Order and quantum phase transitions in the cuprate superconductors

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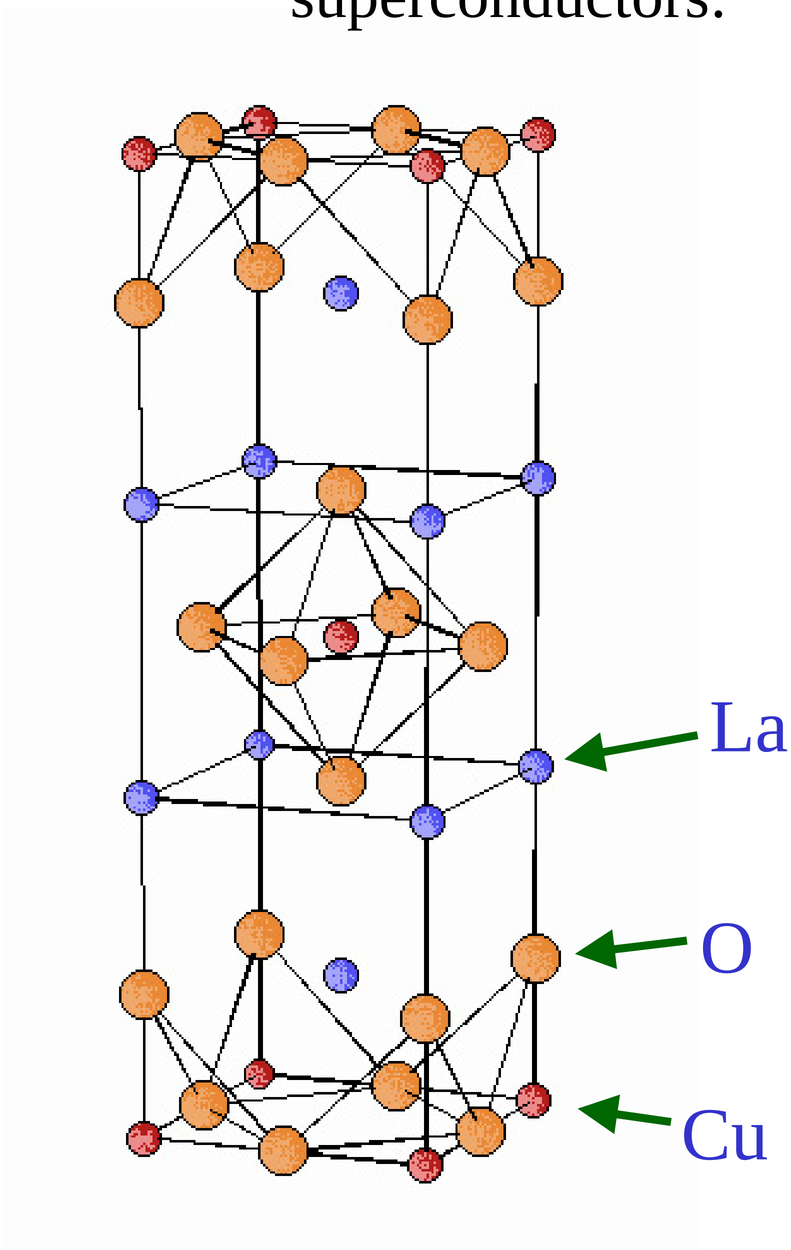
Ying Zhang (Maryland)

