

# Order and quantum phase transitions in the cuprate superconductors

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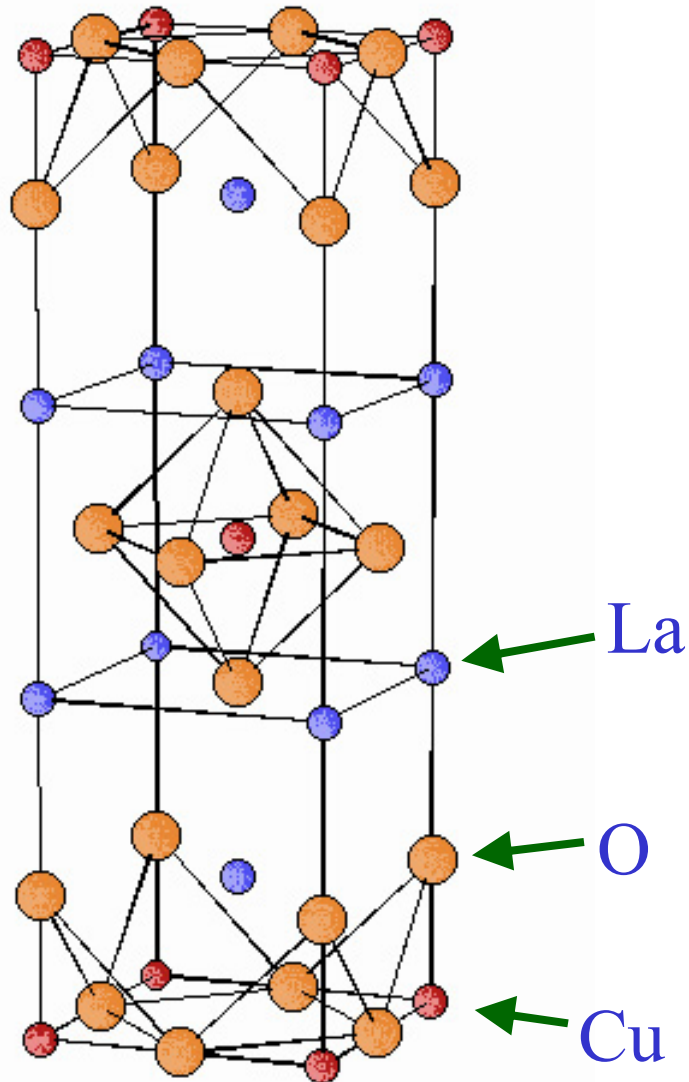
Colloquium article in *Reviews of Modern Physics*, July 2003,  
cond-mat/0211005.



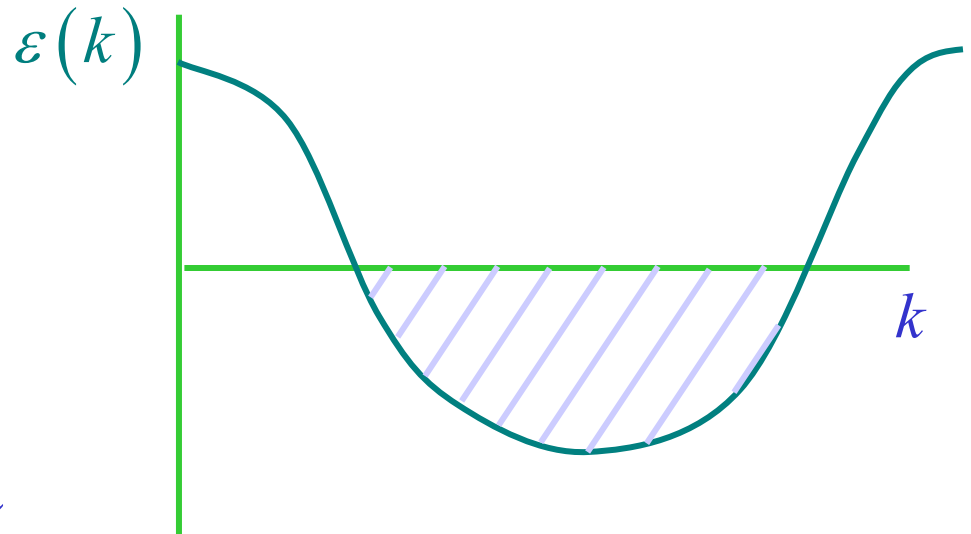
Talk online:  
[Google](#) [Sachdev](#)



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



Band theory

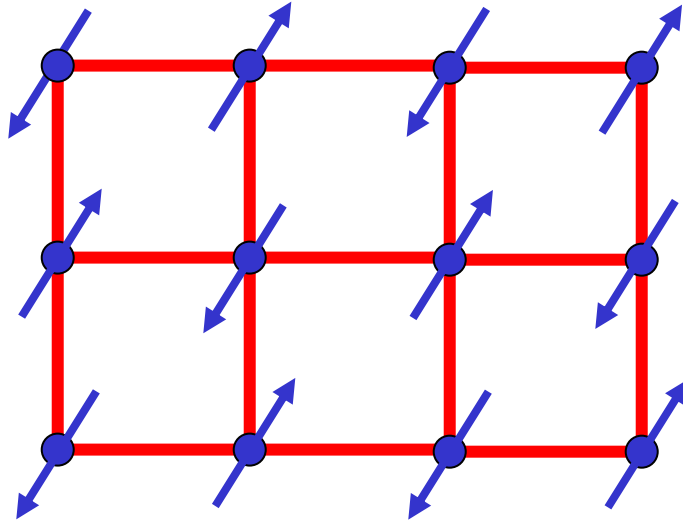


Half-filled band of Cu 3d orbitals –  
ground state is predicted to be a metal.

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

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

A Mott insulator



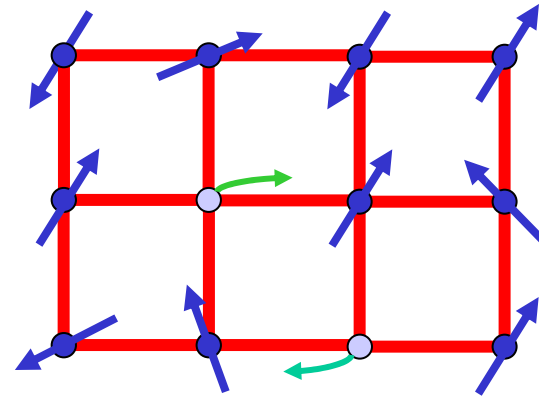
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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.  $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$

