

# Order and quantum phase transitions in the cuprate superconductors

Eugene Demler (Harvard)

Kwon Park (Maryland)

Anatoli Polkovnikov

Subir Sachdev

Matthias Vojta (Karlsruhe)

Ying Zhang (Maryland)



Talk online:

Google™



# Order and quantum phase transitions in the cuprate superconductors

S. Sachdev, *Reviews of Modern Physics*,  
July 2003, cond-mat/0211005.

See also

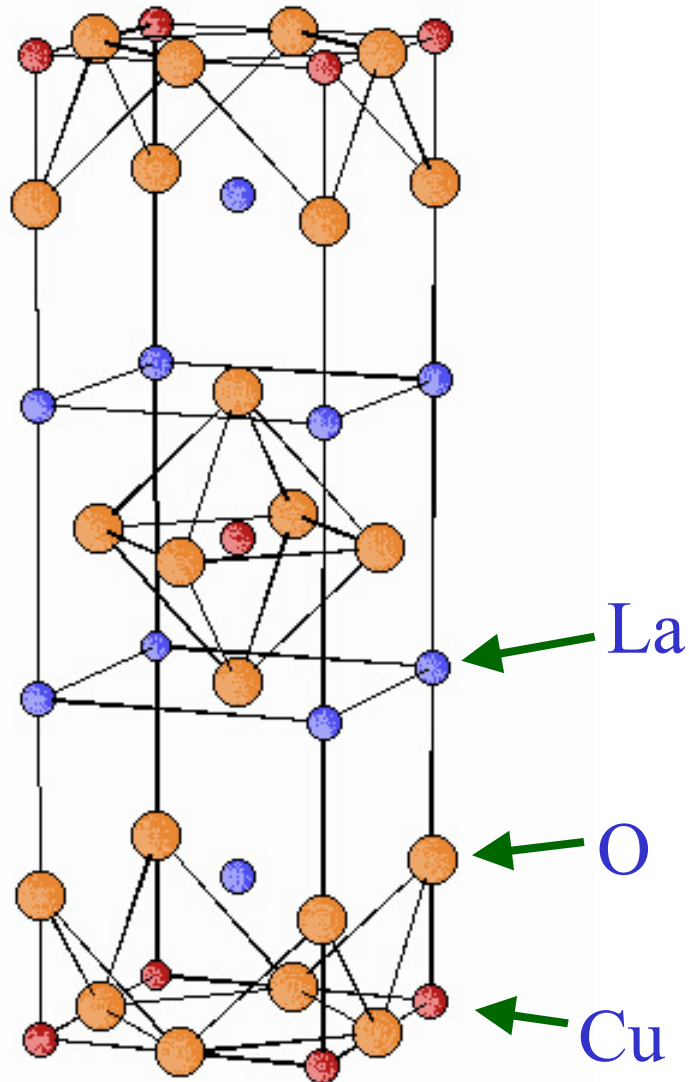
S. A. Kivelson, E. Fradkin, V. Oganesyan,  
I. P. Bindloss, J. M. Tranquada, A. Kapitulnik,  
and C. Howald, cond-mat/0210683.



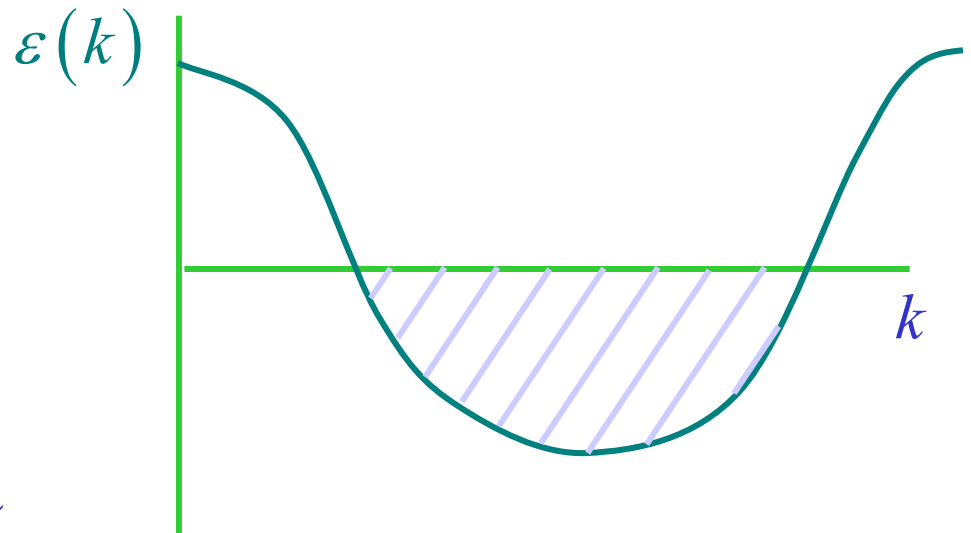
Talk online:  




Parent compound of the high temperature  
superconductors:  $\text{La}_2\text{CuO}_4$



Band theory

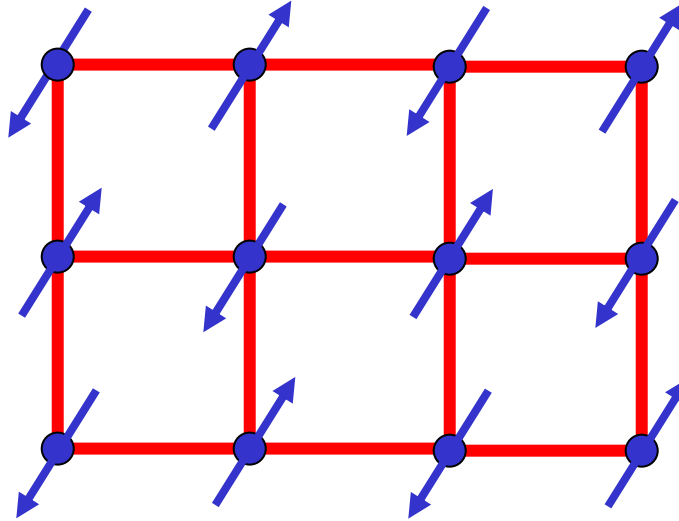


Half-filled band of Cu 3d orbitals –  
ground state is predicted to be a metal.

However,  $\text{La}_2\text{CuO}_4$  is a  
very good insulator

Parent compound of the high temperature  
superconductors:  $\text{La}_2\text{CuO}_4$

Mott insulator: square lattice antiferromagnet



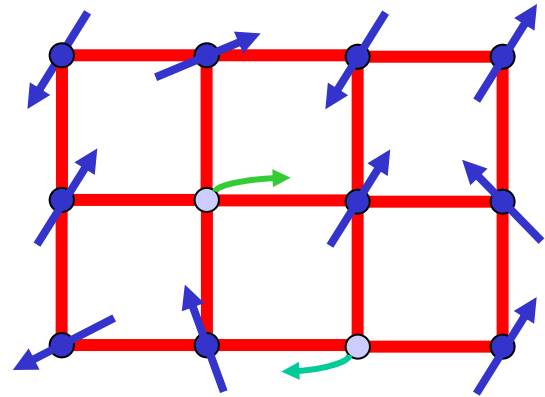
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Ground state has long-range magnetic Néel order,  
or “collinear magnetic (CM) order”

Néel order parameter:  $\vec{\phi} = (-1)^{i_x+i_y} \vec{S}_i$

$$\langle \vec{\phi} \rangle \neq 0 \quad ; \quad \langle \vec{S}_i \rangle \neq 0$$

Introduce mobile carriers of density  $\delta$   
by substitutional doping of out-of-plane  
ions e.g.  $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$

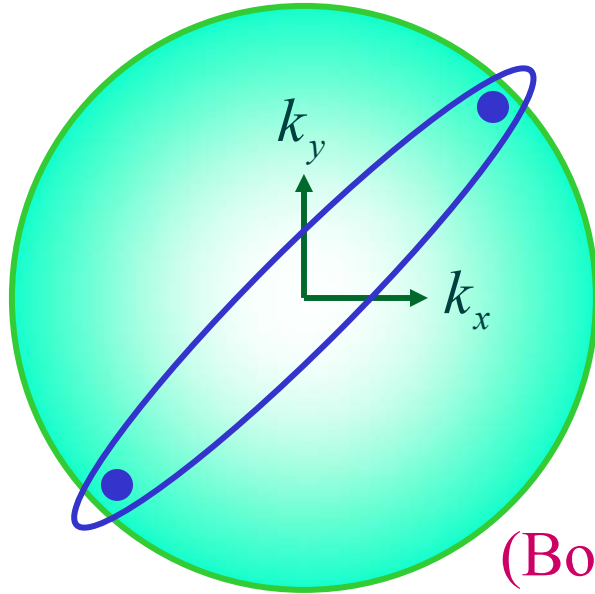


$$\langle \vec{S} \rangle = 0$$

Exhibits superconductivity below a high critical temperature  $T_c$

Superconductivity in a doped Mott insulator

BCS superconductor obtained by the Cooper instability of a *metallic Fermi liquid*



Pair wavefunction

$$\Psi = (k_x^2 - k_y^2) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\langle \vec{S} \rangle = 0$$

(Bose-Einstein) condensation of Cooper pairs

Many low temperature properties of the cuprate superconductors appear to be qualitatively similar to those predicted by BCS theory.

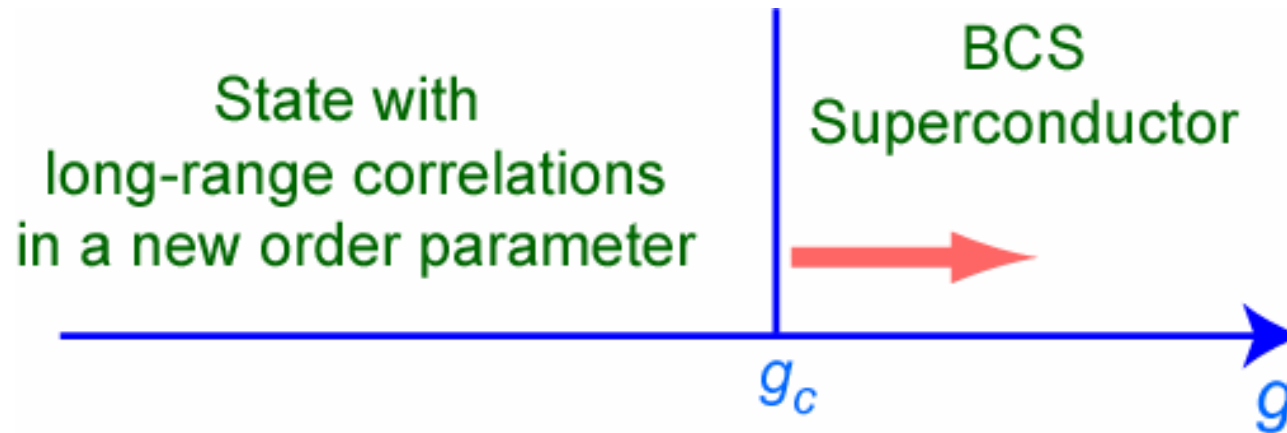
# Superconductivity in a doped Mott insulator

Review: S. Sachdev, *Science* **286**, 2479 (1999).

Hypothesis: cuprate superconductors are characterized by additional order parameters (possibly fluctuating), associated with the proximate Mott insulator, along with the familiar order associated with the condensation of Cooper pairs in BCS theory. These orders lead to new low energy excitations.

# Superconductivity in a doped Mott insulator

Review: S. Sachdev, *Science* **286**, 2479 (1999).



Study physics in a generalized phase diagram which includes new phases (which need not be experimentally accessible) with long-range correlations in the additional order parameters. Expansion away from quantum critical points provides a systematic and controlled theory of the low energy excitations (including their behavior near imperfections such as impurities and vortices and their response to applied fields) and of crossovers into “incoherent” regimes at finite temperature.



# Outline

- I. **Simple model of a quantum phase transition**  
Coupled ladder antiferromagnet
- II. Interplay of CM and SC order in the cuprates: theory and neutron scattering experiments
- III. Microscopic theory: bond order and a global phase diagram (STM experiments)
- IV. Conclusions

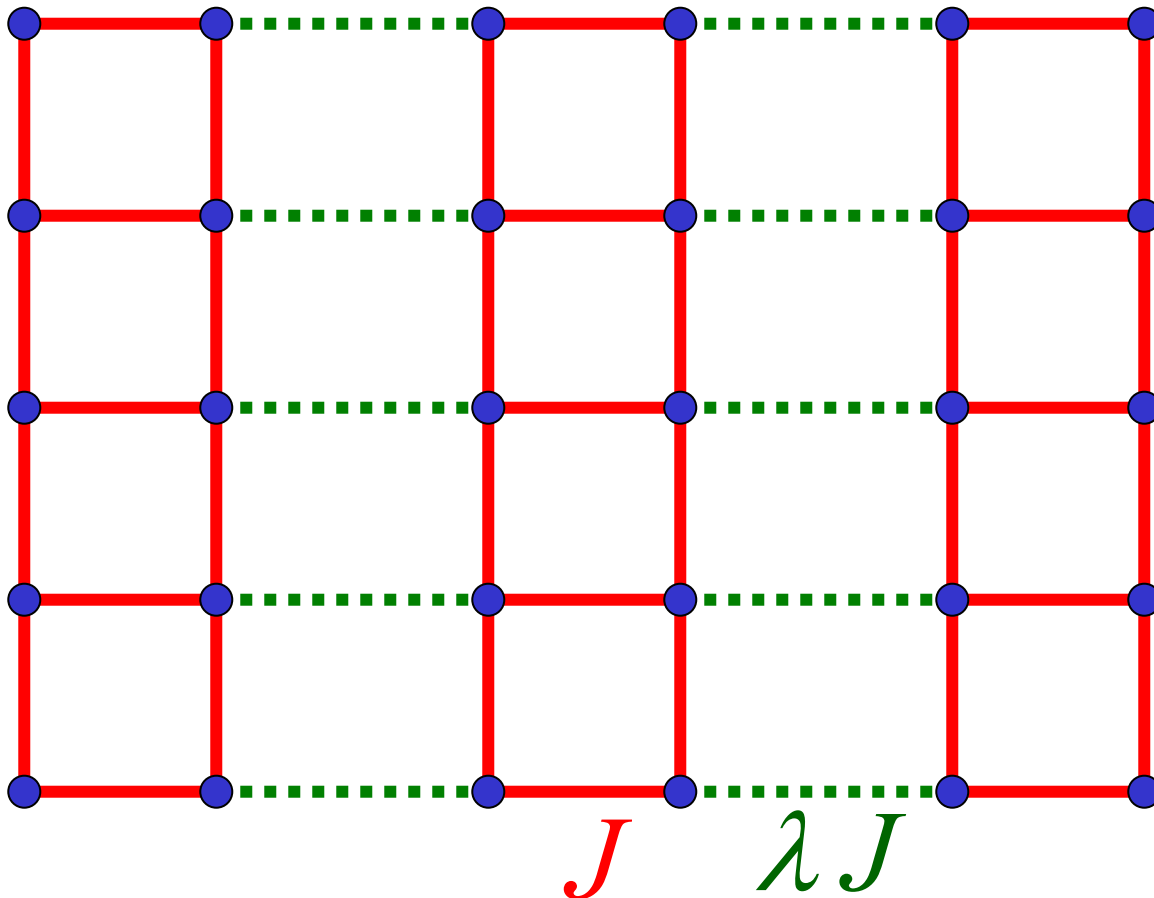
# I. Coupled ladder antiferromagnet

N. Katoh and M. Imada, *J. Phys. Soc. Jpn.* **63**, 4529 (1994).

J. Tworzydło, O. Y. Osman, C. N. A. van Duin, J. Zaanen, *Phys. Rev. B* **59**, 115 (1999).

M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev. B* **65**, 014407 (2002).

