in the AFM regions form spin-singlet bipolarons below T_{PG2}.
- Two-components; localized bipolarons (bosons) and delocalized nodal fermions (Ranninger, Micnas, Bussmann-Holder) produces HTSC.
- Mediation by LO phonons is a possibility.

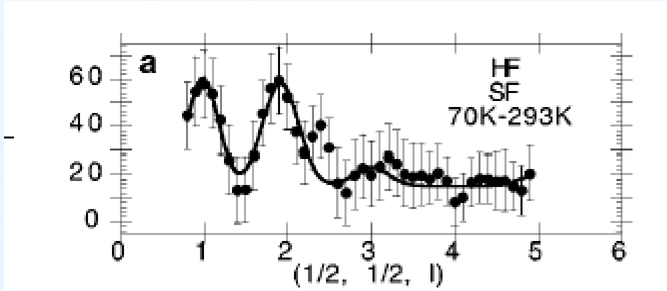


Conclusions

- **Doped cuprates are strongly frustrated systems with high propensity for phase-separation.**
- **Because of low ionic mobility only electrons phase-separate, resulting in nano-scale intermediate order, which is consistent with neutron diffuse scattering.**
- **This state could be the origin of the pseudogap state.**
- **The intermediate state with local AFM order may support spin-singlet bipolarons, and could form the basis for the two-component SC.**
- **Strong frustration and intermediate order could hold the key in HTSC mechanism.**


0
1
2
3
4
l


g
HF
SF
70K
150
100
50
0
0 1 2 3 4 5 6
(1/2, 1/2, l)


a
HF
SF
70K-293K
60
40
20
0
0 1 2 3 4 5 6
(1/2, 1/2, l)