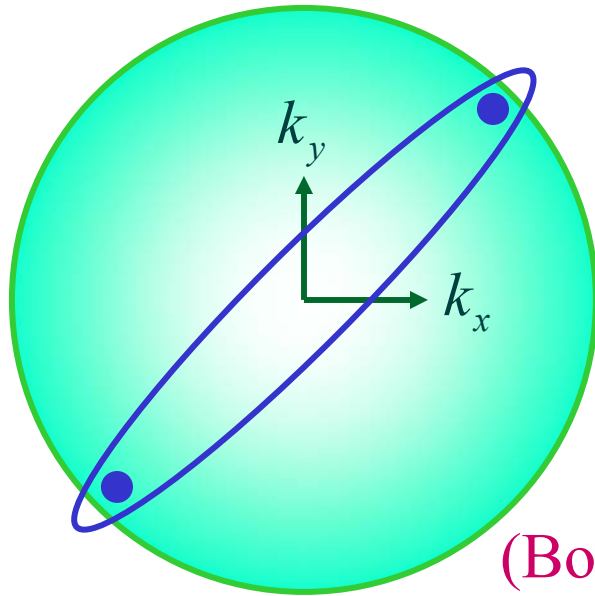


$$\langle \vec{S} \rangle = 0$$

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

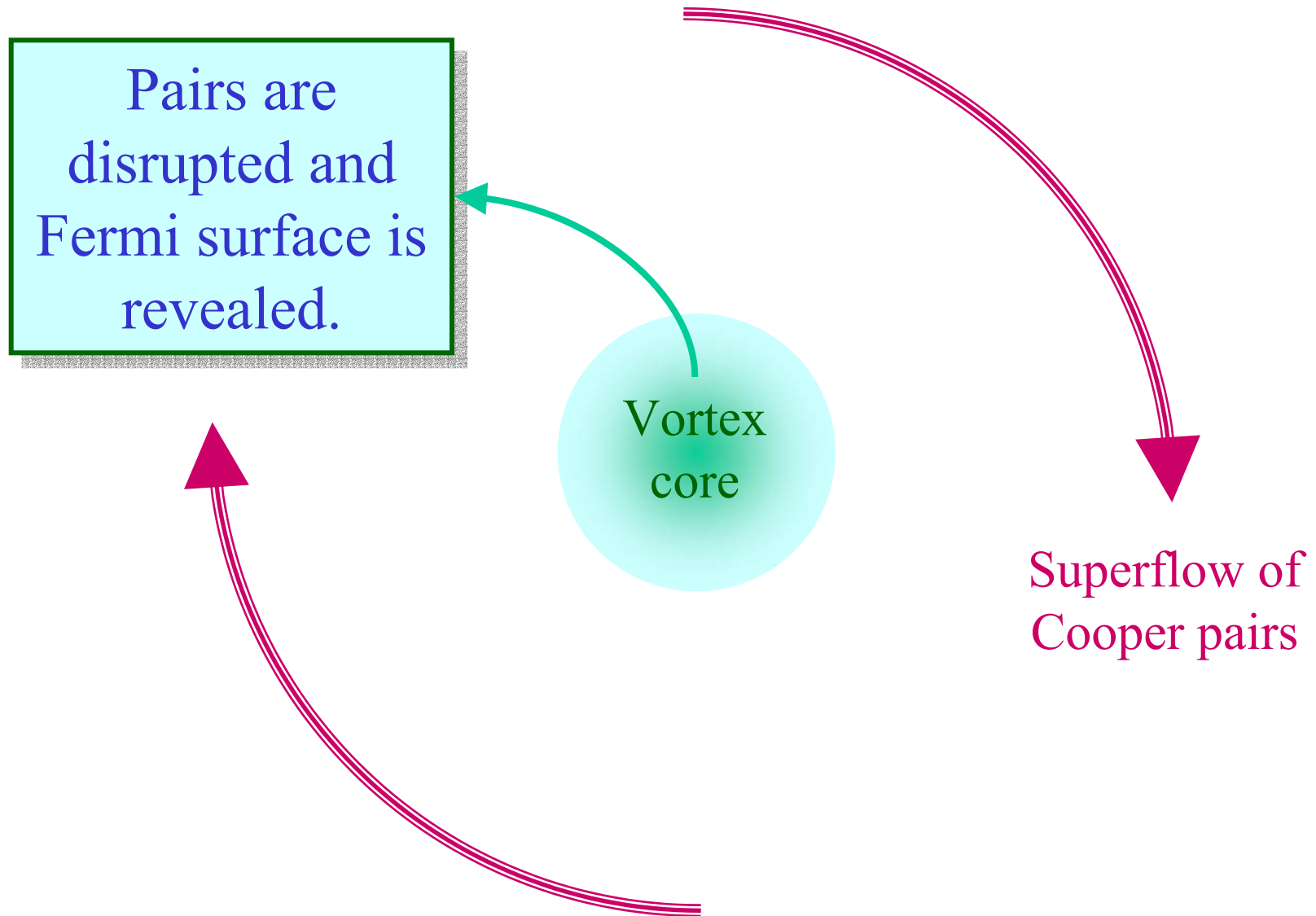
$$\Psi = (k_x^2 - k_y^2) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

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

(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.

# BCS theory of a vortex in the superconductor



# Superconductivity in a doped Mott insulator

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

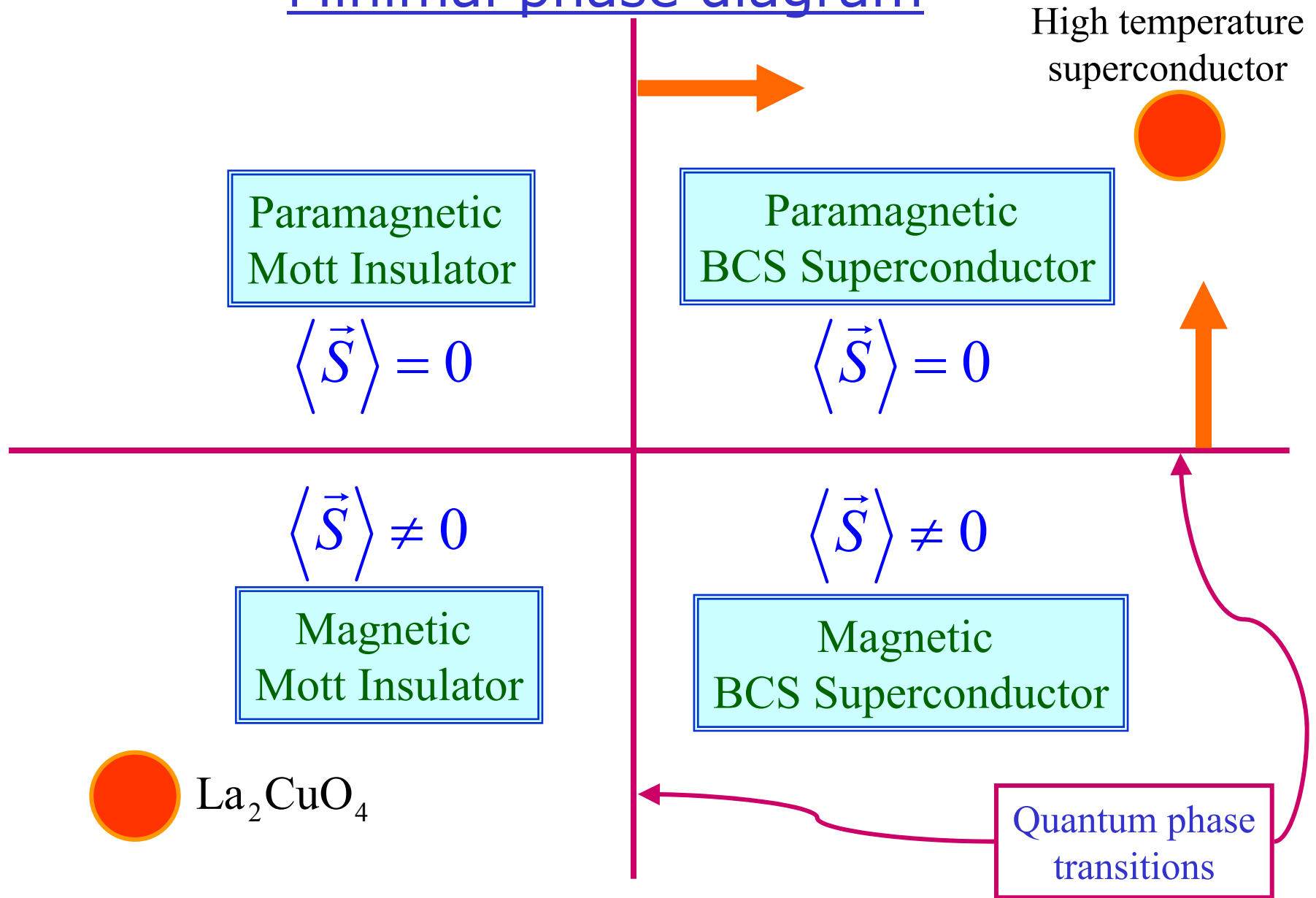
## Hypothesis:

Competition between orders of  
BCS theory (condensation of Cooper pairs)  
and  
Mott insulators

## Needed:

Theory of zero temperature transitions  
between competing ground states.