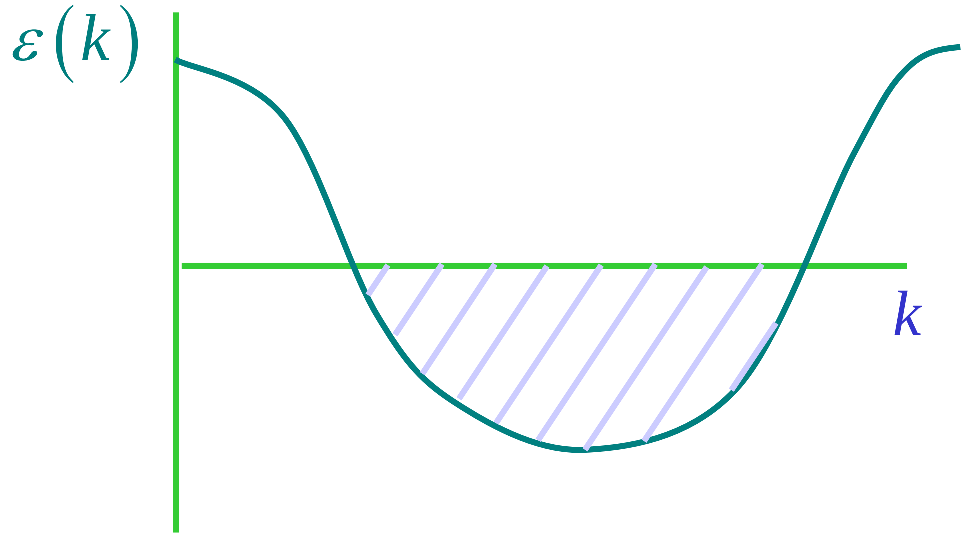
Colloquium article in *Reviews of Modern Physics* **75**, 913 (2003)

Talk online:
Google Sachdev

Parent compound of the high temperature superconductors: La_2CuO_4



Band theory

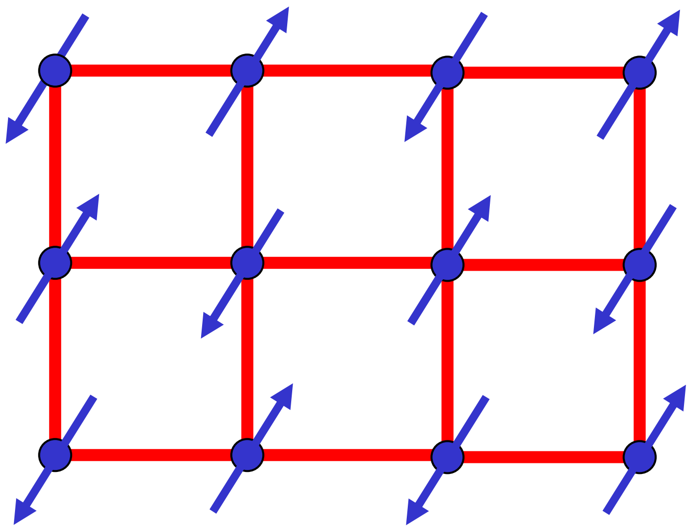


Half-filled band of Cu 3d orbitals – ground state is predicted to be a metal.

However, La_2CuO_4 is a very good insulator

Parent compound of the high temperature superconductors: La_2CuO_4

A Mott insulator



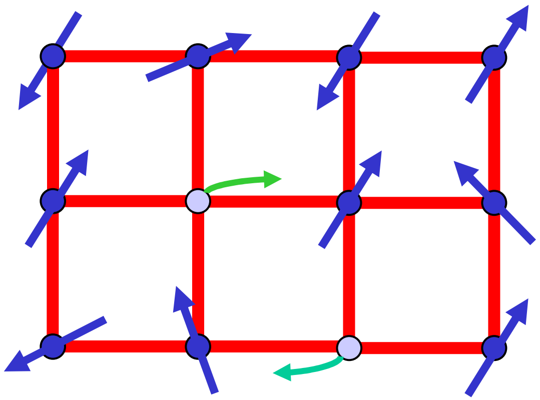
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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 δ by substitutional doping of out-of-plane ions *e.g.* $La_{2-\delta}Sr_{\delta}CuO_4$