$S=1/2$  spins on coupled 2-leg ladders



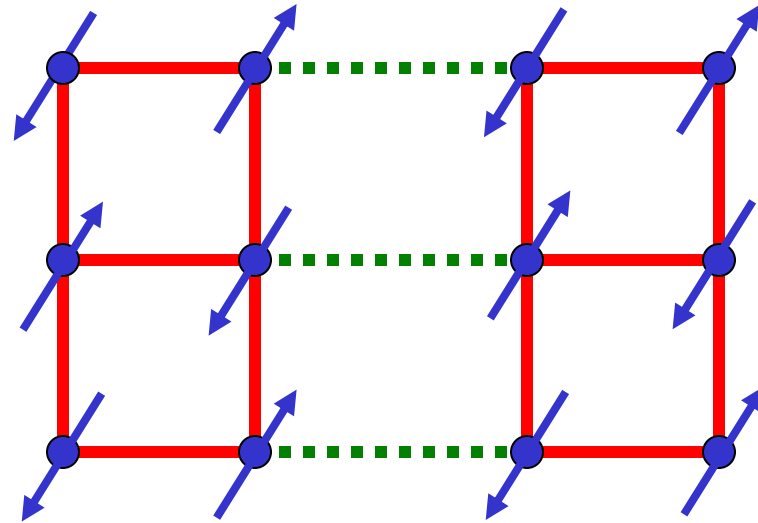
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$0 \leq \lambda \leq 1$$

$\lambda$  close to 1

Square lattice antiferromagnet

Experimental realization:  $La_2CuO_4$



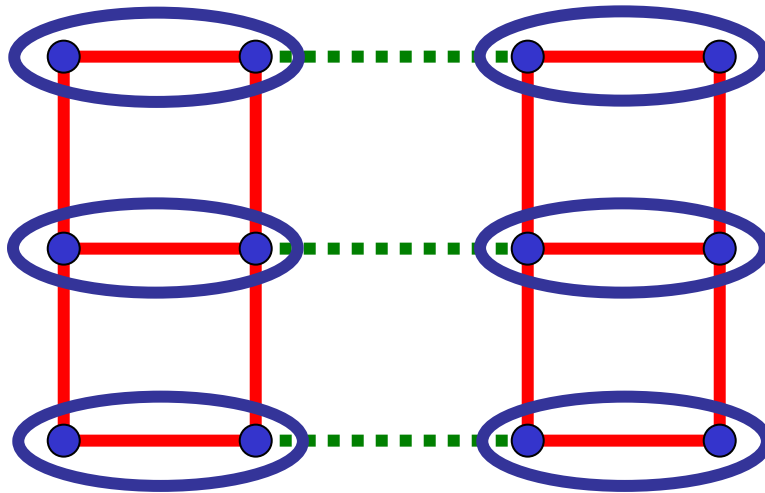
Ground state has long-range  
collinear magnetic (Neel) order

$$\langle \vec{S}_i \rangle = (-1)^{i_x + i_y} N_0 \neq 0$$

Excitations: 2 spin waves  $\varepsilon_p = \sqrt{c_x^2 p_x^2 + c_y^2 p_y^2}$

$\lambda$  close to 0

## Weakly coupled ladders



$$\text{Oval} = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

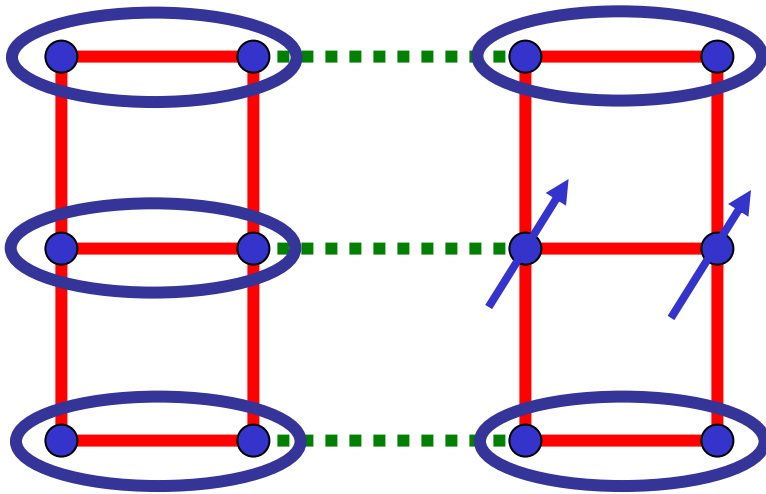
Real space Cooper pairs  
with their charge localized.  
Upon doping, motion and  
condensation of Cooper  
pairs leads to  
superconductivity

Paramagnetic ground state

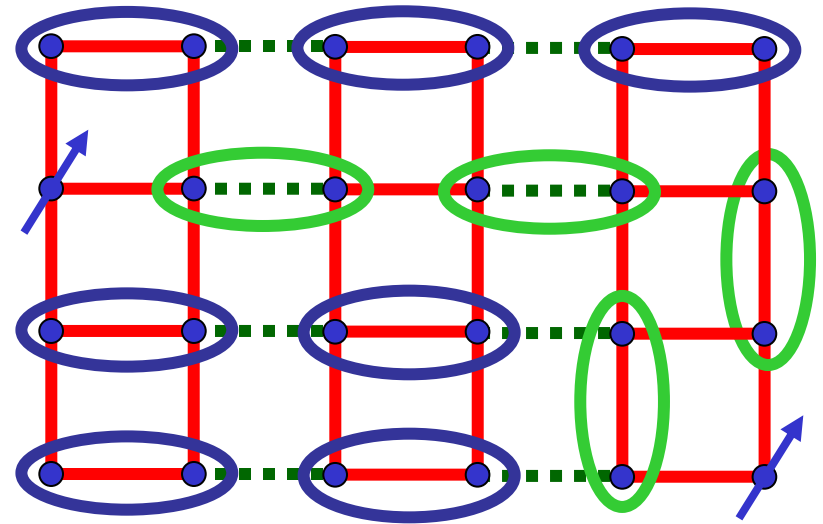
$$\langle \vec{S}_i \rangle = 0$$

$\lambda$  close to 0

## Excitations

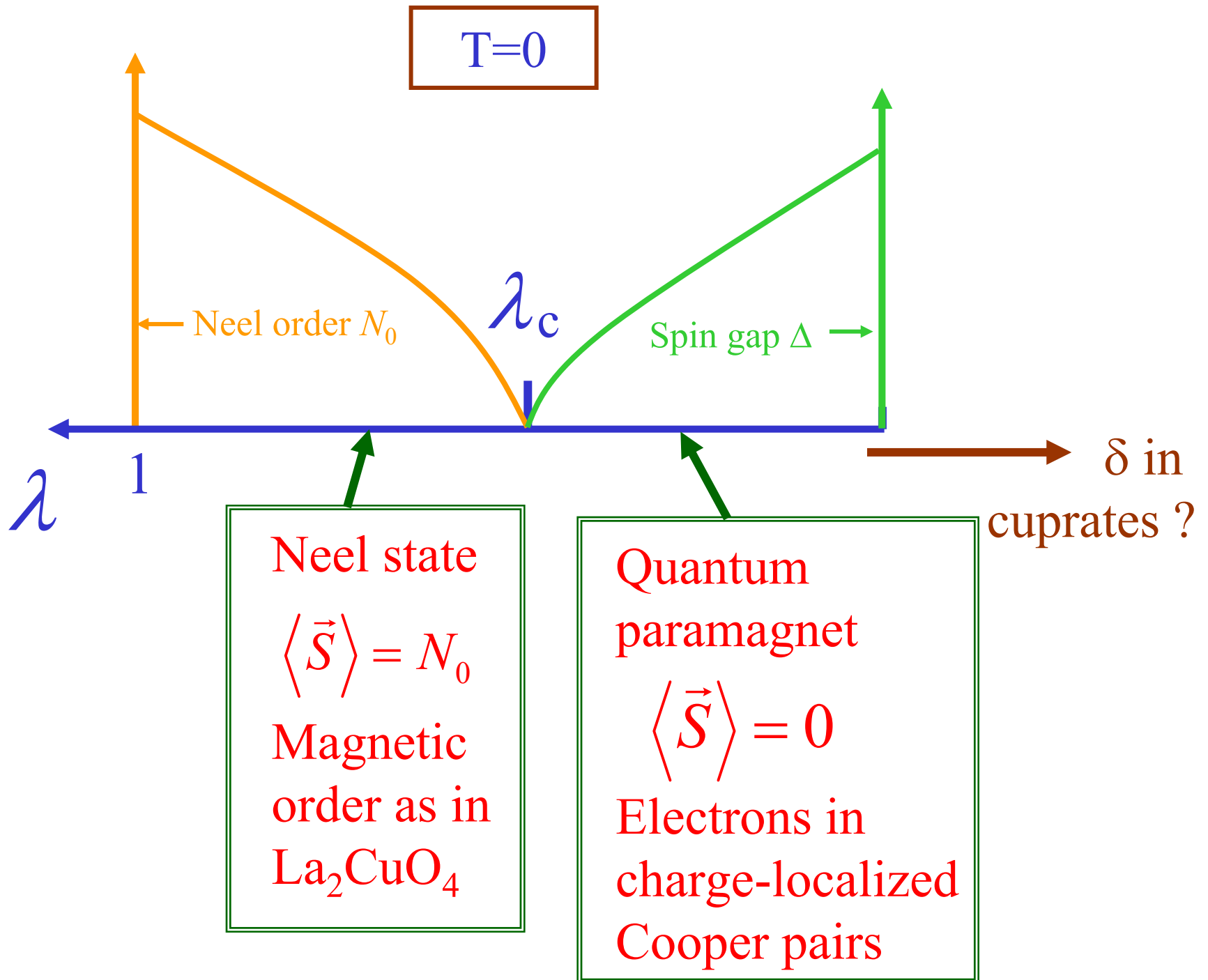


Excitation:  $S=1$  *exciton*  
(spin collective mode)



$S=1/2$  spinons are *confined*  
by a linear potential.

Energy dispersion away from  
antiferromagnetic wavevector  $\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$

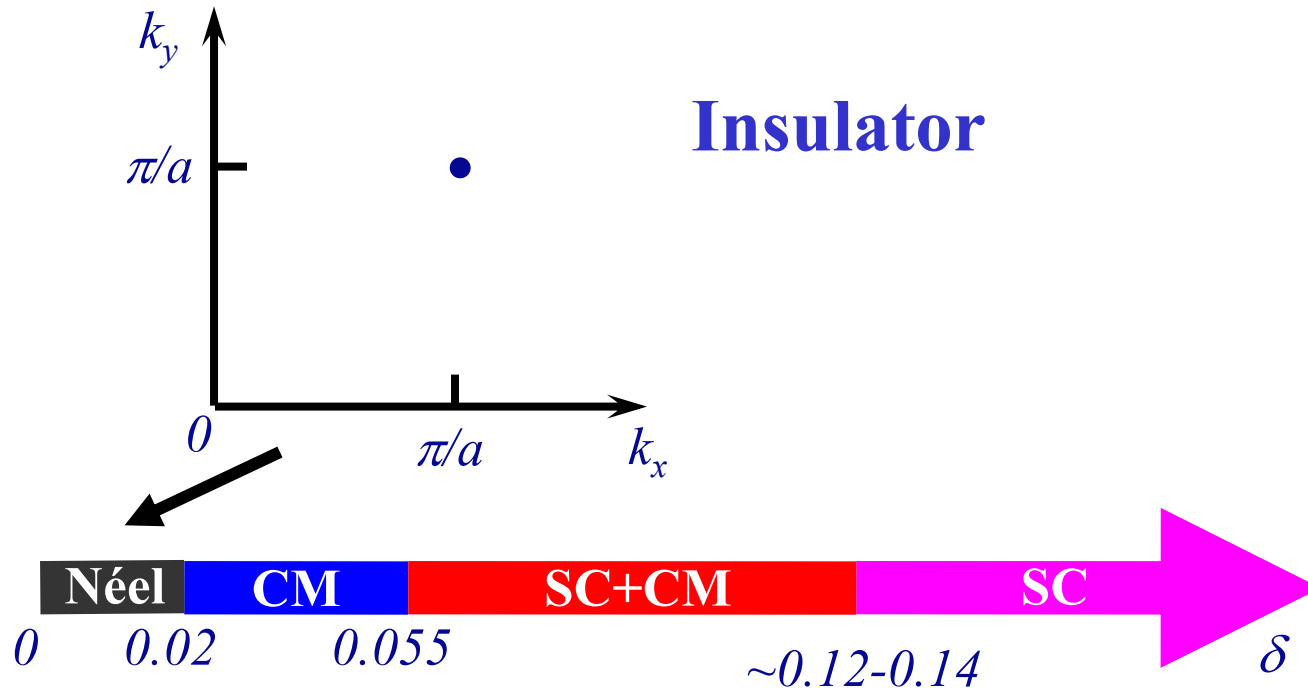


## Outline

- I. Simple model of a quantum phase transition  
Coupled ladder antiferromagnet
- II. Interplay of CM and SC order in the cuprates: theory  
and neutron scattering experiments**
- III. Microscopic theory: bond order and a global phase  
diagram (STM experiments)
- IV. Conclusions

## II. Interplay of CM and SC order in the cuprates

### T=0 phases of LSCO



(additional commensurability effects near  $\delta=0.125$ )

J. M. Tranquada *et al.*, *Phys. Rev. B* **54**, 7489 (1996).

G. Aeppli, T.E. Mason, S.M. Hayden, H.A. Mook, J. Kulda, *Science* **278**, 1432 (1997).

S. Wakimoto, G. Shirane *et al.*, *Phys. Rev. B* **60**, R769 (1999).

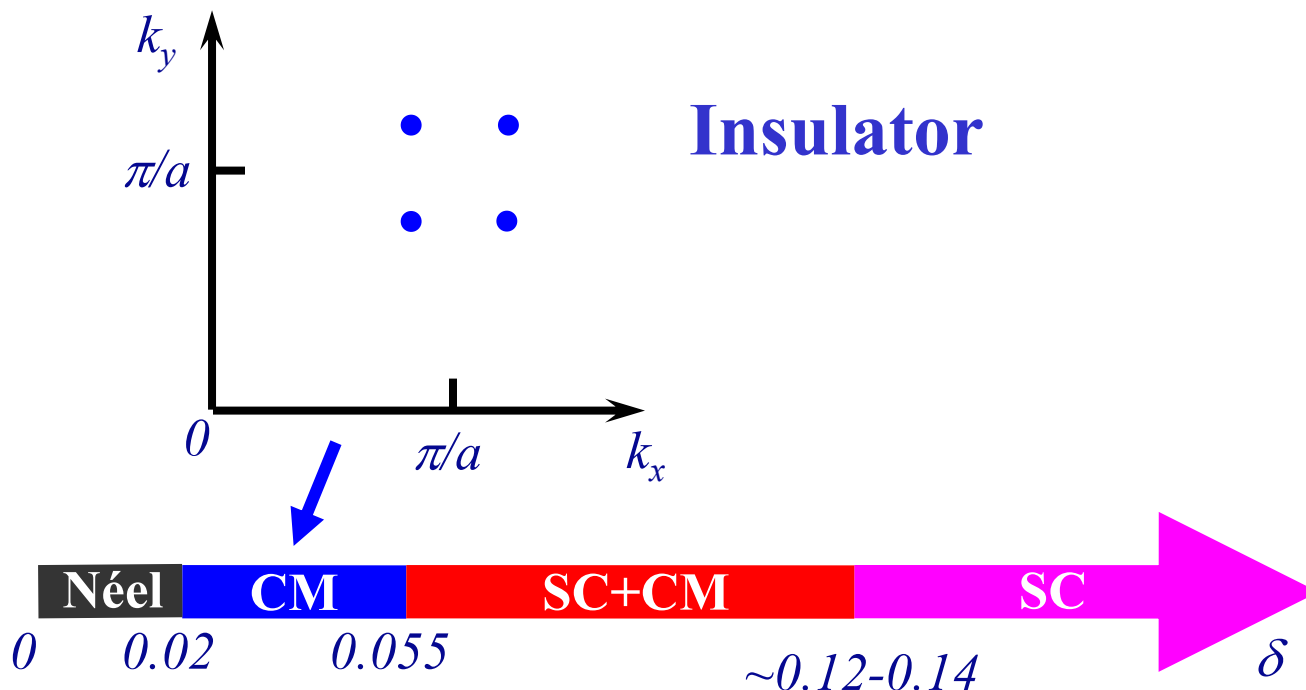
Y.S. Lee, R. J. Birgeneau, M. A. Kastner *et al.*, *Phys. Rev. B* **60**, 3643 (1999)