# Minimal phase diagram





Magnetic-paramagnetic quantum phase  
transition in a Mott insulator

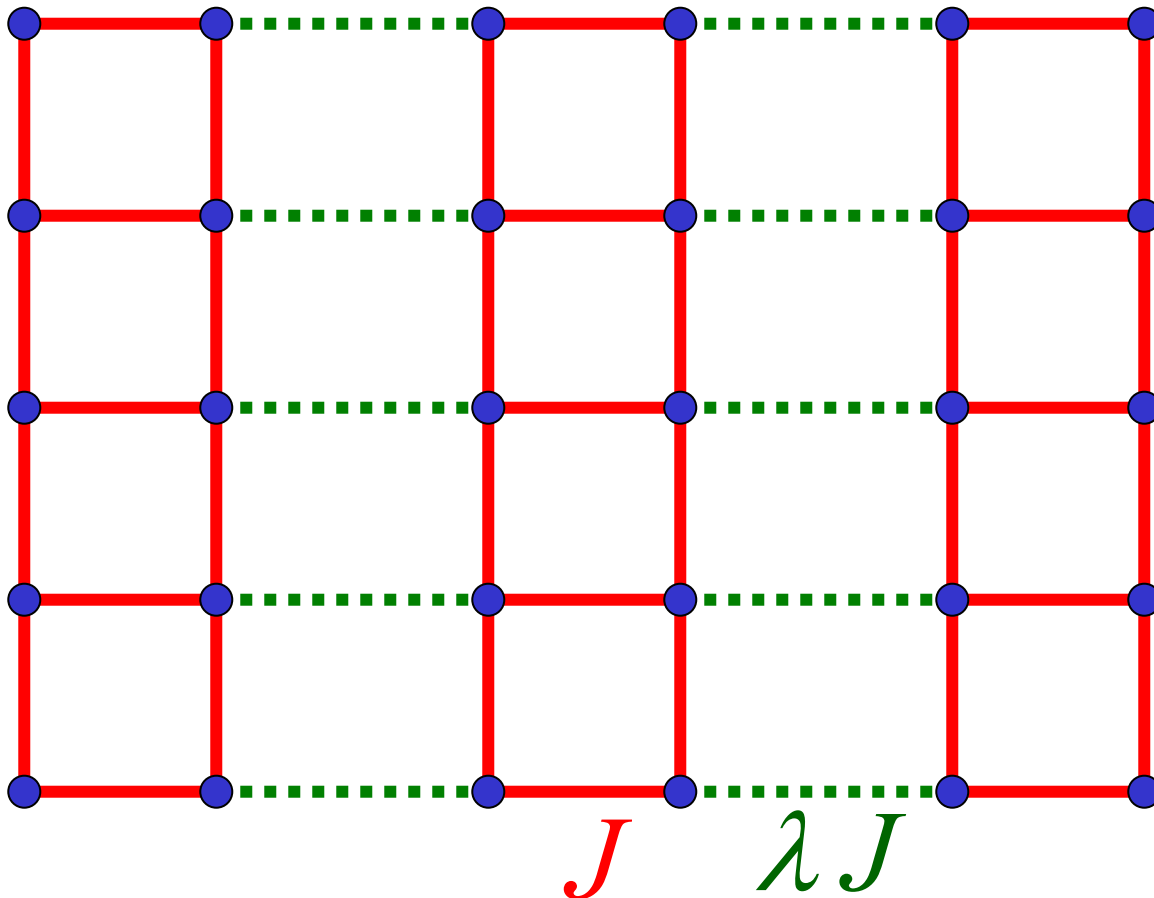
# Coupled ladder antiferromagnet

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



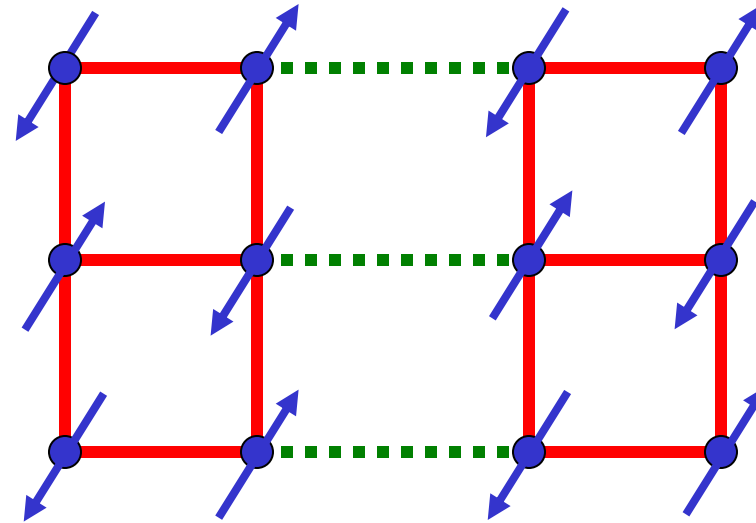
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

$\lambda$  close to 1

Square lattice antiferromagnet

Experimental realization:  $La_2CuO_4$



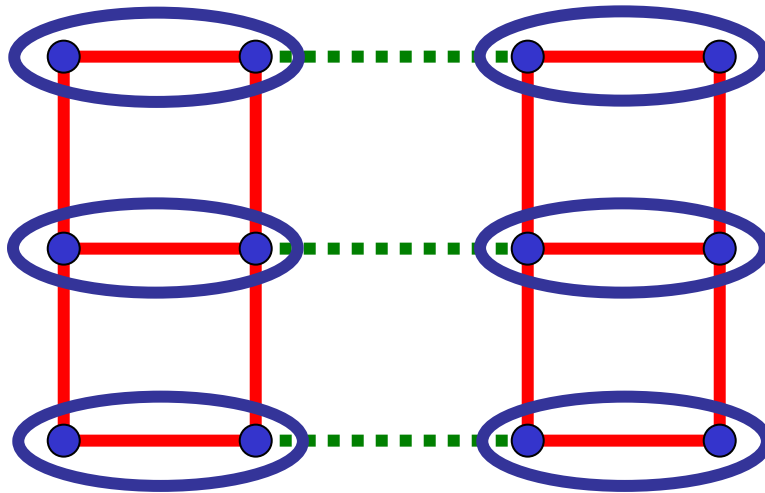
Ground state has long-range  
collinear magnetic (Neel) order

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

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



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

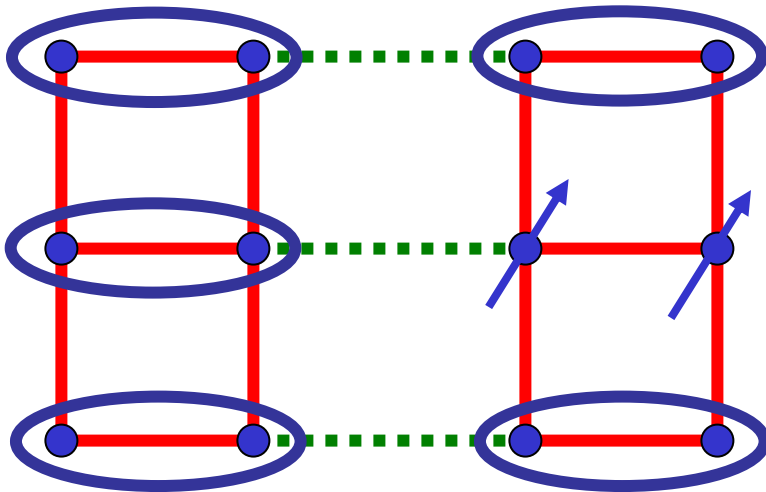
Real space Cooper pairs  
with their charge localized.  
Upon doping, motion and  
condensation of Cooper  
pairs leads to  
superconductivity