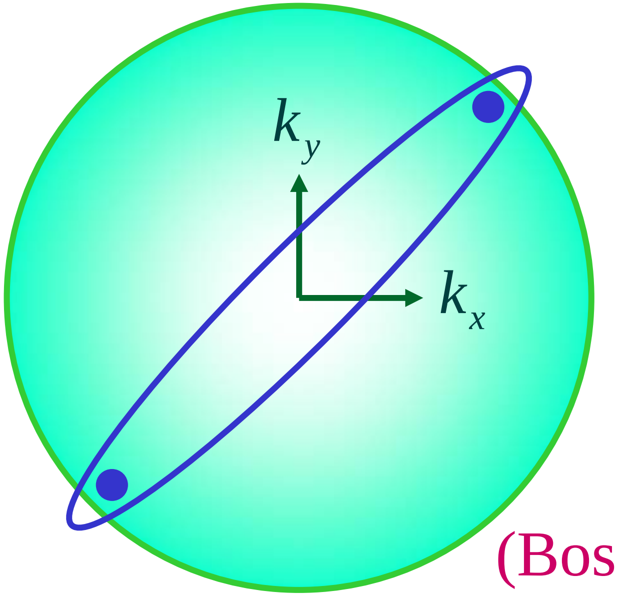


$$\left\langle \vec{S} \right\rangle = 0$$

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

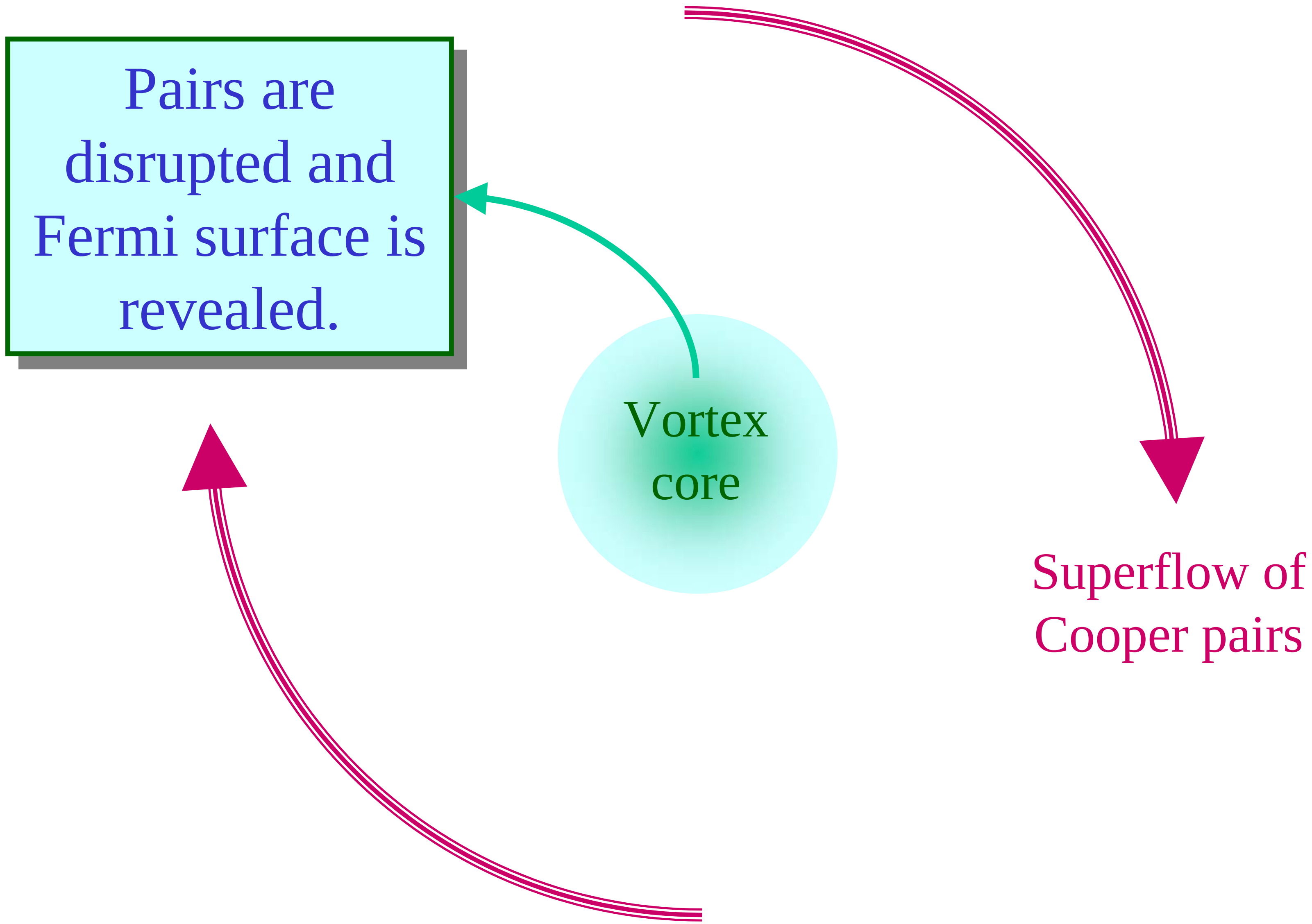
$$\Psi = \left(k_x^2 - k_y^2\right)\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$$