S. Wakimoto, R.J. Birgeneau, Y.S. Lee, and G. Shirane, *Phys. Rev. B* **63**, 172501 (2001).



## II. Interplay of CM and SC order in the cuprates

### T=0 phases of LSCO



(additional commensurability effects near  $\delta=0.125$ )

J. M. Tranquada *et al.*, *Phys. Rev. B* **54**, 7489 (1996).

G. Aeppli, T.E. Mason, S.M. Hayden, H.A. Mook, J. Kulda, *Science* **278**, 1432 (1997).

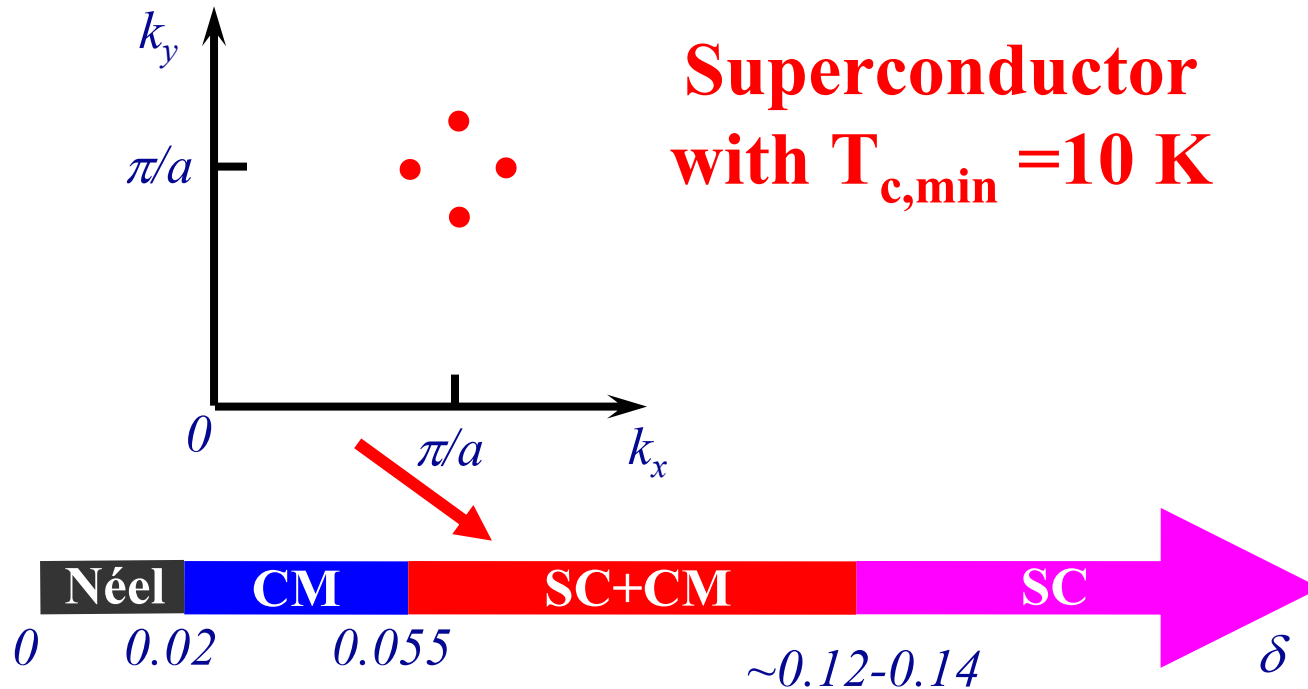
S. Wakimoto, G. Shirane *et al.*, *Phys. Rev. B* **60**, R769 (1999).

Y.S. Lee, R. J. Birgeneau, M. A. Kastner *et al.*, *Phys. Rev. B* **60**, 3643 (1999)

S. Wakimoto, R.J. Birgeneau, Y.S. Lee, and G. Shirane, *Phys. Rev. B* **63**, 172501 (2001).

## II. Interplay of CM and SC order in the cuprates

### T=0 phases of LSCO



(additional commensurability effects near  $\delta=0.125$ )

J. M. Tranquada *et al.*, *Phys. Rev. B* **54**, 7489 (1996).

G. Aeppli, T.E. Mason, S.M. Hayden, H.A. Mook, J. Kulda, *Science* **278**, 1432 (1997).

S. Wakimoto, G. Shirane *et al.*, *Phys. Rev. B* **60**, R769 (1999).

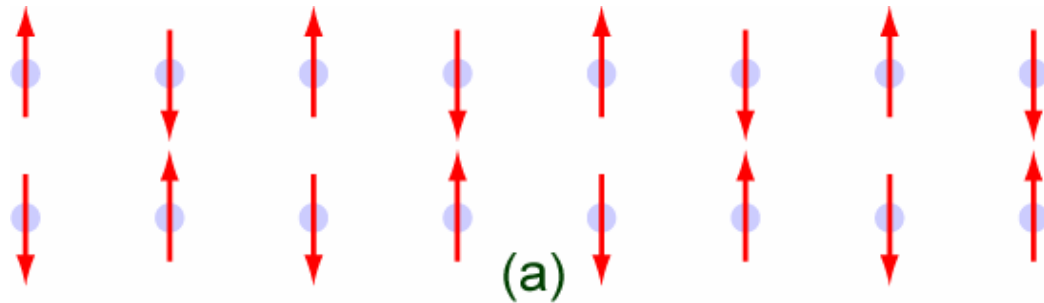
Y.S. Lee, R. J. Birgeneau, M. A. Kastner *et al.*, *Phys. Rev. B* **60**, 3643 (1999)

S. Wakimoto, R.J. Birgeneau, Y.S. Lee, and G. Shirane, *Phys. Rev. B* **63**, 172501 (2001).

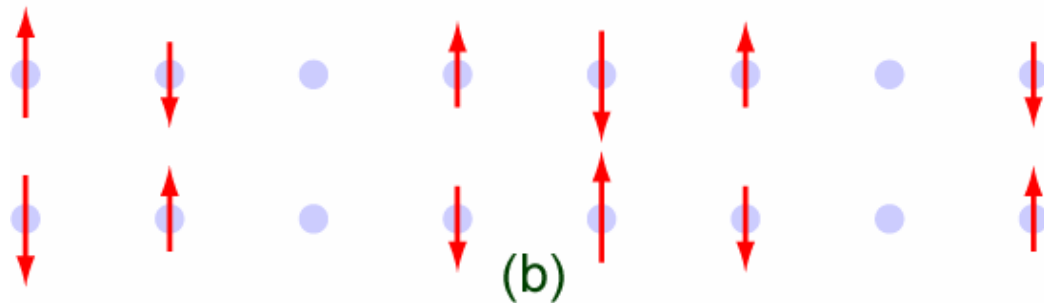
Collinear magnetic (spin density wave) order

$$\langle \mathbf{S}_j \rangle = N_1 \cos(\vec{K} \cdot \vec{r}_j) + N_2 \sin(\vec{K} \cdot \vec{r}_j)$$

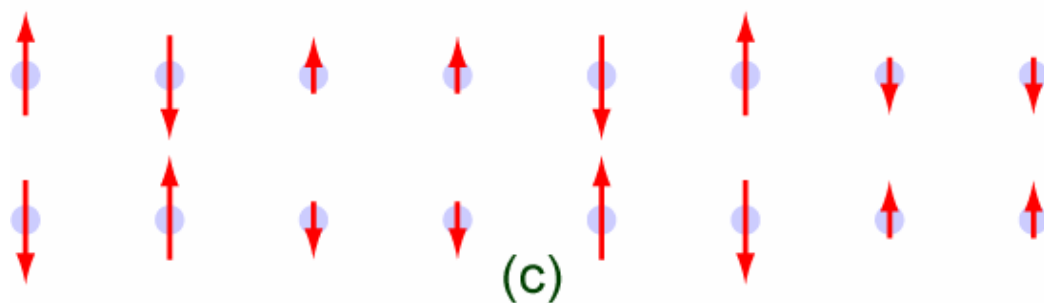
Collinear spins



$$\vec{K} = (\pi, \pi) ; N_2 = 0$$



$$\vec{K} = (3\pi/4, \pi) ; N_2 = 0$$

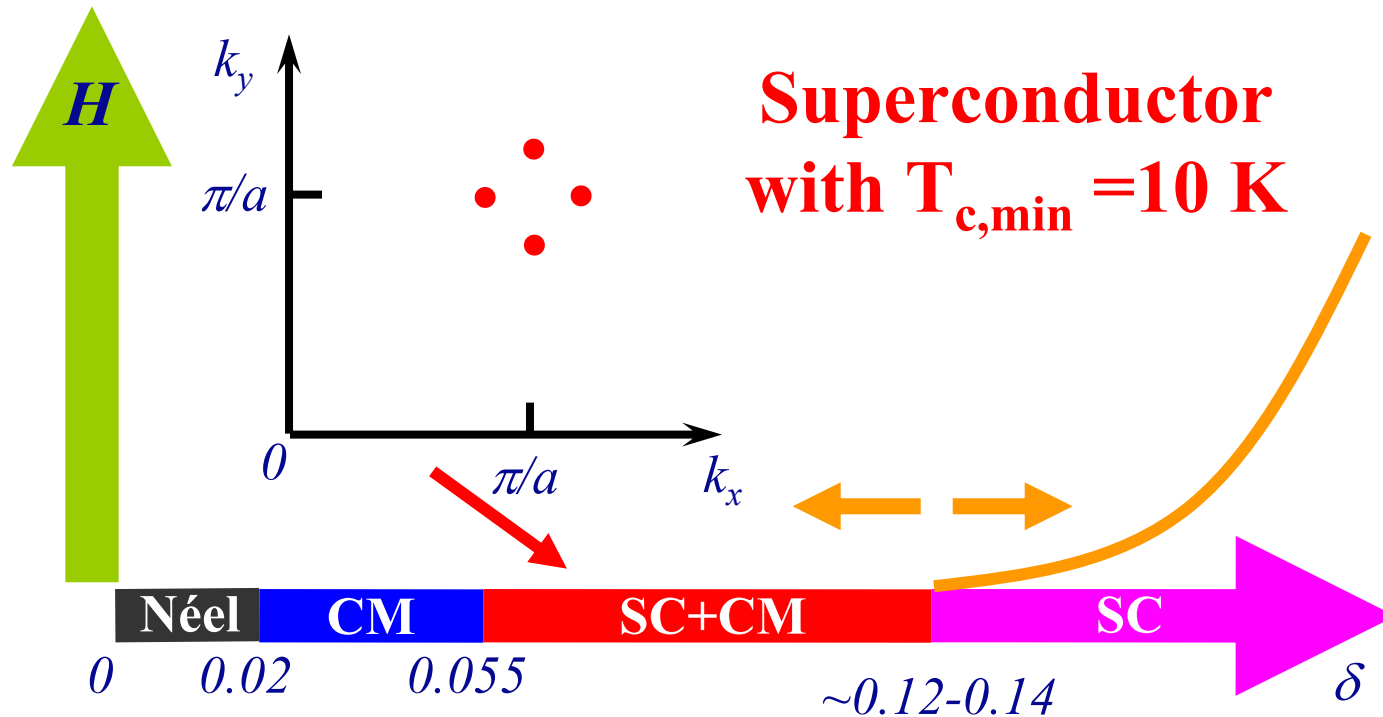


$$\vec{K} = (3\pi/4, \pi) ;$$

$$N_2 = (\sqrt{2} - 1) N_1$$

## II. Interplay of CM and SC order in the cuprates

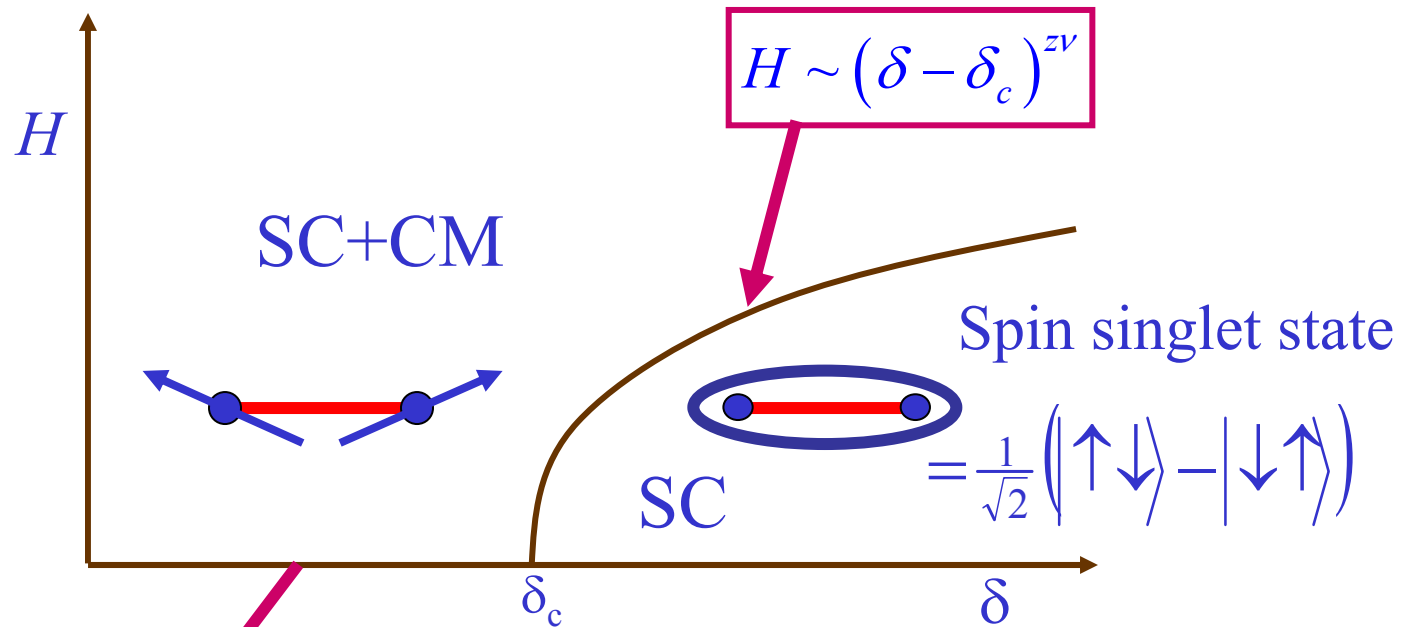
### T=0 phases of LSCO



Use simplest assumption of a direct second-order quantum phase transition between SC and SC+CM phases