Paramagnetic ground state

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

$\lambda$  close to 0

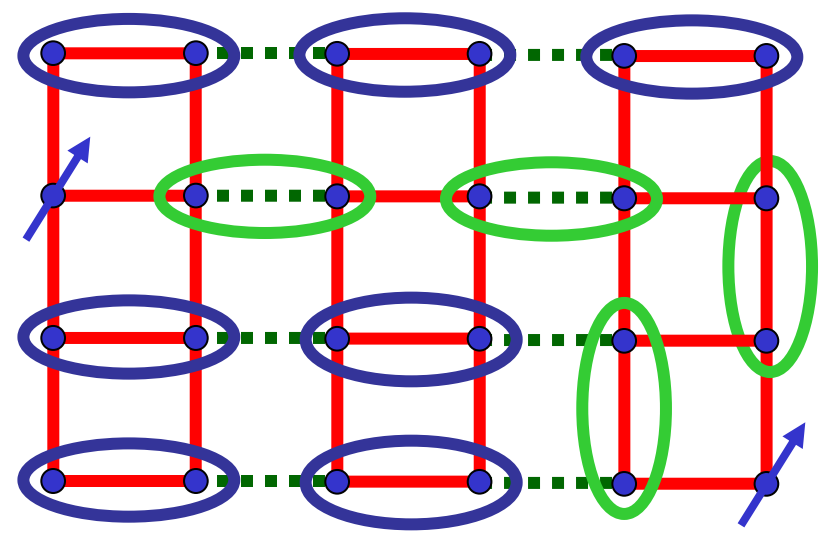
Excitations



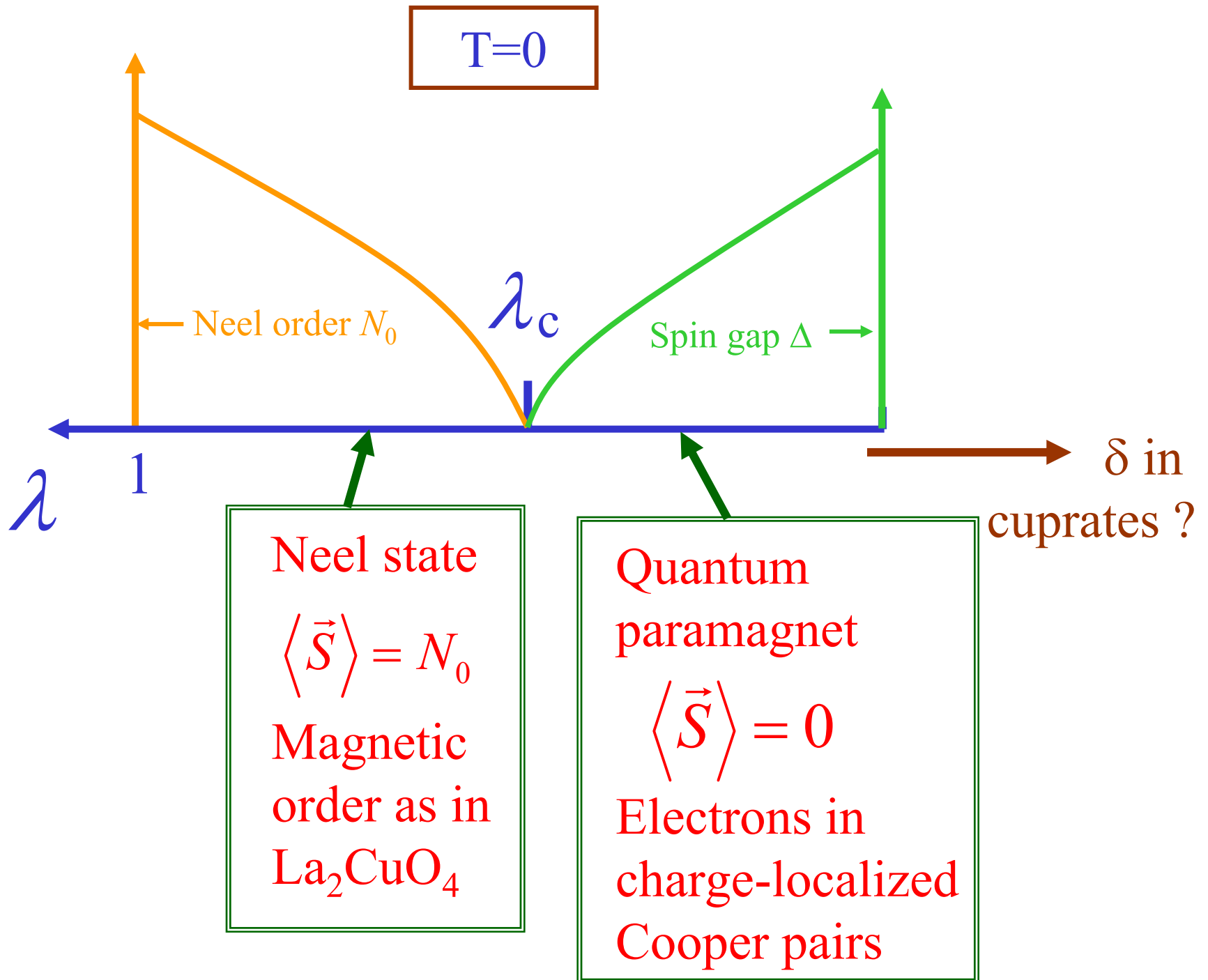
Excitation:  $S=1$  *exciton*  
 (vector  $N$  particle of  
 paramagnetic state )

Energy dispersion away from  
 antiferromagnetic wavevector

$$\epsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$$

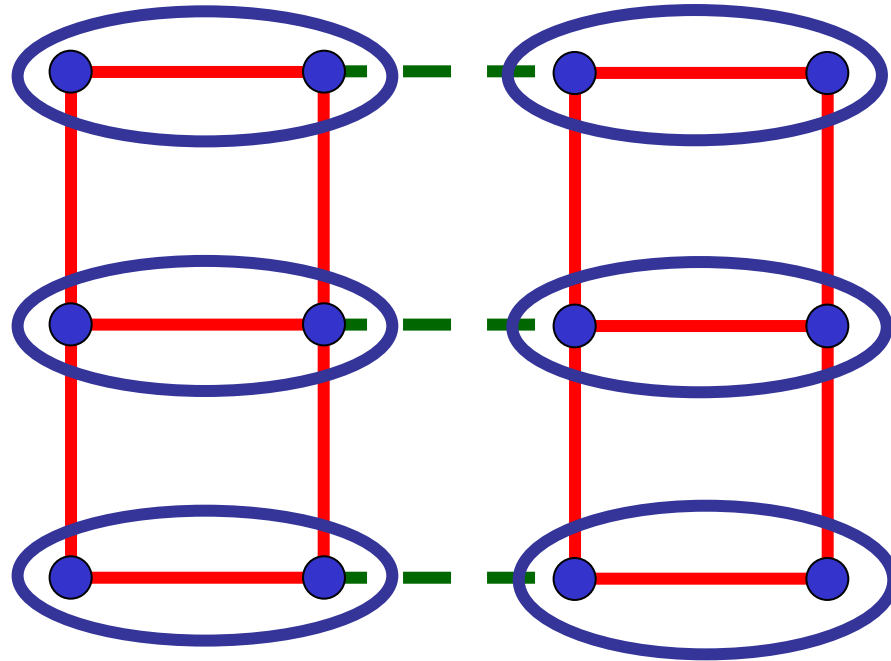


$S=1/2$  spinons are *confined*  
 by a linear potential.



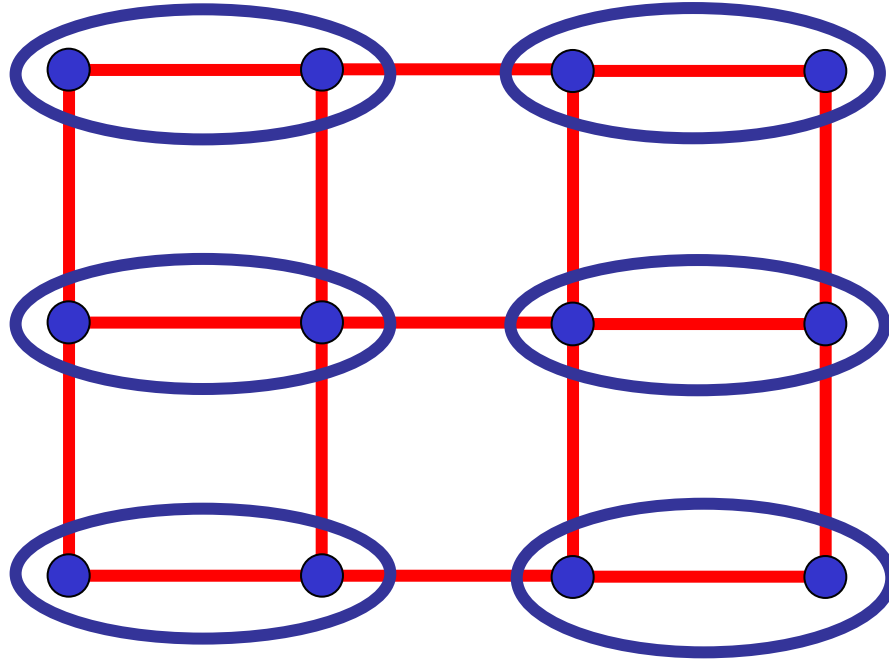
Bond and charge order Mott insulator

## Paramagnetic ground state of coupled ladder model

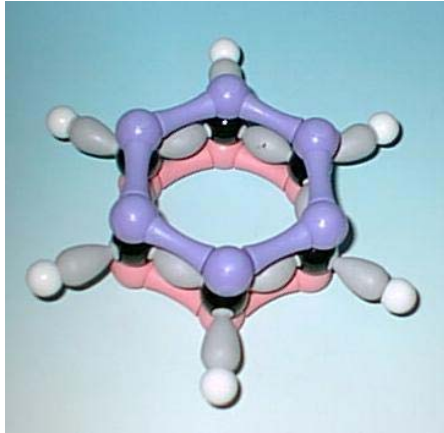
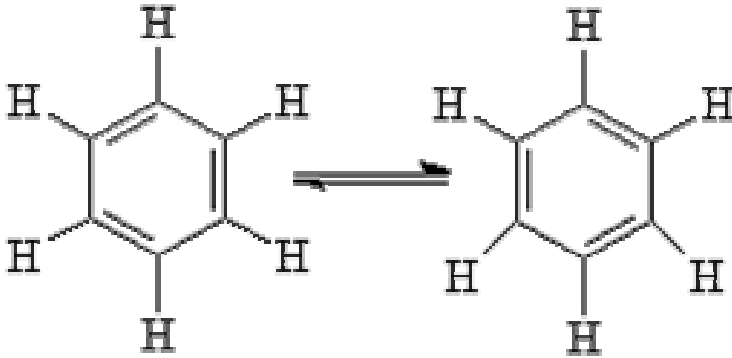




Can such a state with *bond order* be the ground state of a system with full square lattice symmetry ?