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

(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



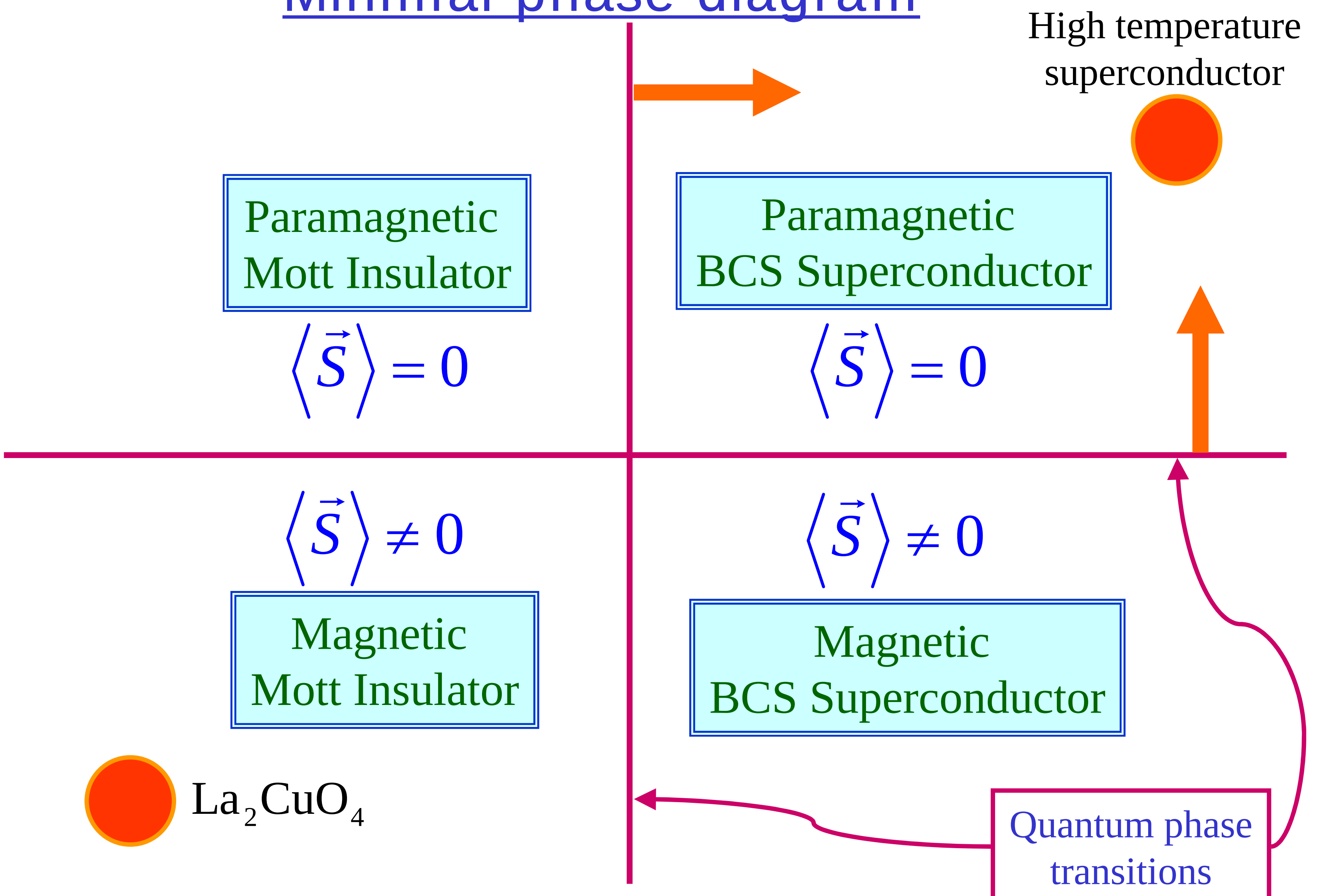
Superconductivity in a doped Mott insulator