Follow intensity of elastic Bragg spots in a magnetic field

# Zeeman term: only effect in coupled ladder system

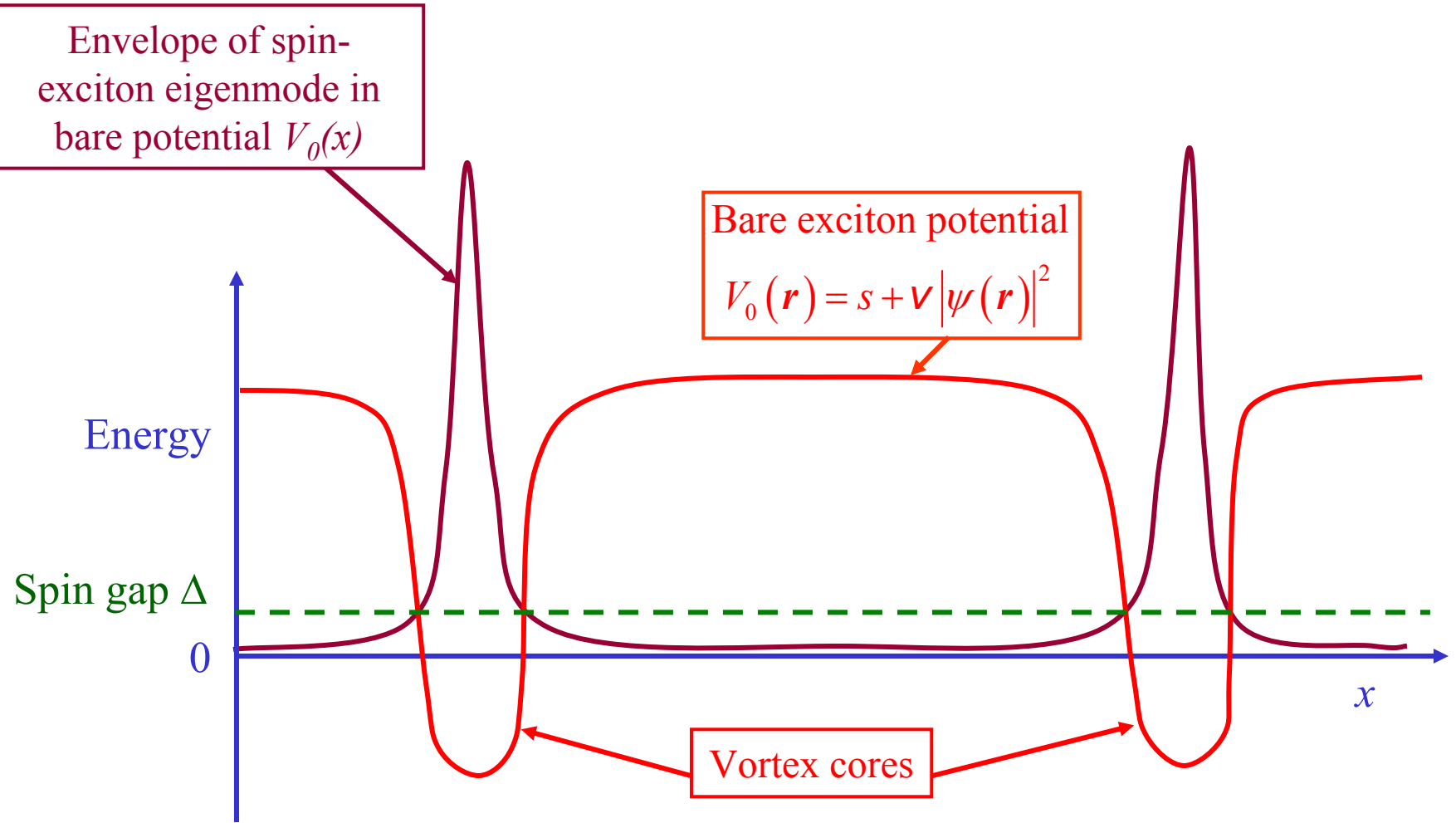


Characteristic field  $g\mu_B H = \Delta$ , the spin gap  
 1 Tesla = 0.116 meV

Effect is negligible over experimental field scales

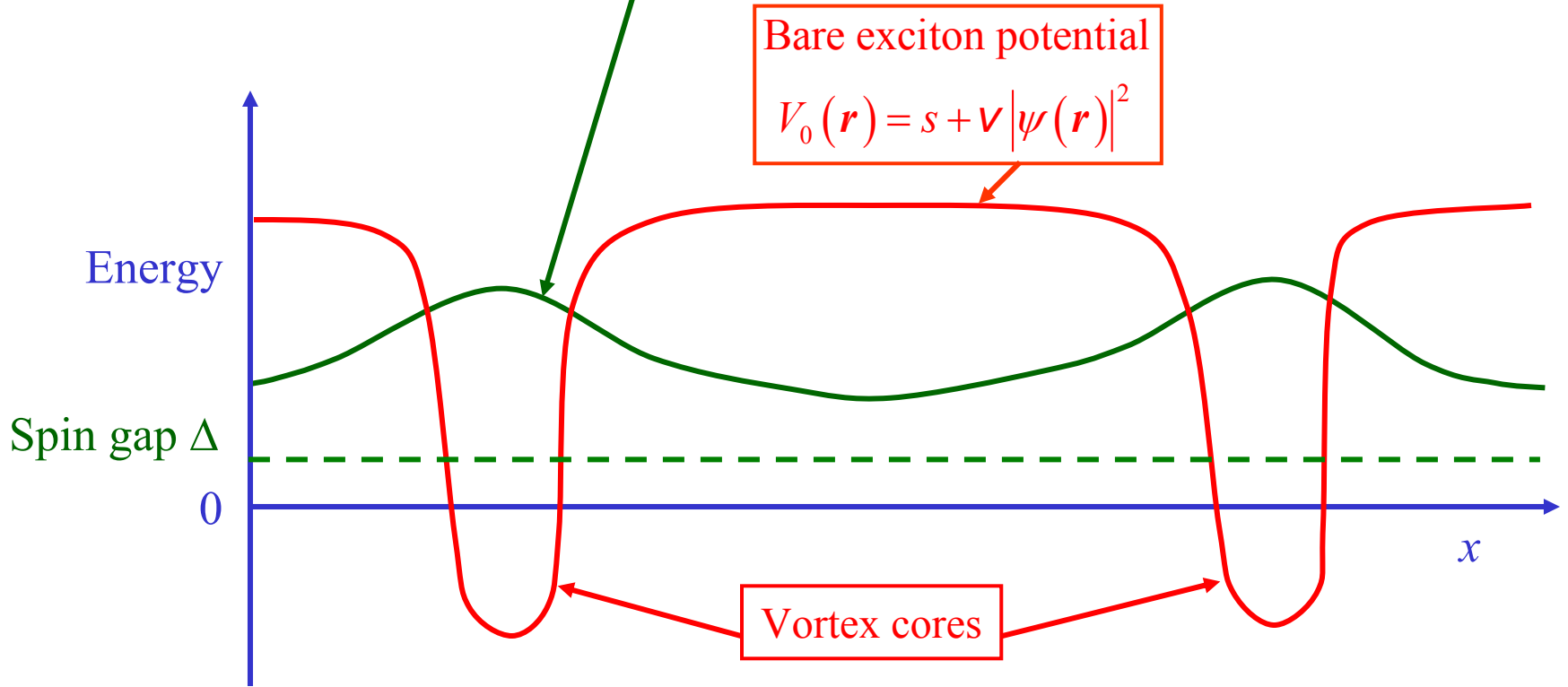
Elastic scattering intensity

$$I(H) = I(0) + a \left( \frac{H}{J} \right)^2$$



D. P. Arovas, A. J. Berlinsky, C. Kallin, and S.-C. Zhang,  
*Phys. Rev. Lett.* **79**, 2871 (1997) proposed static magnetism  
 (with  $\Delta=0$ ) localized within vortex cores

Envelope of lowest energy spin-exciton eigenmode  $\Phi_\alpha$   
 after including exciton interactions:  $V(\mathbf{r}) = V_0(\mathbf{r}) + g \langle |\Phi_\alpha(\mathbf{r})|^2 \rangle$



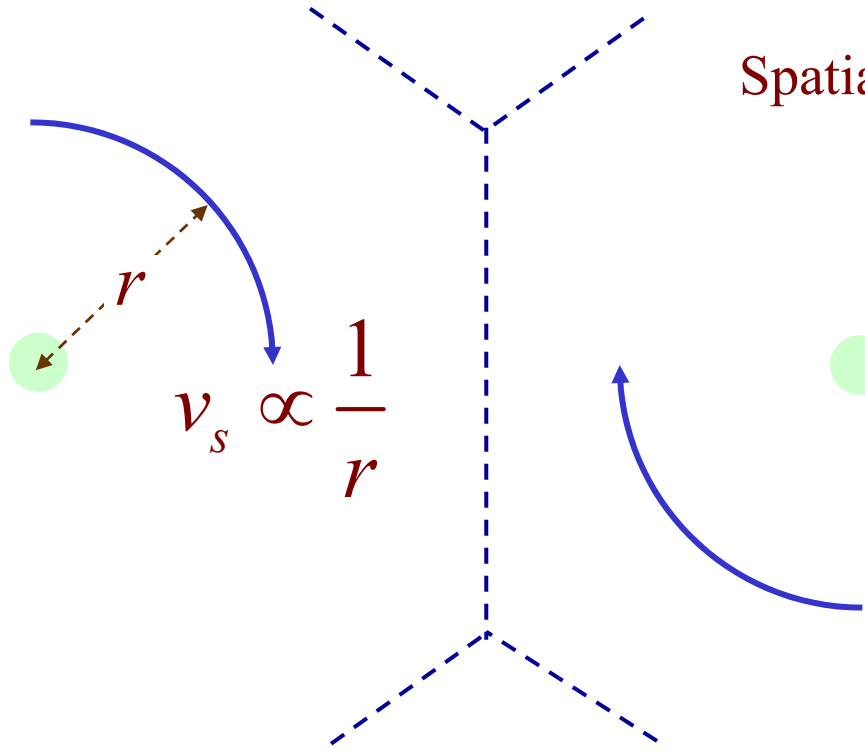
*Strongly relevant* repulsive interactions between excitons imply that excitons must be extended as  $\Delta \rightarrow 0$ .

E. Demler, S. Sachdev, and Y. Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

A.J. Bray and M.A. Moore, *J. Phys. C* **15**, L7 65 (1982).

J.A. Hertz, A. Fleishman, and P.W. Anderson, *Phys. Rev. Lett.* **43**, 942 (1979).

A magnetic field applied to a superconductor induces a lattice of vortices in superflow

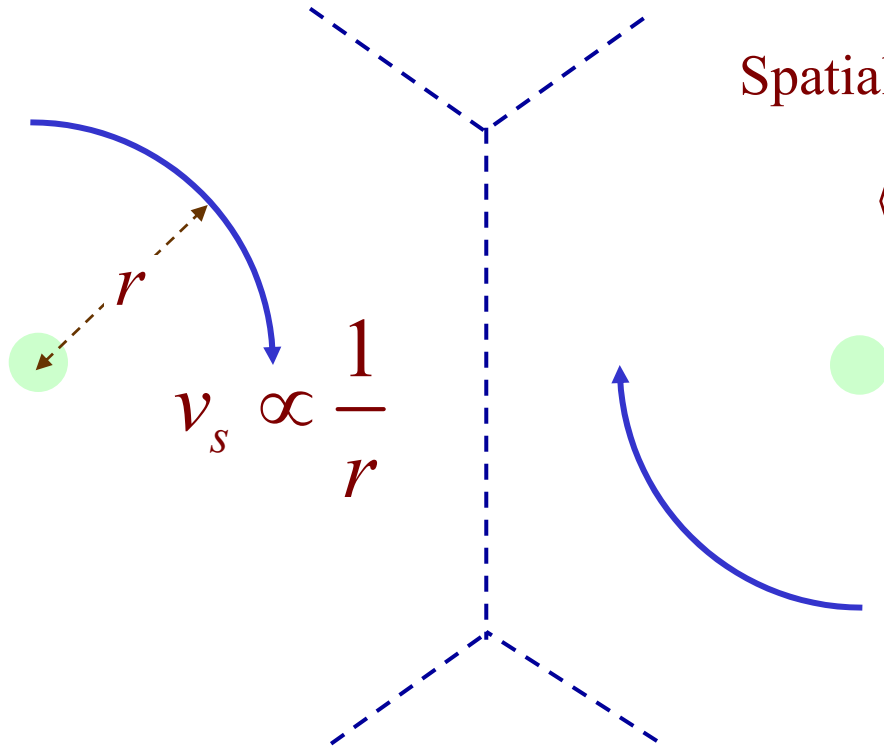


Spatially averaged superflow kinetic energy

$$\langle v_s^2 \rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H}$$



# Dominant effect with coexisting superconductivity: uniform softening of spin excitations by superflow kinetic energy



Spatially averaged superflow kinetic energy

$$\langle v_s^2 \rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H}$$

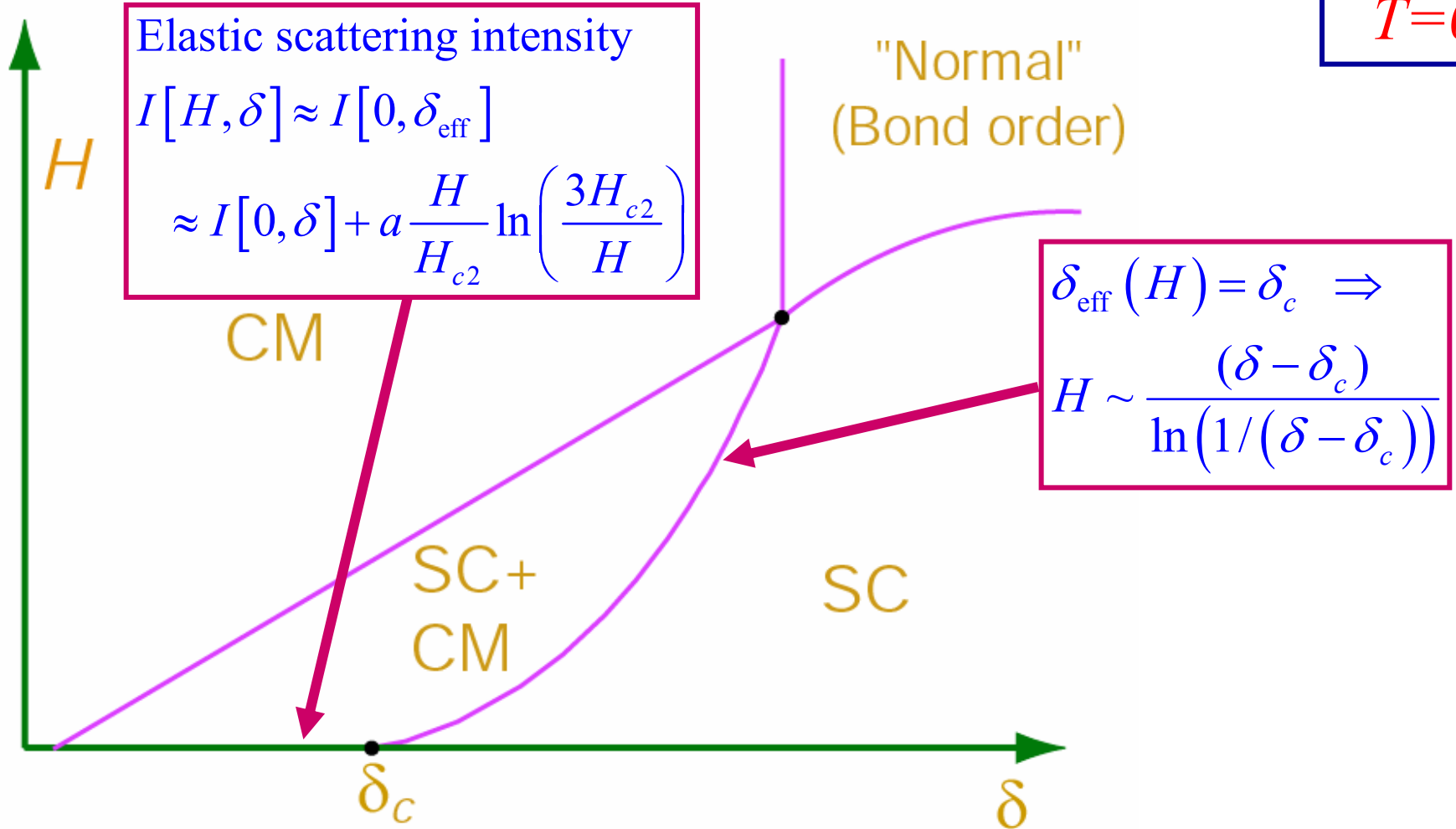
The suppression of SC order appears to the CM order as an effective  $\delta$  :

$$\delta_{\text{eff}}(H) = \delta - C \frac{H}{H_{c2}} \ln \left( \frac{3H_{c2}}{H} \right)$$