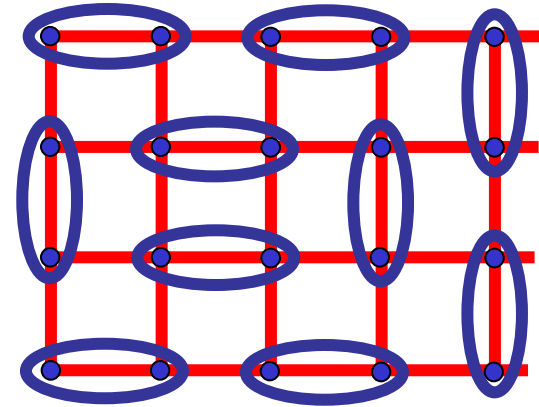


## Resonating valence bonds



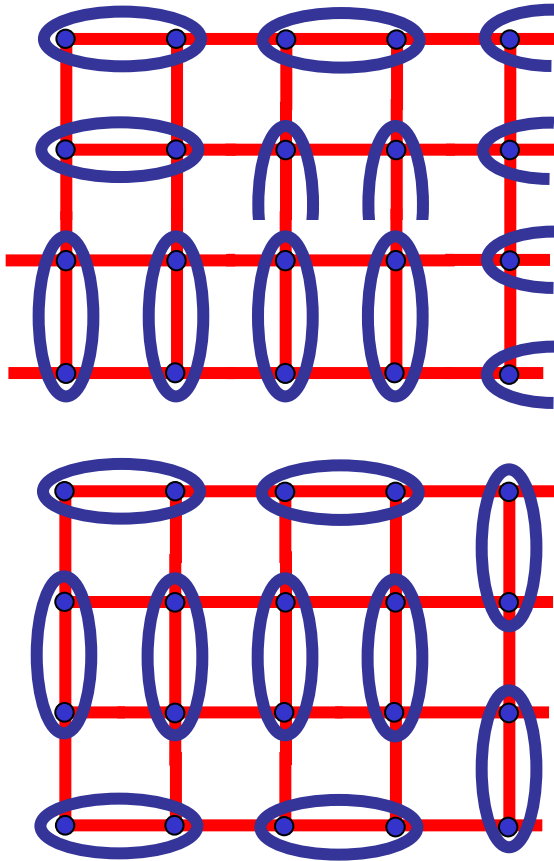
Resonance in benzene leads to a symmetric configuration of valence bonds

*(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)*



## 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.

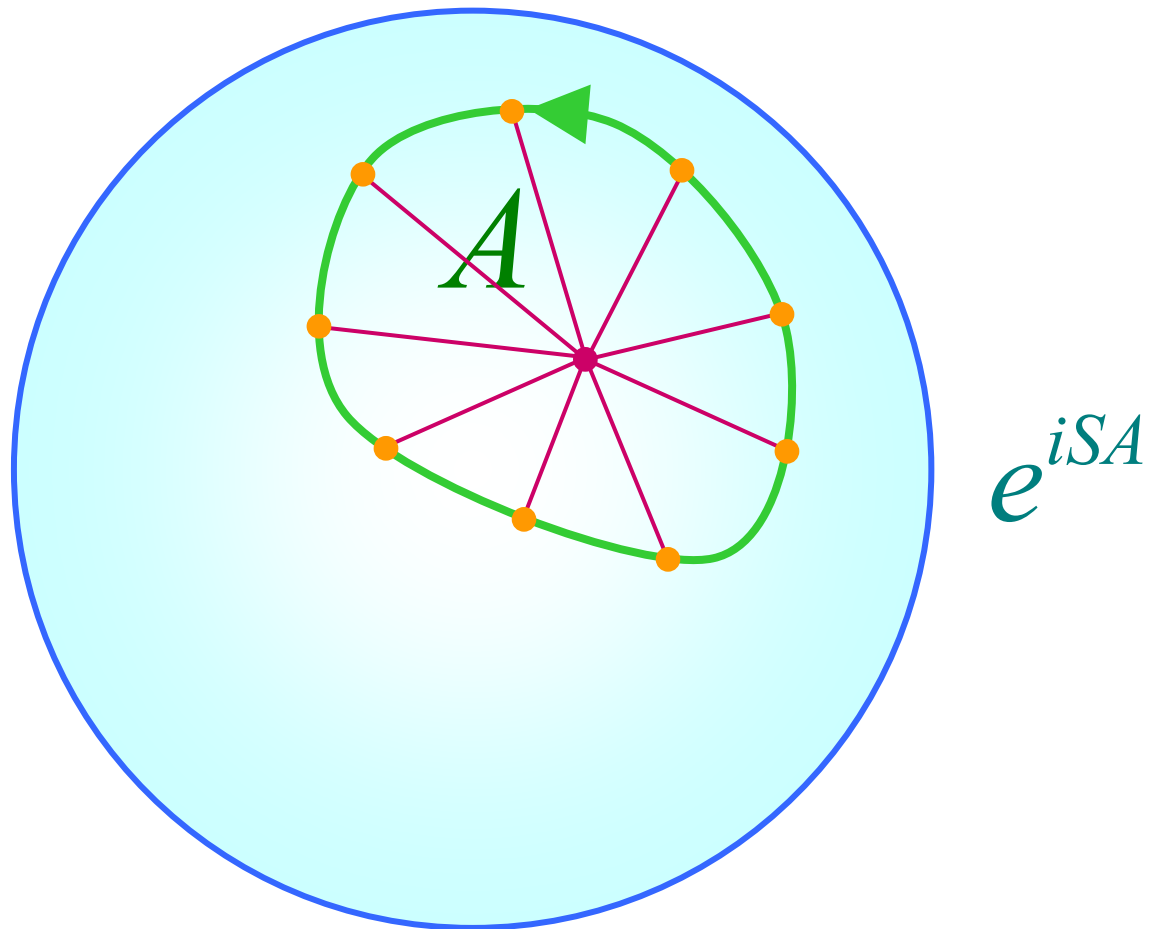
These effects lead to a broken square lattice symmetry near the transition to the magnetically ordered states with collinear spins.

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).

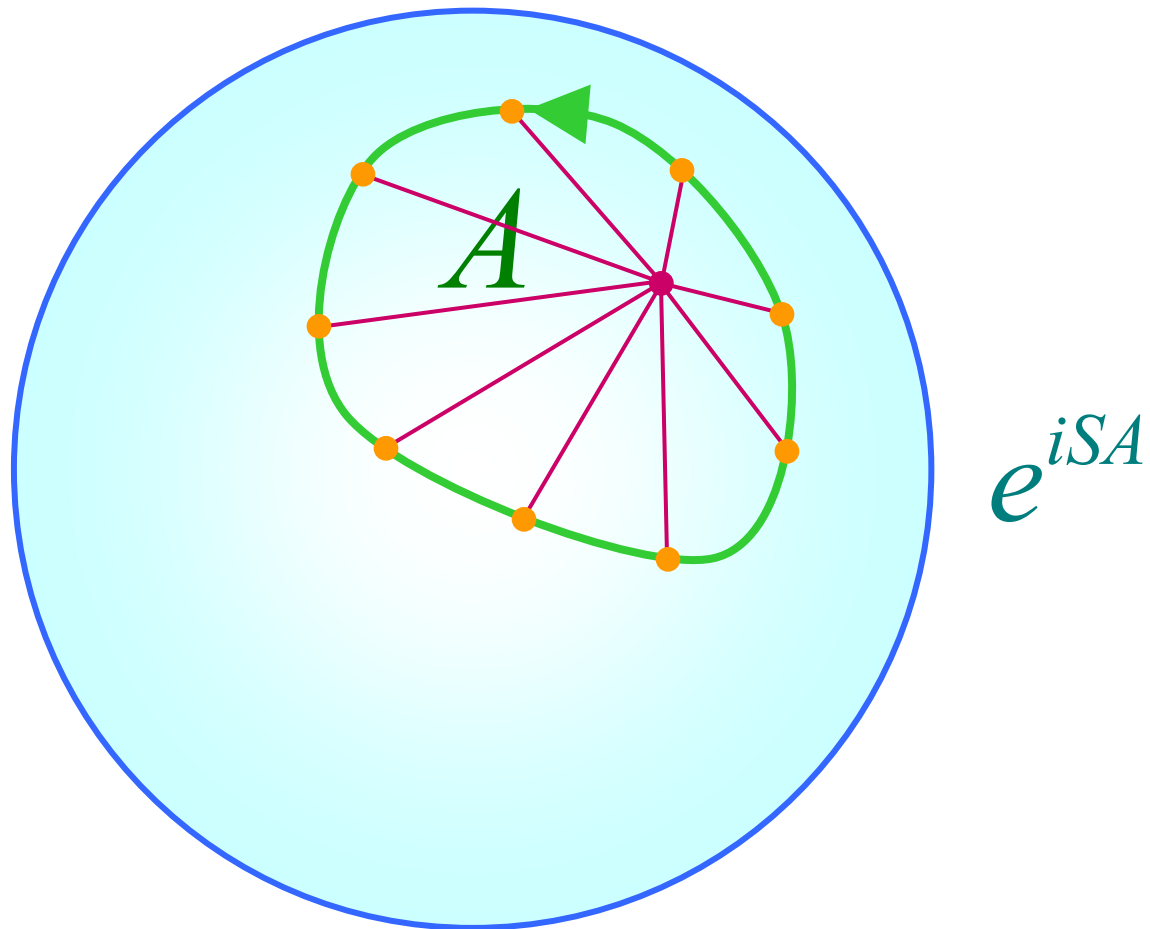
(Slightly) Technical interlude:  
*Quantum theory for bond order*