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

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

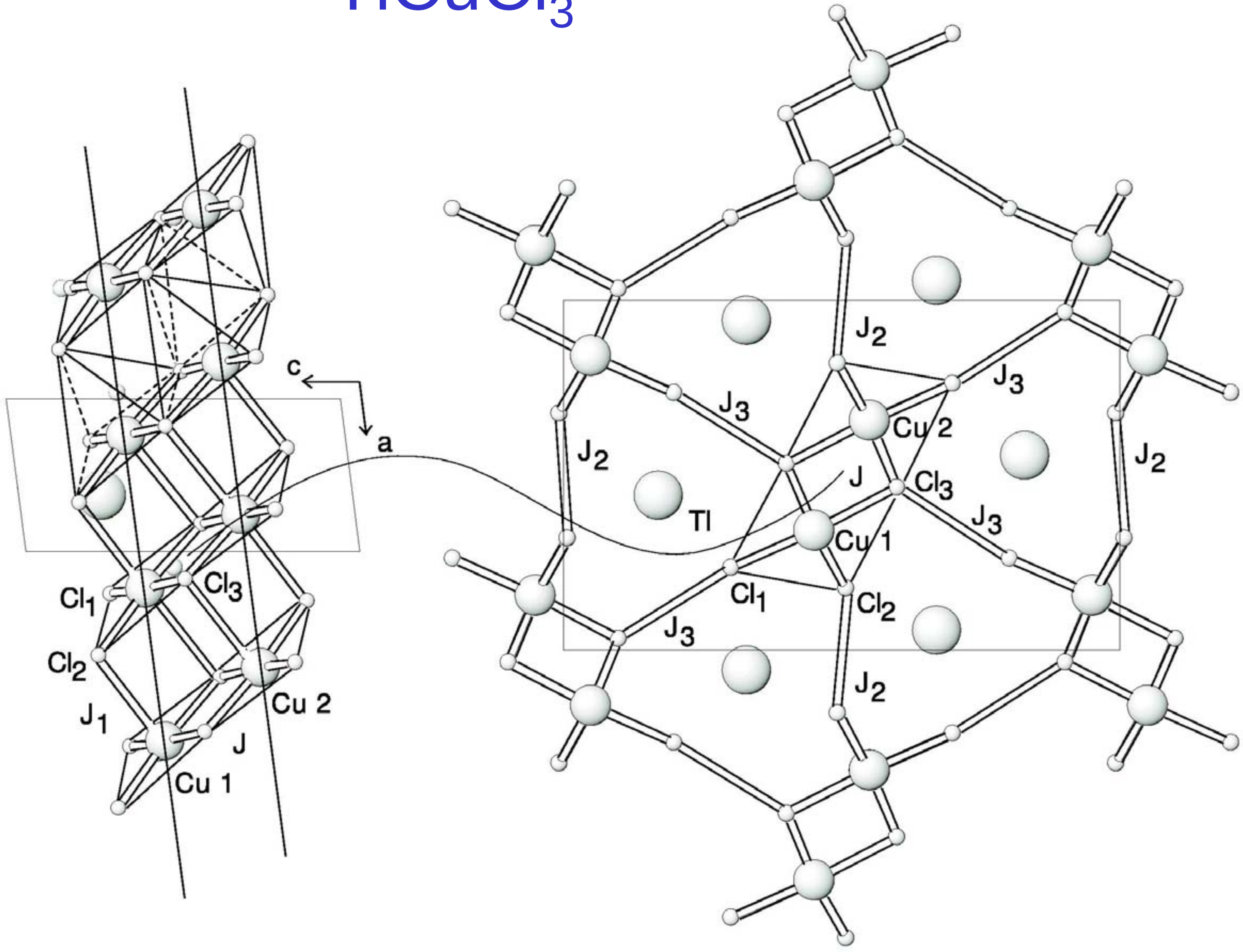
Needed:
Theory of zero temperature transitions
between competing ground states.