Competing order is enhanced in a “halo” around each vortex

# Main results

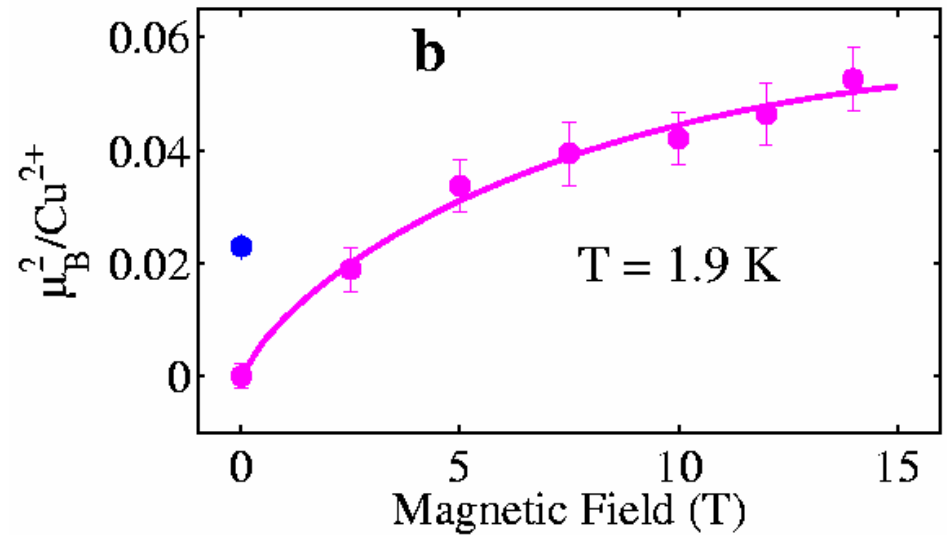
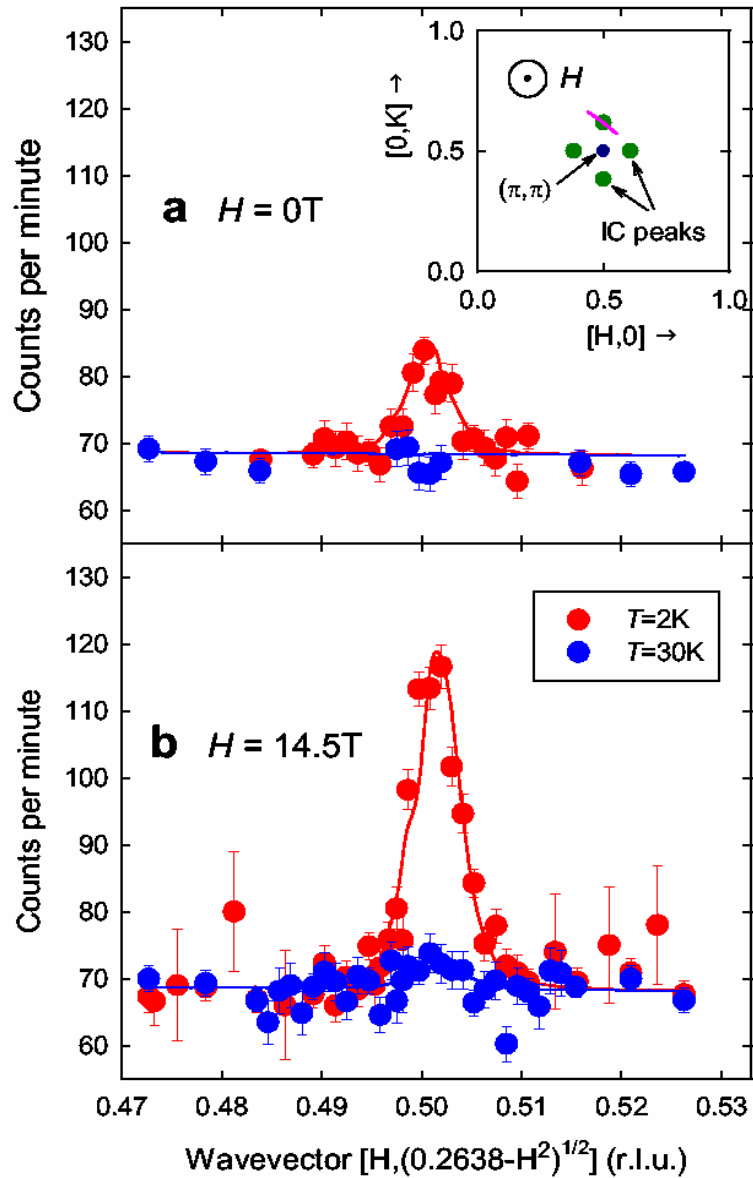
$T=0$



E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

# Neutron scattering of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at $x=0.1$

B. Lake, H. M. Rønnow, N. B. Christensen, G. Aeppli, K. Lefmann, D. F. McMorrow, P. Vorderwisch, P. Smeibidl, N. Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, T. E. Mason, *Nature*, **415**, 299 (2002).



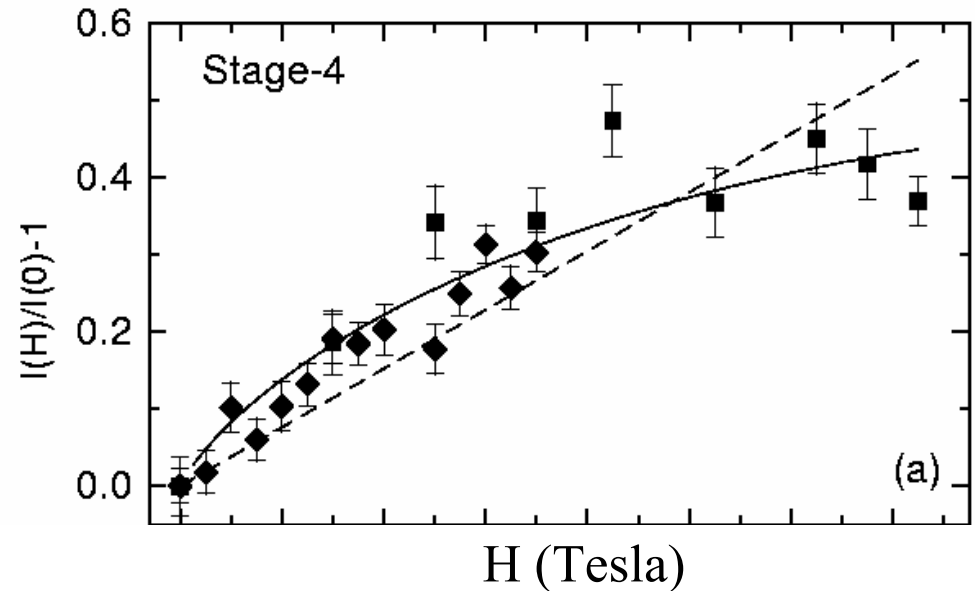
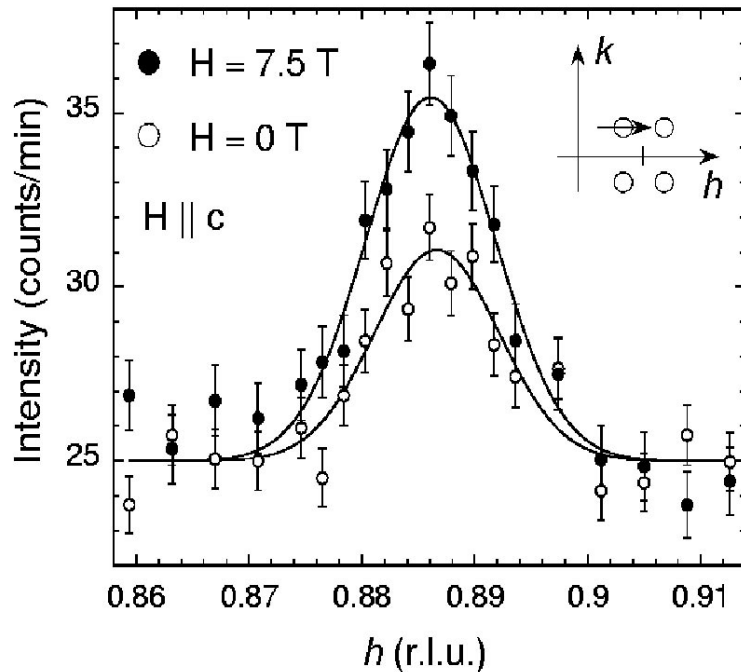
Solid line - fit to : 
$$I(H) = a \frac{H}{H_{c2}} \ln \left( \frac{H_{c2}}{H} \right)$$

See also S. Katano, M. Sato, K. Yamada, T. Suzuki, and T. Fukase, *Phys. Rev. B* **62**, R14677 (2000).

# Neutron scattering measurements of static spin correlations of the superconductor+spin-density-wave (SC+CM) in a magnetic field

Elastic neutron scattering off  $\text{La}_2\text{CuO}_{4+y}$

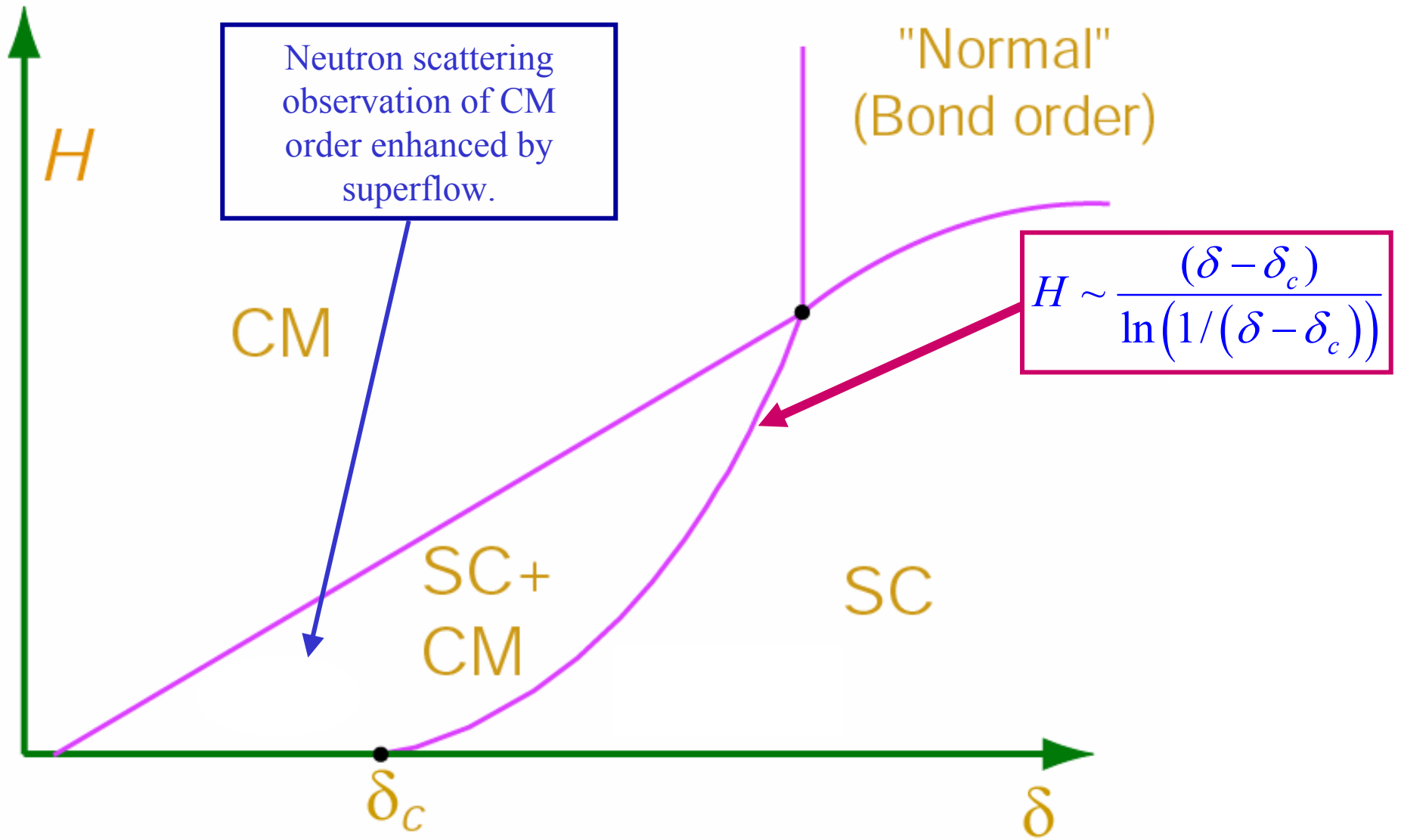
B. Khaykovich, Y. S. Lee, S. Wakimoto,  
K. J. Thomas, M. A. Kastner,  
and R.J. Birgeneau, *Phys. Rev. B* **66**,  
014528 (2002).