Key ingredient: Spin Berry Phases



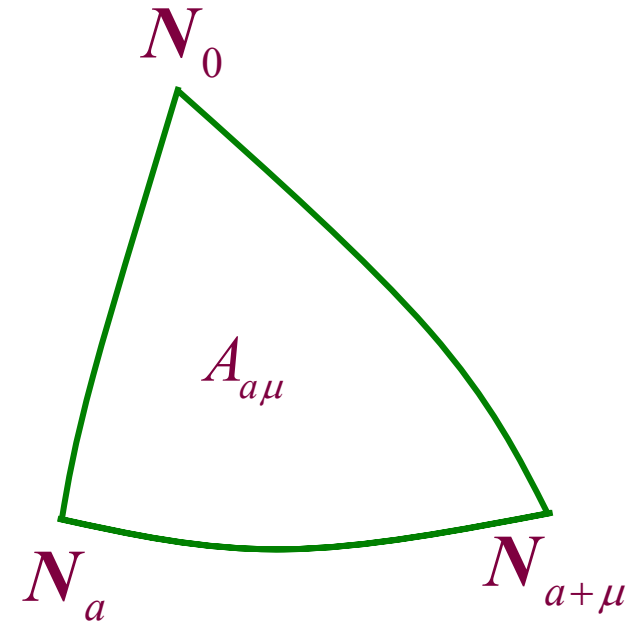
(Slightly) Technical interlude:  
*Quantum theory for bond order*

Key ingredient: Spin Berry Phases



$A_{a\mu} \rightarrow$  oriented area of spherical triangle

formed by  $N_a$ ,  $N_{a+\mu}$ , and an arbitrary reference point  $N_0$



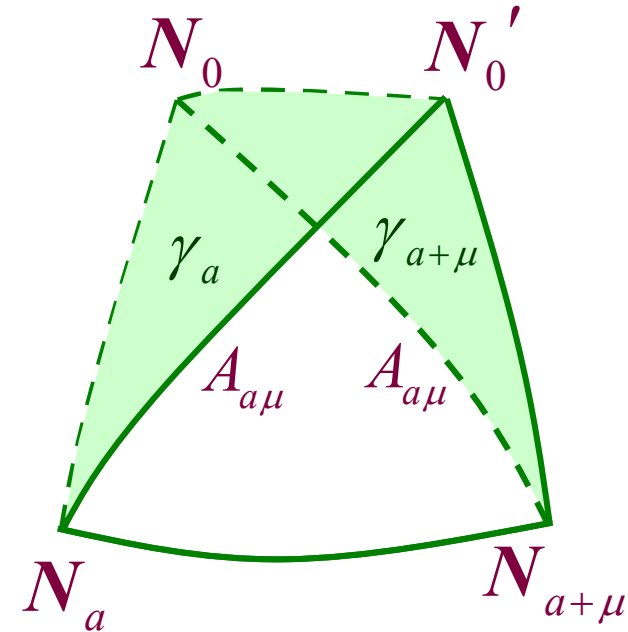
$A_{a\mu} \rightarrow$  oriented area of spherical triangle

formed by  $N_a$ ,  $N_{a+\mu}$ , and an arbitrary reference point  $N_0$

Change in choice of  $n_0$  is like a “gauge transformation”

$$A_{a\mu} \rightarrow A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

( $\gamma_a$  is the oriented area of the spherical triangle formed by  $N_a$  and the two choices for  $N_0$ ).



The area of the triangle is uncertain modulo  $4\pi$ , and the action is invariant under

$$A_{a\mu} \rightarrow A_{a\mu} + 4\pi$$

These principles strongly constrain the effective action for  $A_{a\mu}$  which provides description of the paramagnetic phase

Simplest effective action for  $A_{a\mu}$  fluctuations in the paramagnet

$$Z = \prod_{a,\mu} \int dA_{a\mu} \exp \left( \frac{1}{2e^2} \sum_{\square} \cos \left( \frac{1}{2} (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) - \frac{i}{2} \sum_a \eta_a A_{a\tau} \right)$$

$\eta_a \rightarrow \pm 1$  on two square sublattices.

This is compact QED in  $d+1$  dimensions with static charges  $\pm 1$  on two sublattices.

This theory can be reliably analyzed by a duality mapping.

**$d=2$** : The gauge theory is *always* in a *confining* phase and there is bond order in the ground state.

**$d=3$** : A deconfined phase with a gapless “photon” is possible.

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

S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990).

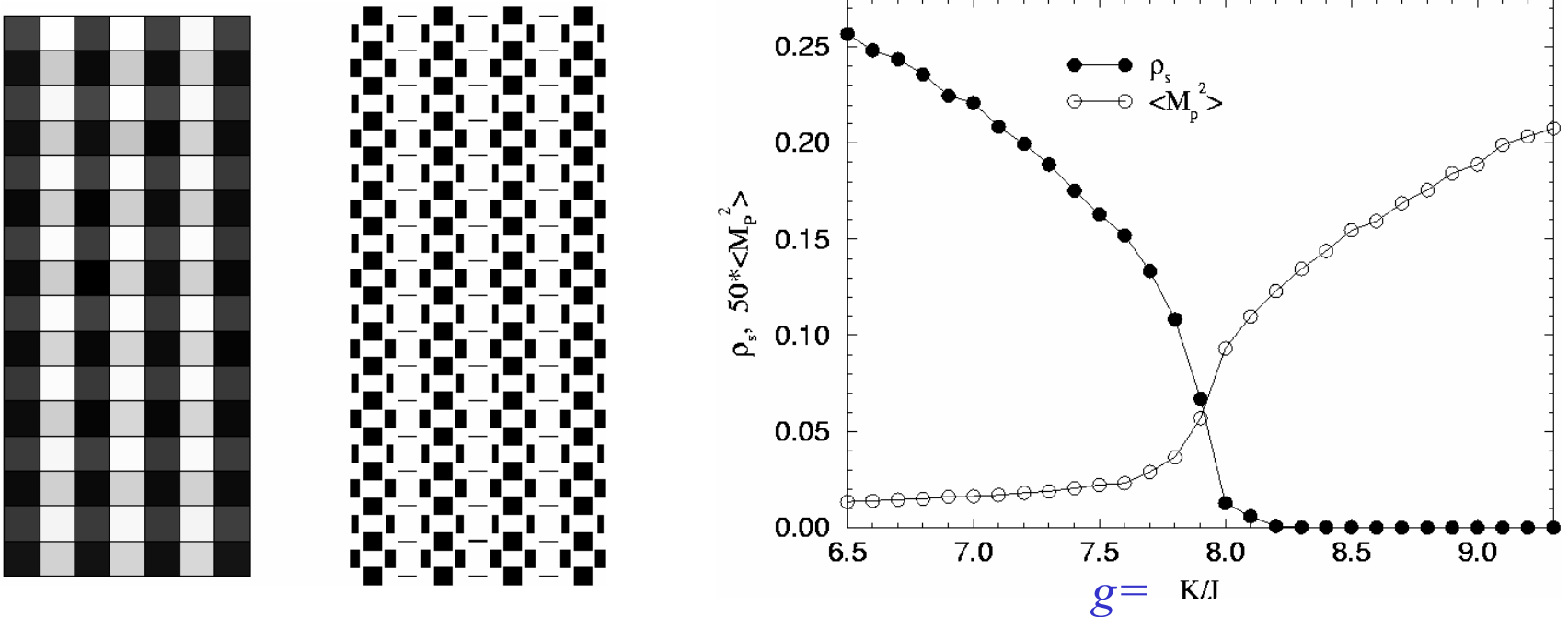
K. Park and S. Sachdev, *Phys. Rev. B* **65**, 220405 (2002).



# Bond order in a frustrated $S=1/2$ XY magnet

A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, *Phys. Rev. Lett.* **89**, 247201 (2002)

First *large scale* numerical study of the destruction of Neel order in a  $S=1/2$  antiferromagnet with full square lattice symmetry

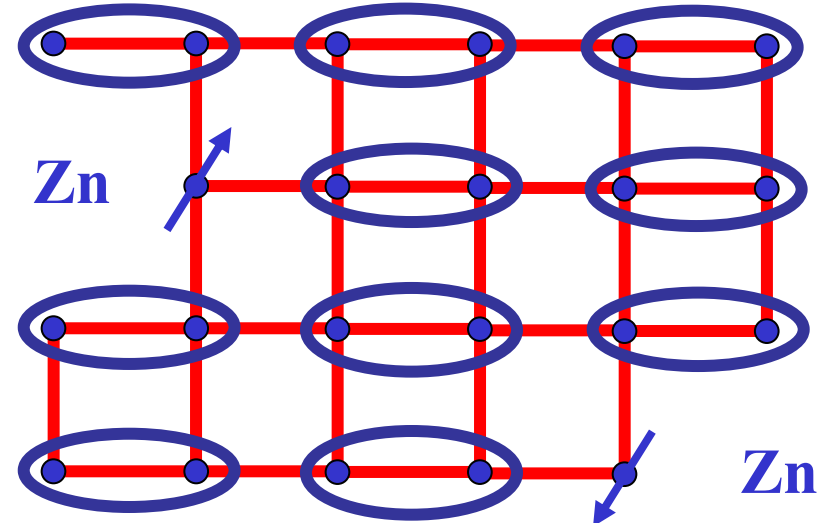
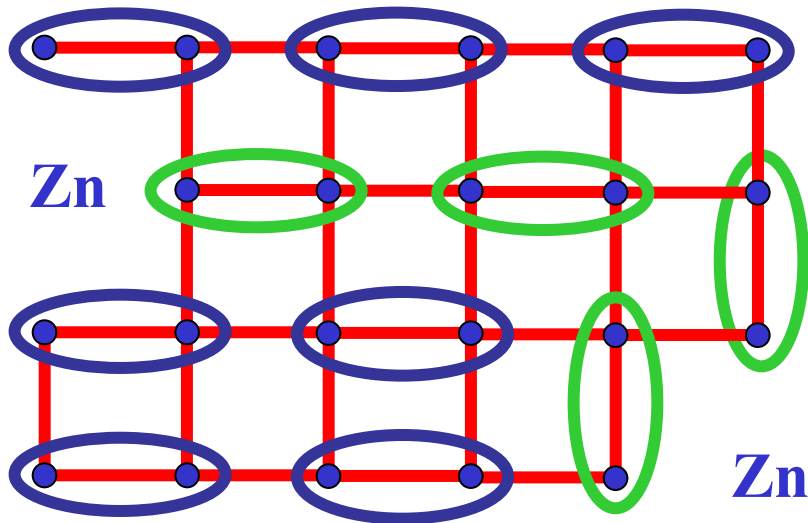


$$H = 2J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - K \sum_{\langle ijkl \rangle \square} (S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+)$$

See also C. H. Chung, Hae-Young Kee, and Yong Baek Kim, cond-mat/0211299.

Experiments on the superconductor revealing  
order inherited from the Mott insulator

## Effect of static non-magnetic impurities (Zn or Li)



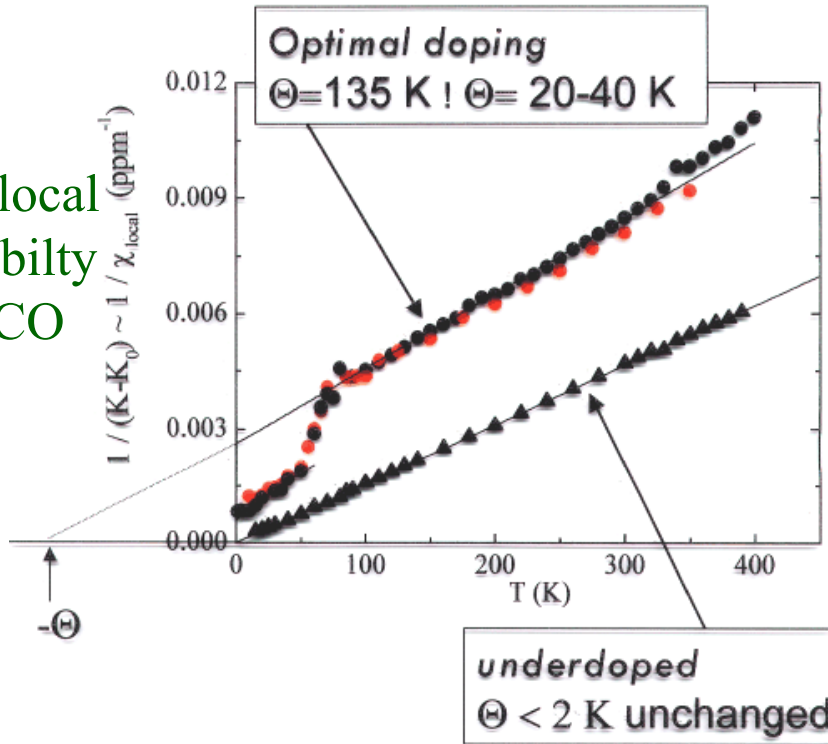
Spinon confinement implies that free  $S=1/2$  moments form near each impurity

$$\chi_{\text{impurity}}(T \rightarrow 0) = \frac{S(S+1)}{3k_B T}$$

# Spatially resolved NMR of Zn/Li impurities in the superconducting state

$^7\text{Li}$  NMR below  $T_c$

J. Bobroff, H. Alloul, W.A. MacFarlane, P. Mendels, N. Blanchard, G. Collin, and J.-F. Marucco, *Phys. Rev. Lett.* **86**, 4116 (2001).



Inverse local susceptibility in YBCO

Measured  $\chi_{\text{impurity}}(T \rightarrow 0) = \frac{S(S+1)}{3k_B T}$  with  $S = 1/2$  in underdoped sample.

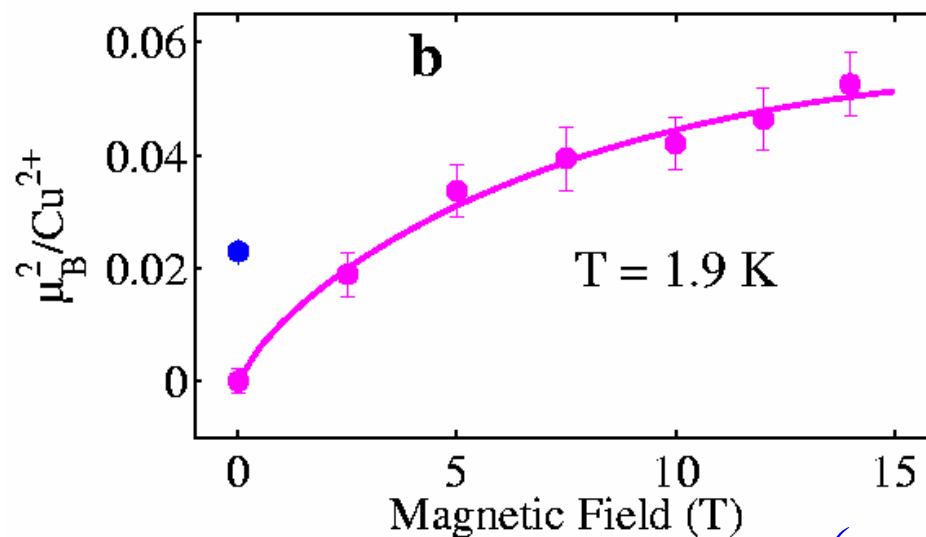
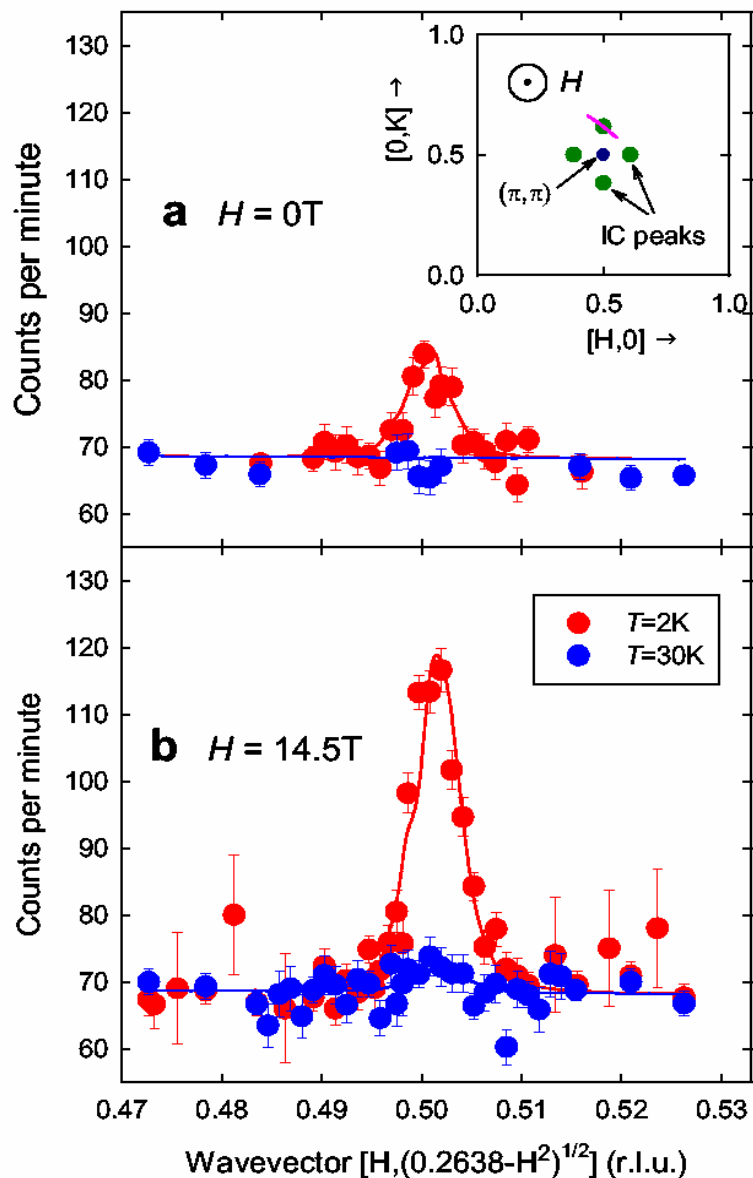
This behavior does not emerge out of BCS theory.