Solid line --- fit to :  $\frac{I(H)}{I(0)} = 1 + a \frac{H}{H_{c2}} \ln\left(\frac{3.0H_{c2}}{H}\right)$

$a$  is the only fitting parameter

Best fit value -  $a = 2.4$  with  $H_{c2} = 60 \text{ T}$

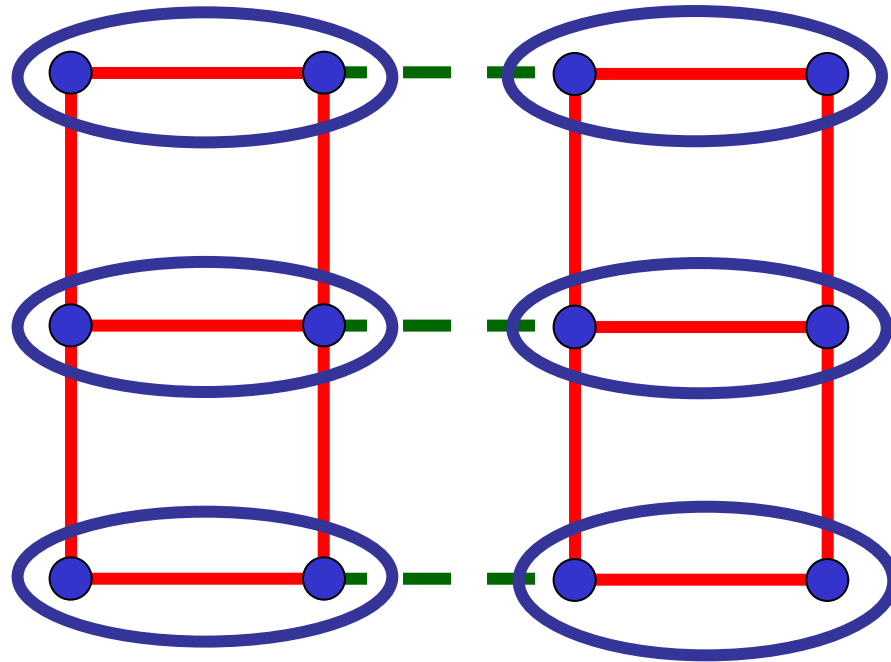


E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

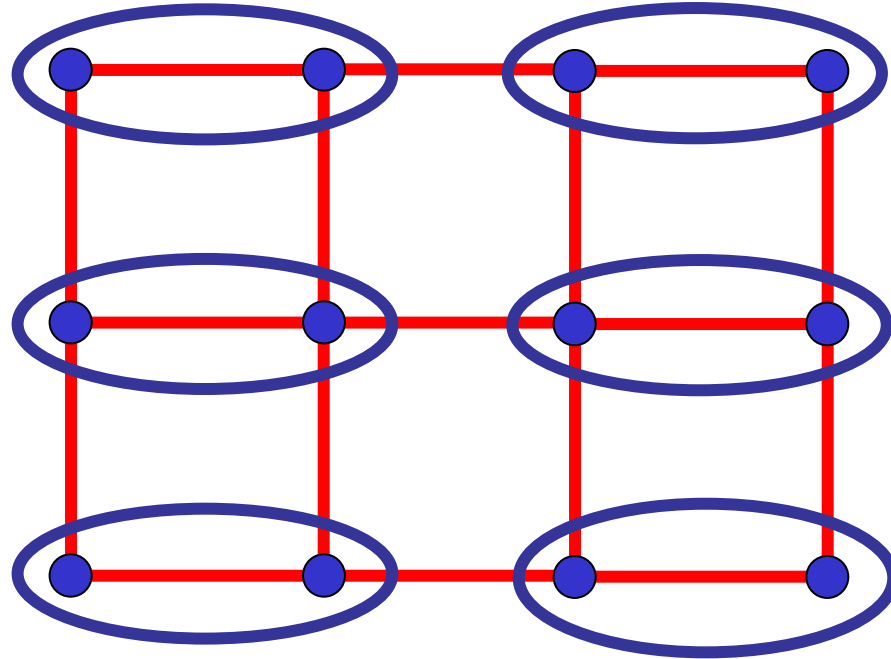
## Outline

- I. Simple model of a quantum phase transition  
Coupled ladder antiferromagnet
- II. Interplay of CM and SC order in the cuprates: theory  
and neutron scattering experiments
- III. Microscopic theory: bond order and a global phase  
diagram (STM experiments)**
- IV. Conclusions

## Paramagnetic ground state of coupled ladder model

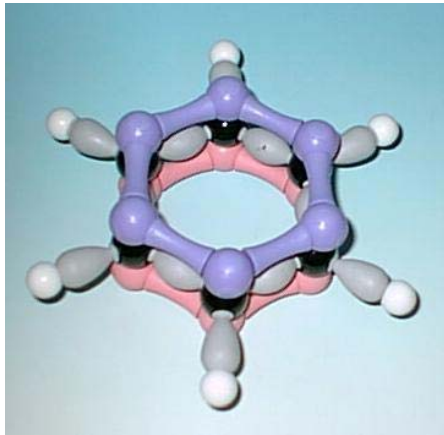
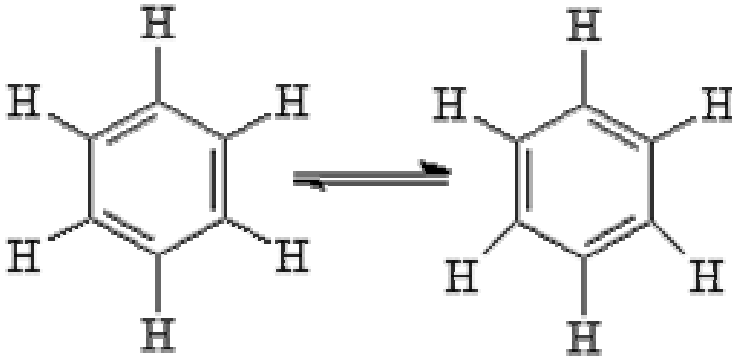


Can such a state with *bond order* be the ground state of a system with full square lattice symmetry ?



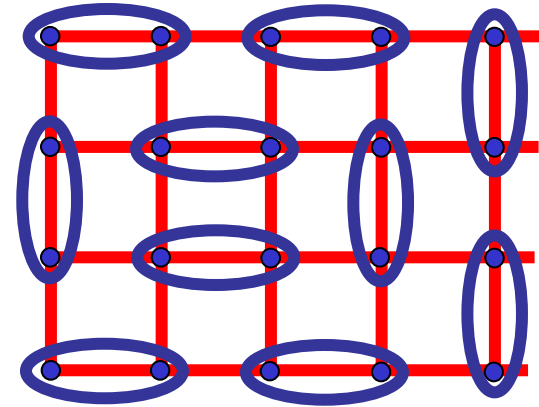


## Resonating valence bonds



Resonance in benzene leads to a symmetric configuration of valence bonds

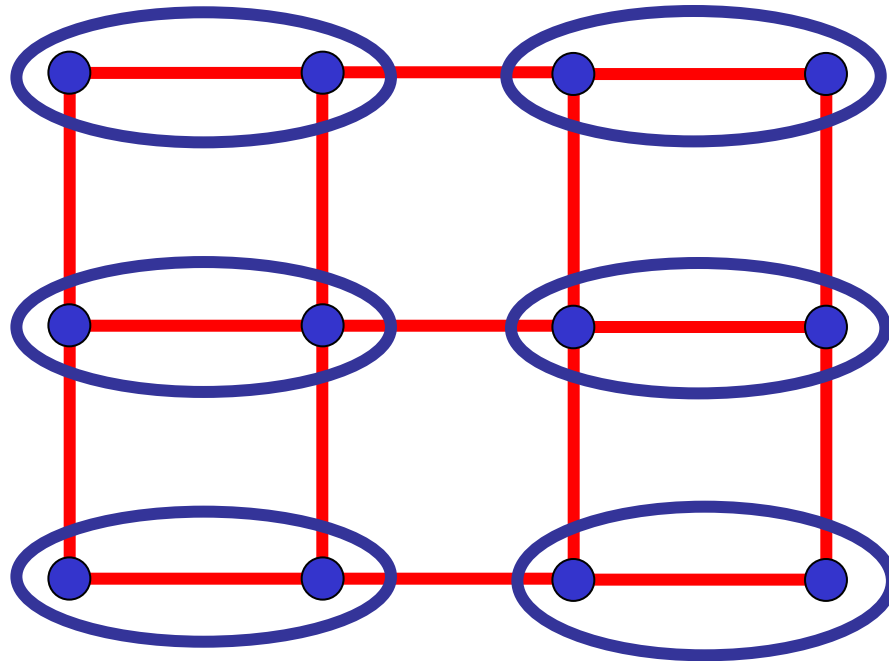
*(F. Kekulé, L. Pauling)*



The paramagnet on the square lattice should also allow other valence bond pairings, and this leads to a “resonating valence bond liquid”

*(P.W. Anderson, 1987)*

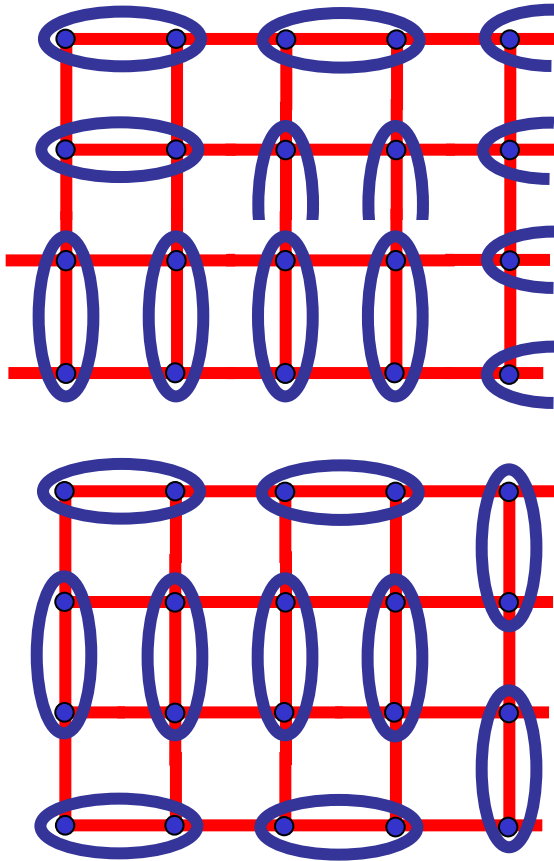
Can such a state with *bond order* be the ground state of a system with full square lattice symmetry ?



Surprising answer: **Yes** ! Here resonance acts to produce a state which breaks lattice symmetry by the appearance of *bond order*

Such *bond order* is generic in paramagnetic states proximate to a magnetic state with collinear spins

N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).



## Origin of bond order

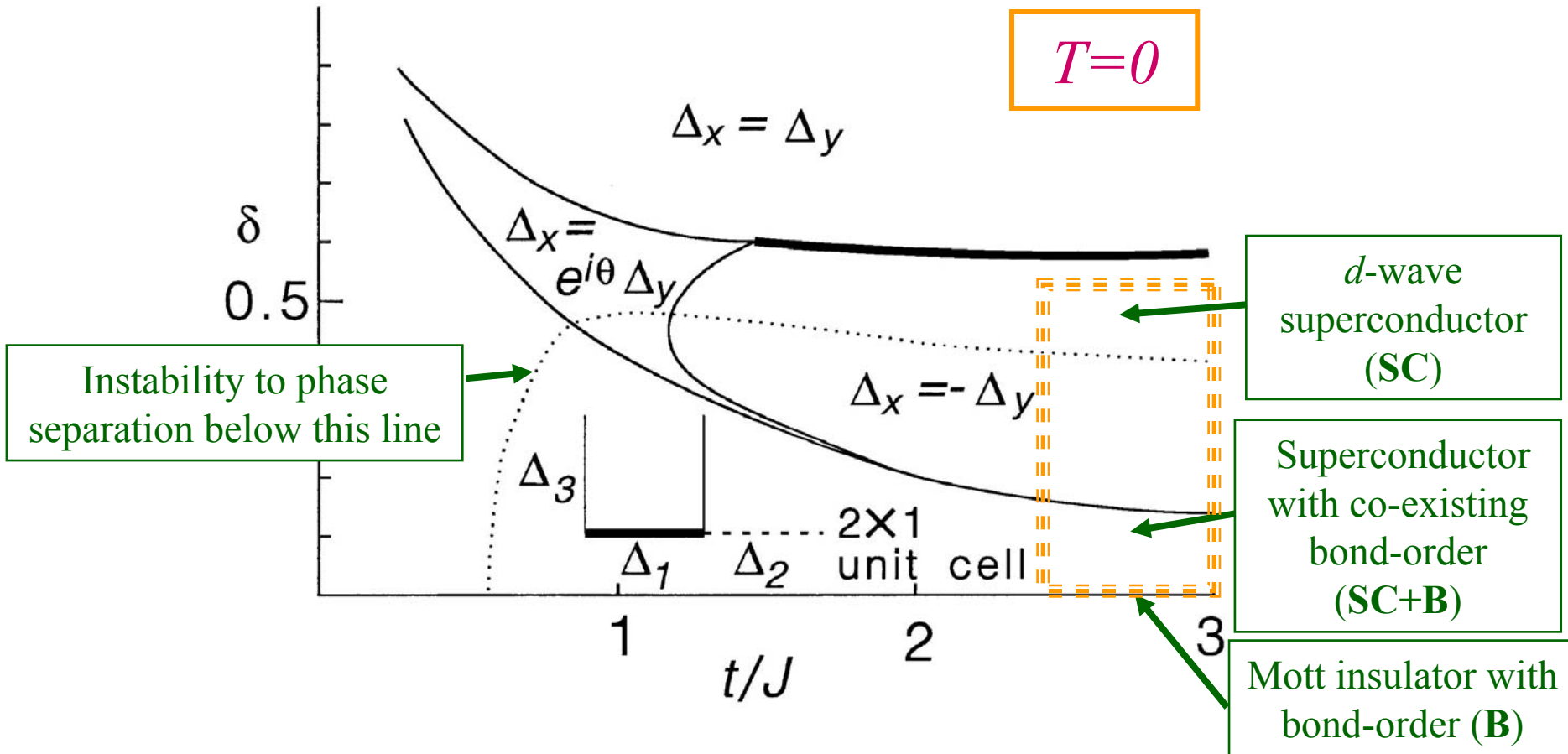
Quantum “entropic” effects prefer bond-ordered configurations in which the largest number of singlet pairs can resonate. The state on the upper left has more flippable pairs of singlets than the one on the lower left.

These effects lead to a broken square lattice symmetry near the transition to the magnetically ordered states with collinear spins.

The quantum dimer model (D. Rokhsar and S.A. Kivelson, *Phys. Rev. Lett.* **61**, 2376 (1988); E. Fradkin and S. A. Kivelson, *Mod. Phys. Lett. B* **4**, 225 (1990)) and semiclassical theories provide dual descriptions of this physics

N. Read and S. Sachdev, *Phys. Rev. B* **42**, 4568 (1990).

# Doping a paramagnetic bond-ordered Mott insulator

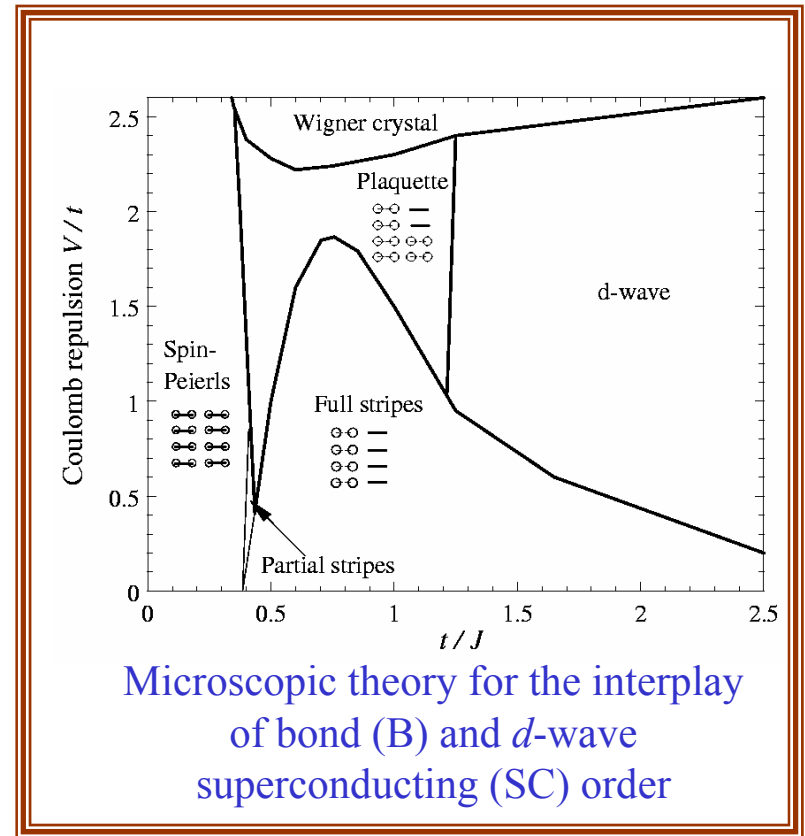
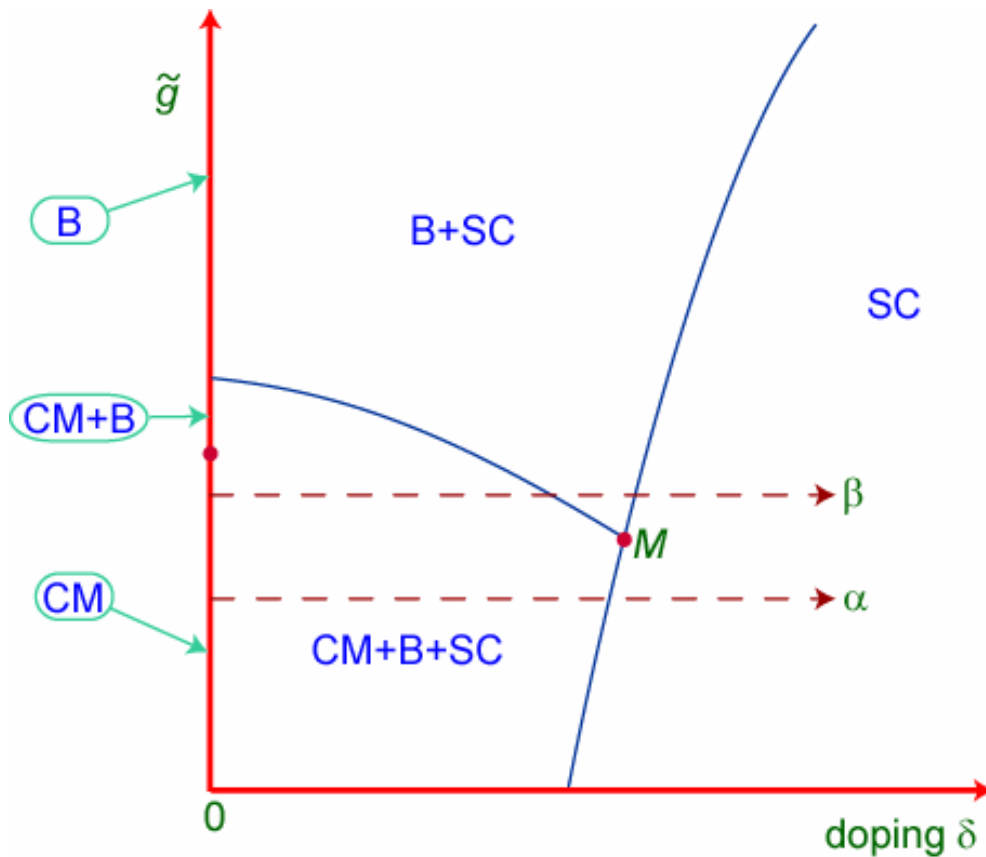