# Tuning across the phase diagram by an applied magnetic field

## 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, Kim Lefmann, D. F. McMorrow, P. Vorderwisch, P. Smeibidl, N. Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, T. E. Mason, *Nature*, **415**, 299 (2002).

**Talk today at 11:00 AM**

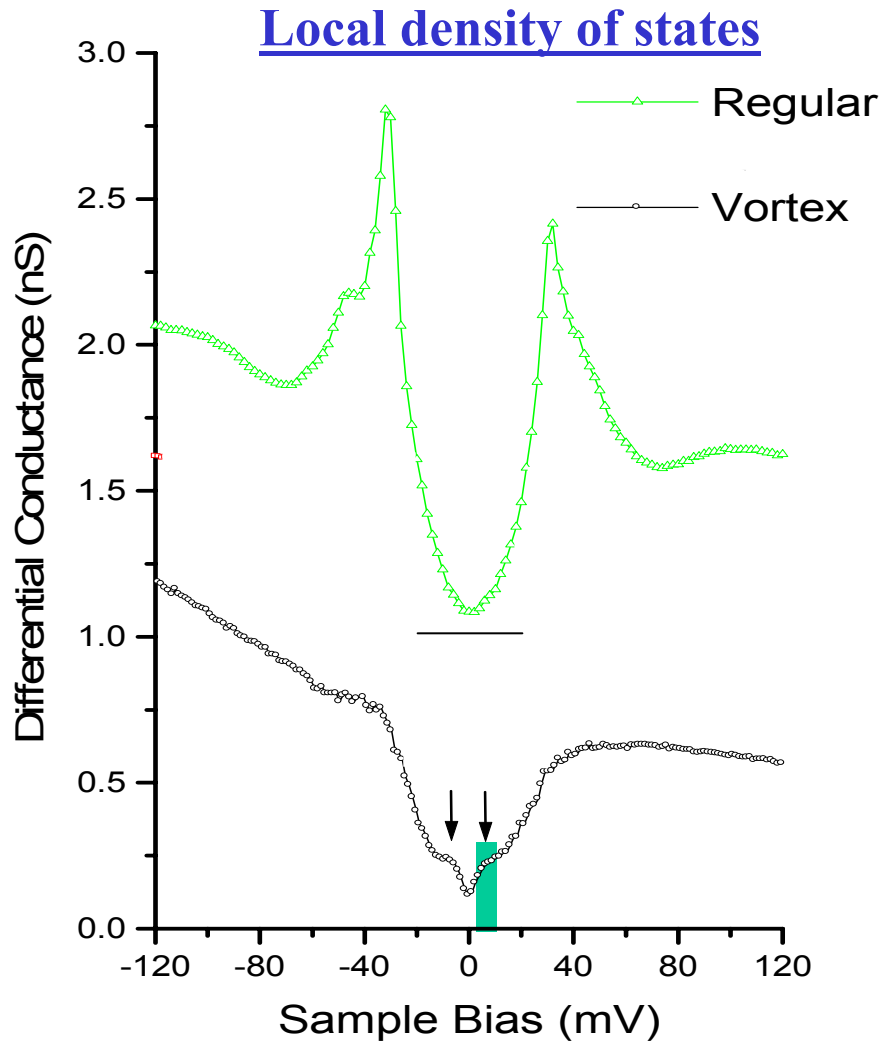


Solid line - fit to :  $I(H) = a \frac{H}{H_{c2}} \ln\left(\frac{H_{c2}}{H}\right)$

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

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

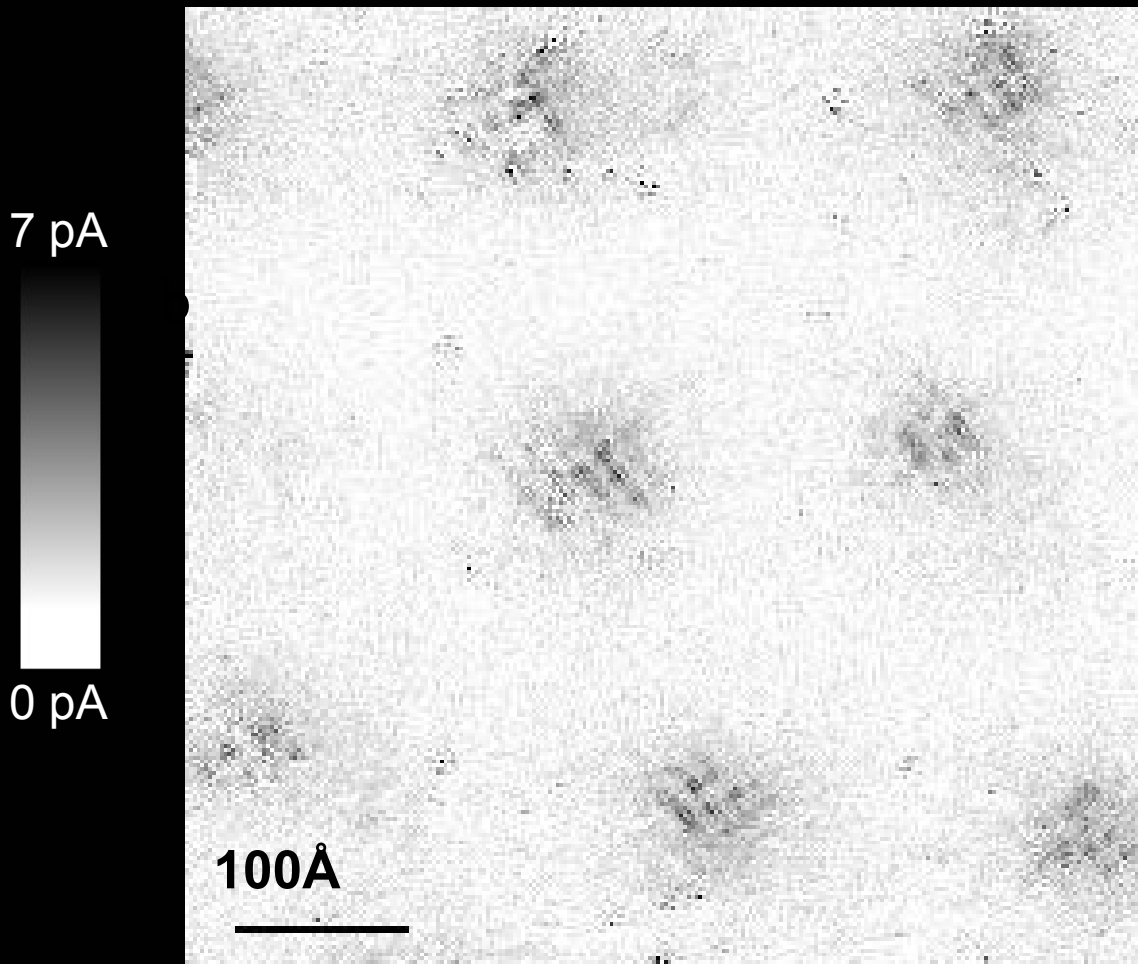
J. E. Hoffman, E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan,  
H. Eisaki, S. Uchida, and J. C. Davis, *Science* **295**, 466 (2002).



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



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

See also:

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

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).

## 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.