S. Sachdev and N. Read, *Int. J. Mod. Phys. B* **5**, 219 (1991).

# A global phase diagram

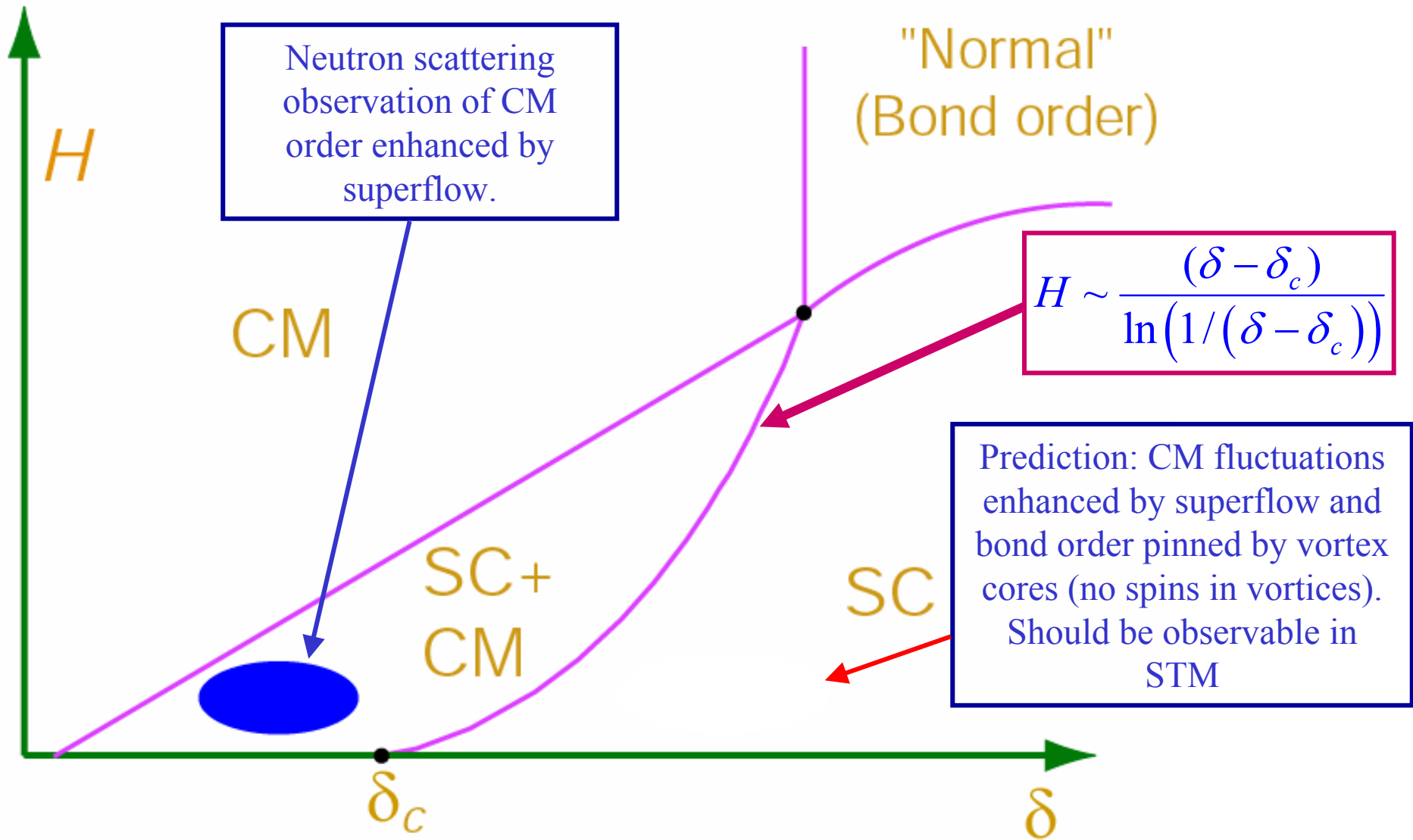
Vertical axis is any microscopic parameter which suppresses

CM order



- Pairing order of BCS theory (SC)
- Collinear magnetic order (CM)
- Bond order (B)

S. Sachdev and N. Read, *Int. J. Mod. Phys. B* **5**, 219 (1991).  
 M. Vojta and S. Sachdev, *Phys. Rev. Lett.* **83**, 3916 (1999);  
 M. Vojta, Y. Zhang, and S. Sachdev, *Phys. Rev. B* **62**, 6721 (2000);  
 M. Vojta, *Phys. Rev. B* **66**, 104505 (2002).

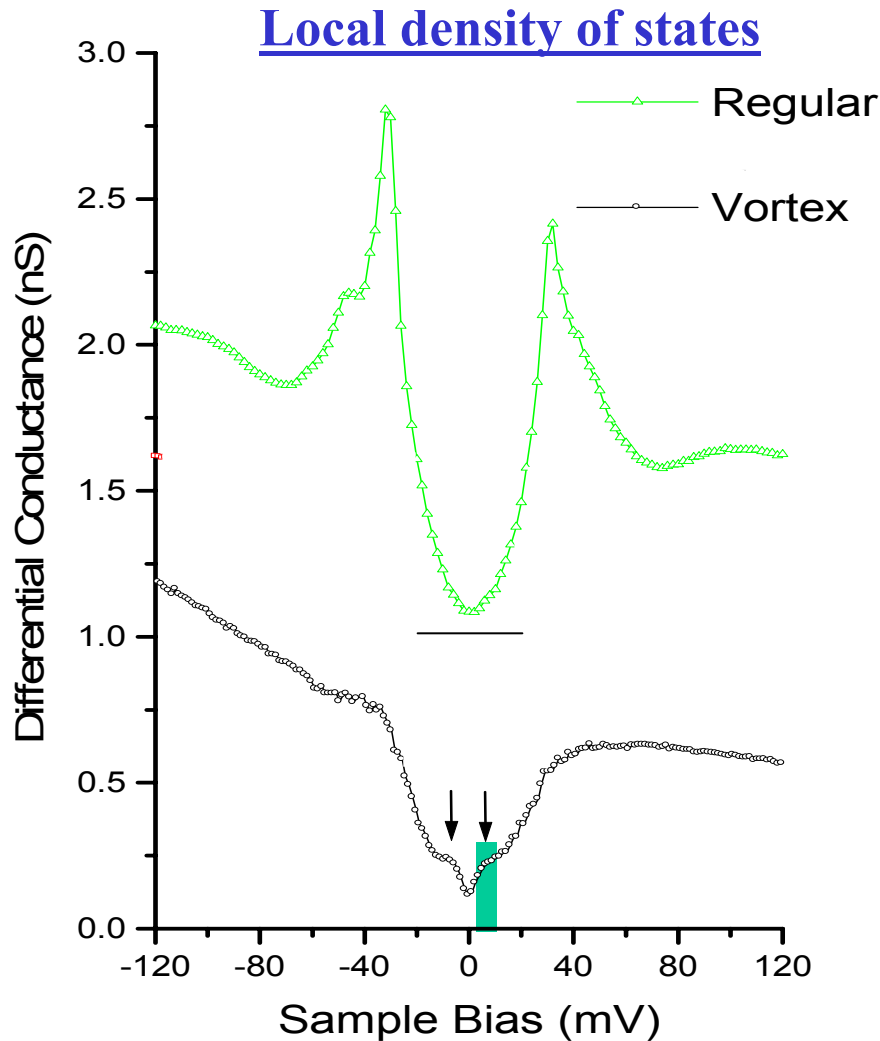


K. Park and S. Sachdev *Phys. Rev. B* **64**, 184510 (2001).

Y. Zhang, E. Demler and S. Sachdev, *Phys. Rev. B* **66**, 094501 (2002).

# STM around vortices induced by a magnetic field in the superconducting state

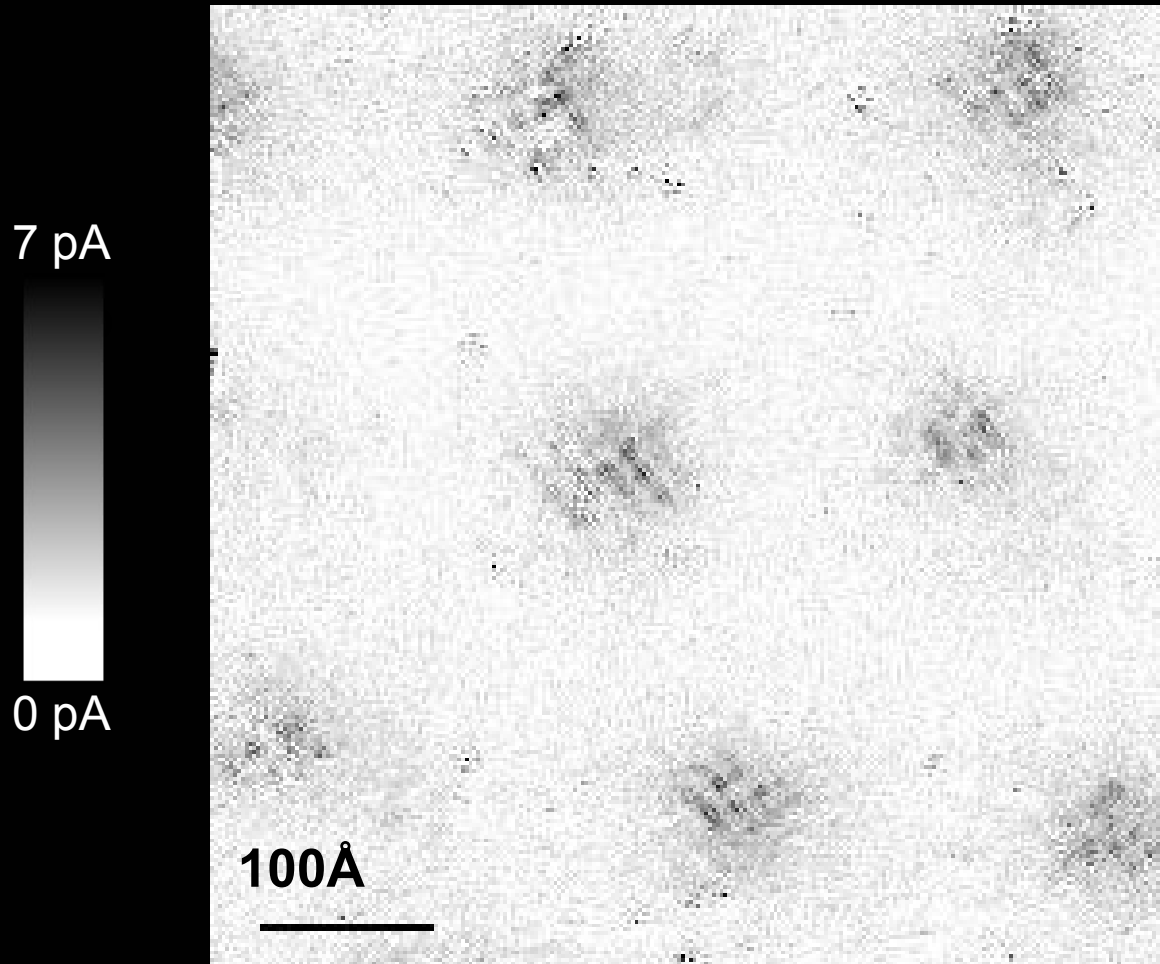
J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan,  
H. Eisaki, S. Uchida, and J. C. Davis, *Science* **295**, 466 (2002).



1Å spatial resolution  
image of integrated  
LDOS of  
 $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$   
( 1meV to 12 meV)  
at B=5 Tesla.

S.H. Pan *et al.* *Phys. Rev. Lett.* **85**, 1536 (2000).

Vortex-induced LDOS of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  integrated  
from 1meV to 12meV

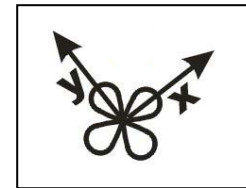
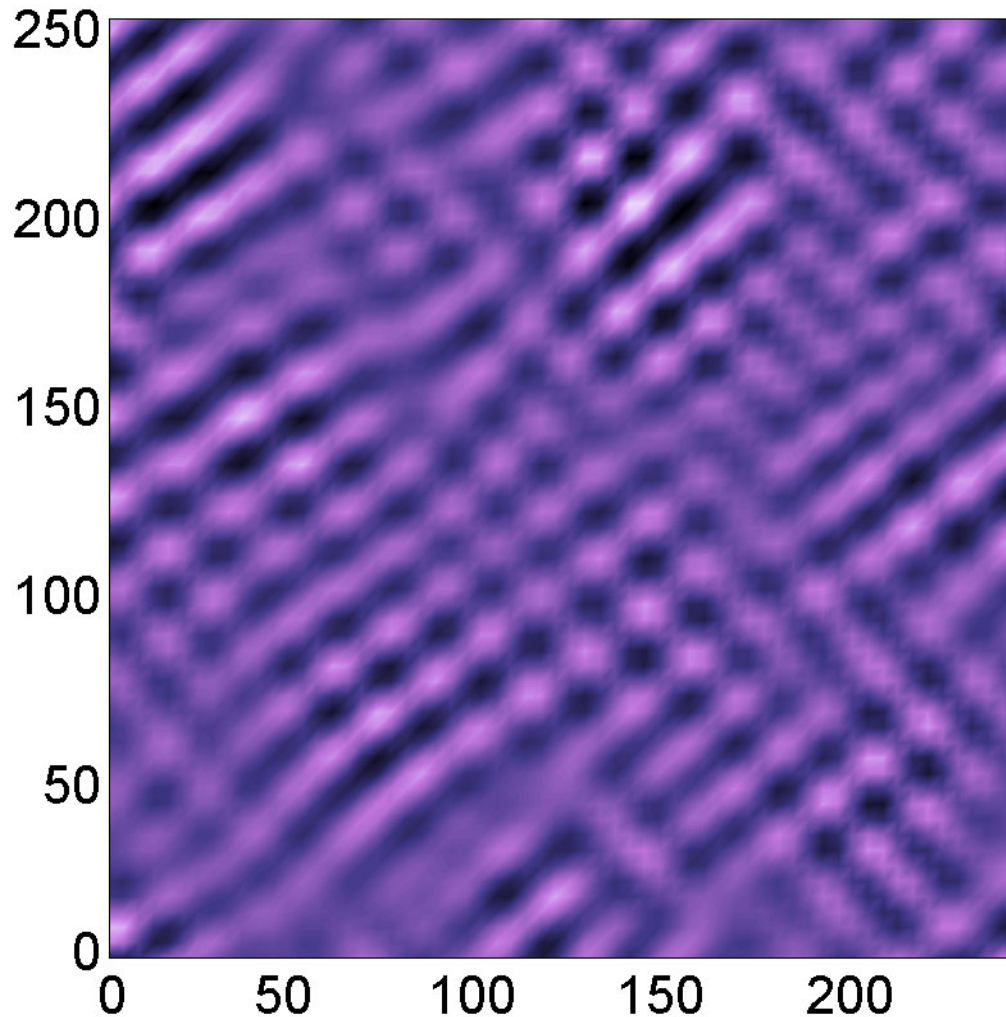


J. Hoffman E. W. Hudson,  
K. M. Lang, V. Madhavan,  
S. H. Pan, H. Eisaki,  
S. Uchida, and J. C. Davis,  
*Science* 295, 466 (2002).

Our interpretation: LDOS modulations are signals of  
bond order of period 4 revealed in vortex halo



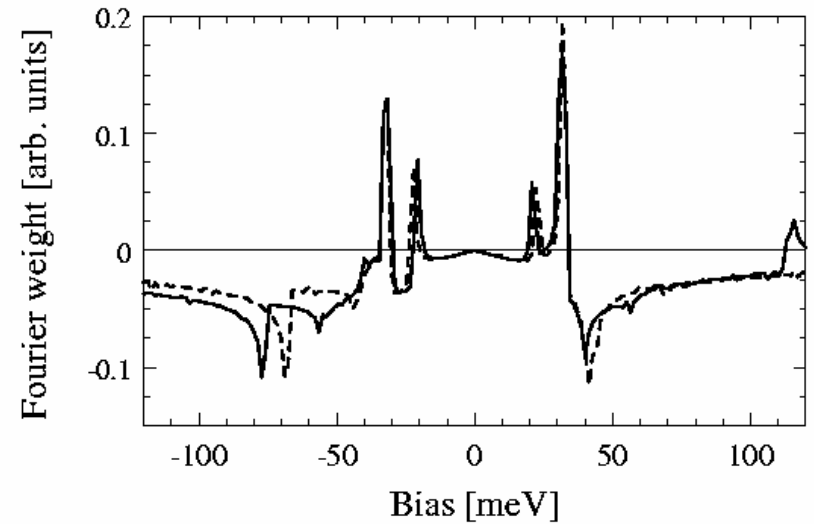
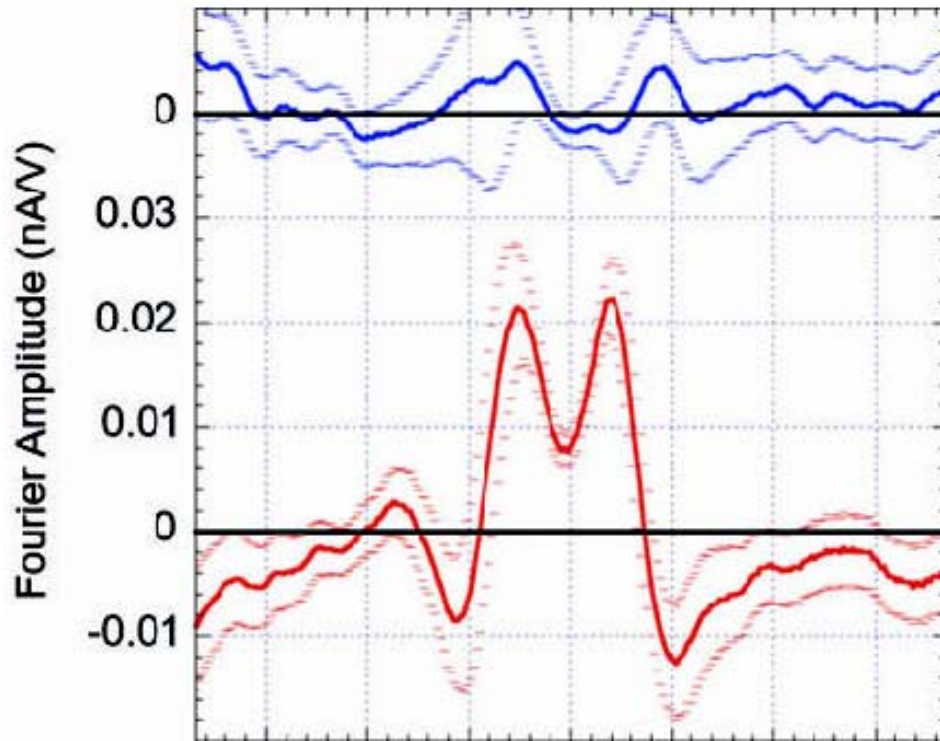
### III. STM image of LDOS modulations in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ in zero magnetic field



Period = 4 lattice spacings

C. Howald, H. Eisaki, N. Kaneko, M. Greven, and A. Kapitulnik,  
*Phys. Rev. B* **67**, 014533 (2003).

# Spectral properties of the STM signal are sensitive to the microstructure of the charge order

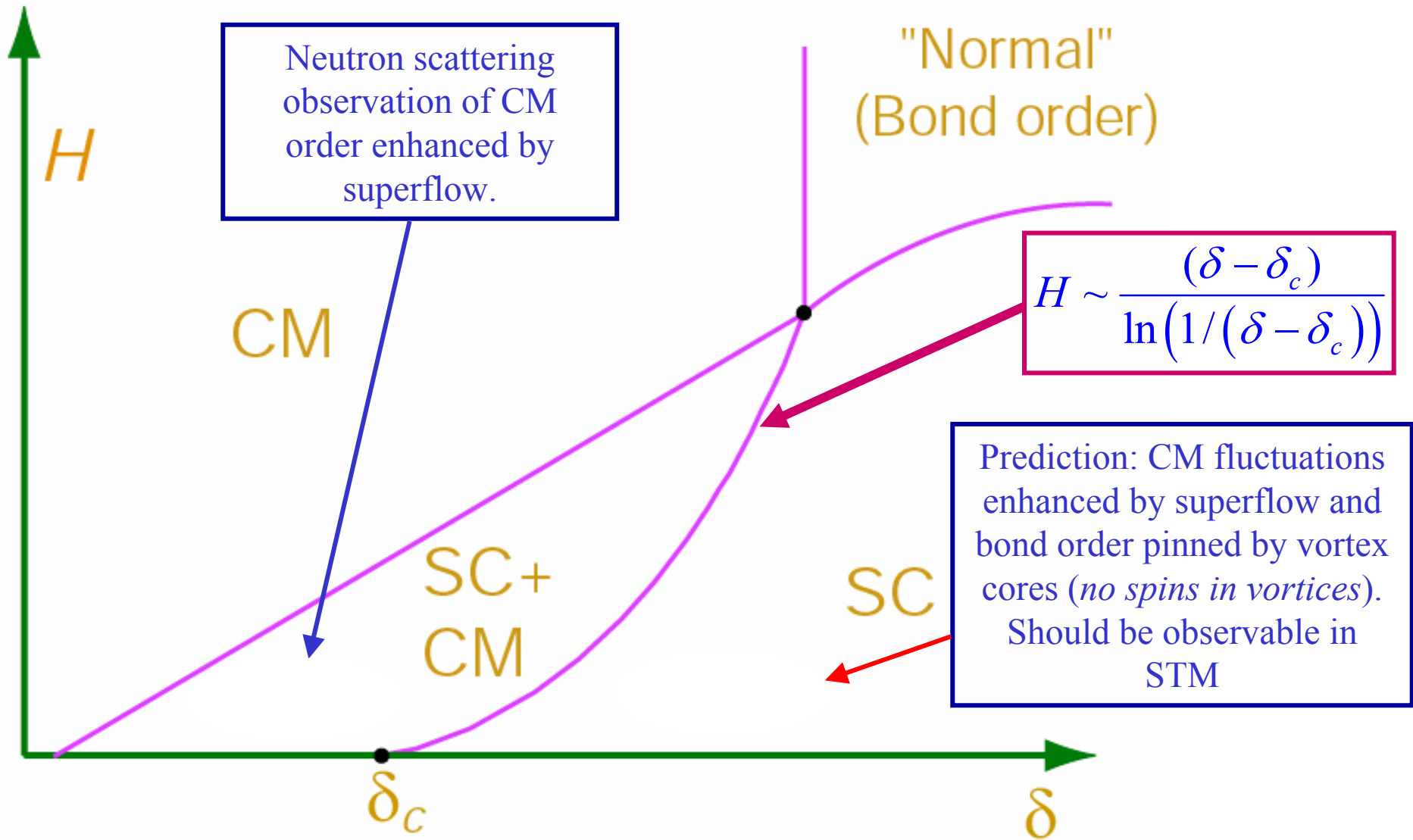


Theoretical modeling shows that this spectrum is best obtained by a modulation of bond variables, such as the exchange, kinetic or pairing energies.

Measured energy dependence of the Fourier component of the density of states which modulates with a period of 4 lattice spacings

C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, *Phys. Rev. B* **67**, 014533 (2003).

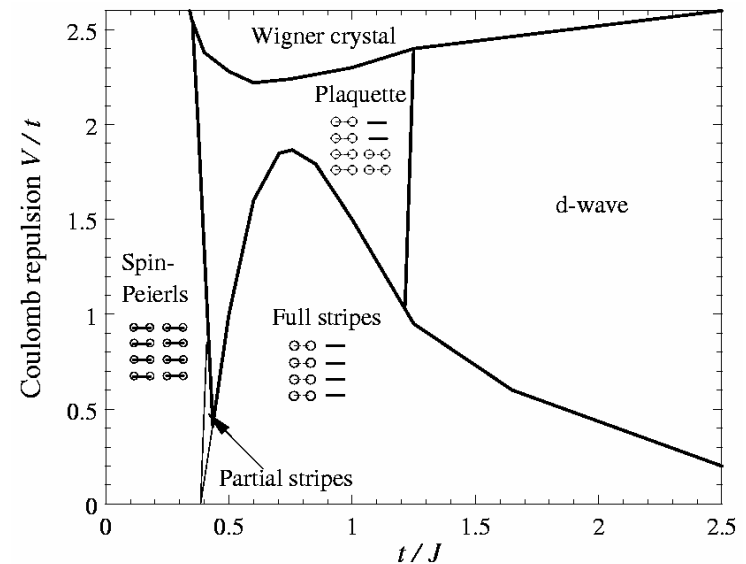
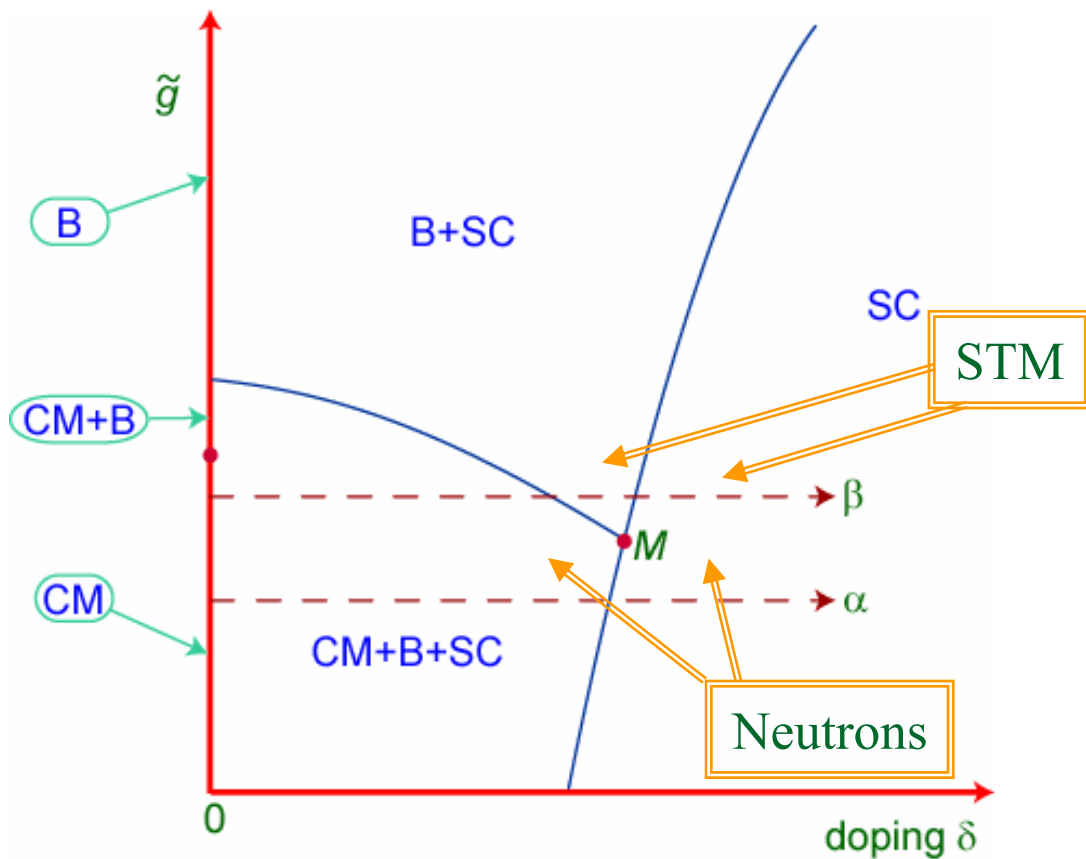
M. Vojta, *Phys. Rev. B* **66**, 104505 (2002);  
D. Podolsky, E. Demler, K. Damle, and B.I. Halperin, *Phys. Rev. B* in press, cond-mat/0204011



K. Park and S. Sachdev *Phys. Rev. B* **64**, 184510 (2001).

Y. Zhang, E. Demler and S. Sachdev, *Phys. Rev. B* **66**, 094501 (2002).

# Global phase diagram



S. Sachdev and N. Read, *Int. J. Mod. Phys. B* **5**, 219 (1991). M. Vojta and S. Sachdev, *Phys. Rev. Lett.* **83**, 3916 (1999); M. Vojta, Y. Zhang, and S. Sachdev, *Phys. Rev. B* **62**, 6721 (2000); M. Vojta, *Phys. Rev. B* **66**, 104505 (2002).

See also S. Mazumdar, R.T. Clay, and D.K. Campbell, *Phys. Rev. B* **62**, 13400 (2000).  
J. Zaanen, *Physica C* **217**, 317 (1999).

S.A. Kivelson, E. Fradkin, and V. Emery, *Nature* **393**, 550 (1998).

S. White and D. Scalapino, *Phys. Rev. Lett.* **80**, 1272 (1998).

C. Castellani, C. Di Castro, and M. Grilli, *Phys. Rev. Lett.* **75**, 4650 (1995).

## Conclusions

- I. Cuprate superconductivity is associated with doping Mott insulators with charge carriers.
- II. Order parameters characterizing the Mott insulator compete with the order associated with the (Bose-Einstein) condensation of Cooper pairs.
- III. Classification of Mott insulators shows that the appropriate order parameters are collinear magnetism and bond order.
- IV. Theory of quantum phase transitions provides semi-quantitative predictions for neutron scattering measurements of spin-density-wave order in superconductors; theory also proposes a connection to STM experiments.
- V. Future experiments should search for SC+CM to SC quantum transition driven by a magnetic field.