Minimal phase diagram



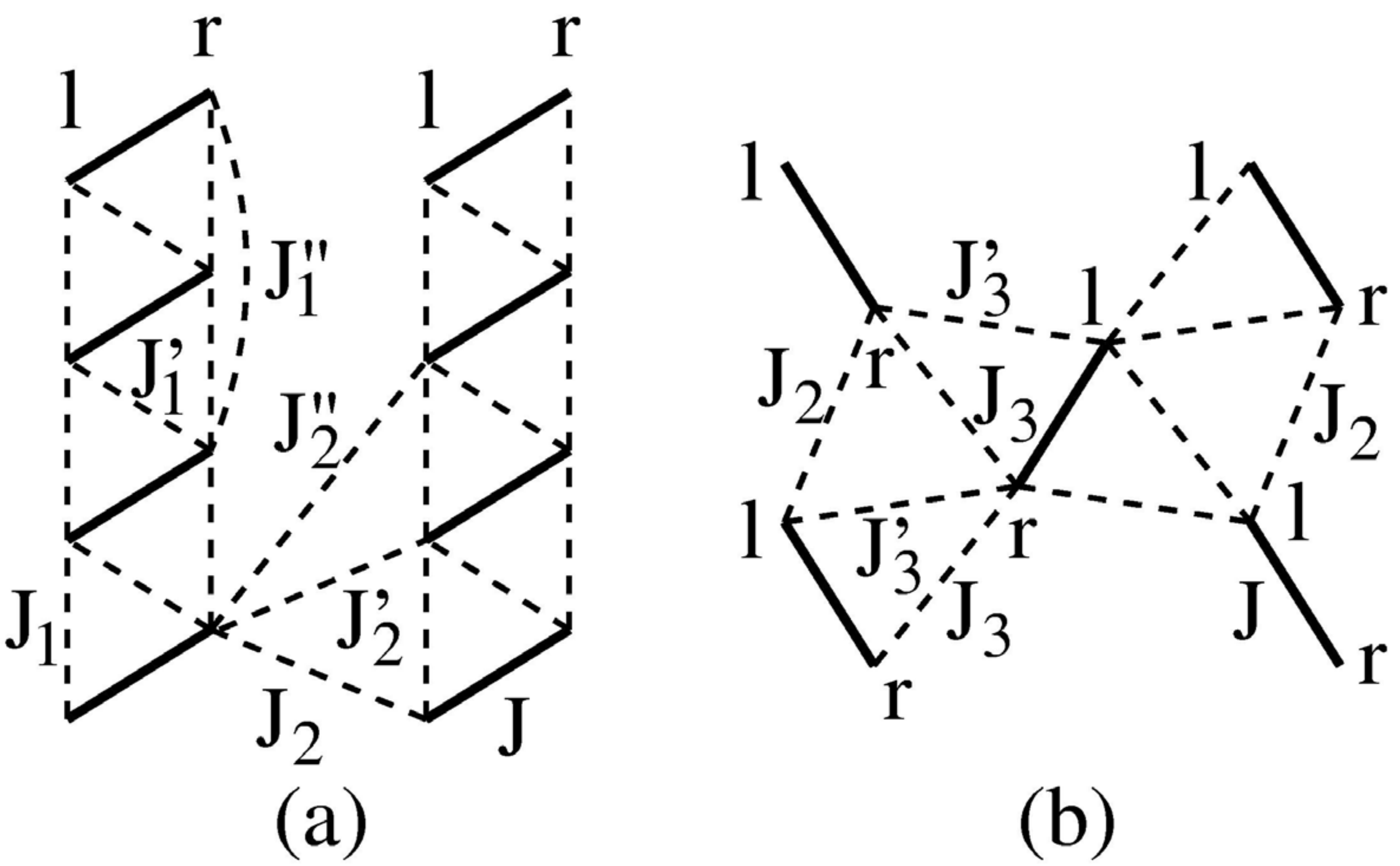
Magnetic-paramagnetic quantum phase transition in a Mott insulator

$TlCuCl_3$



M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, cond-mat/0309440.

$TlCuCl_3$

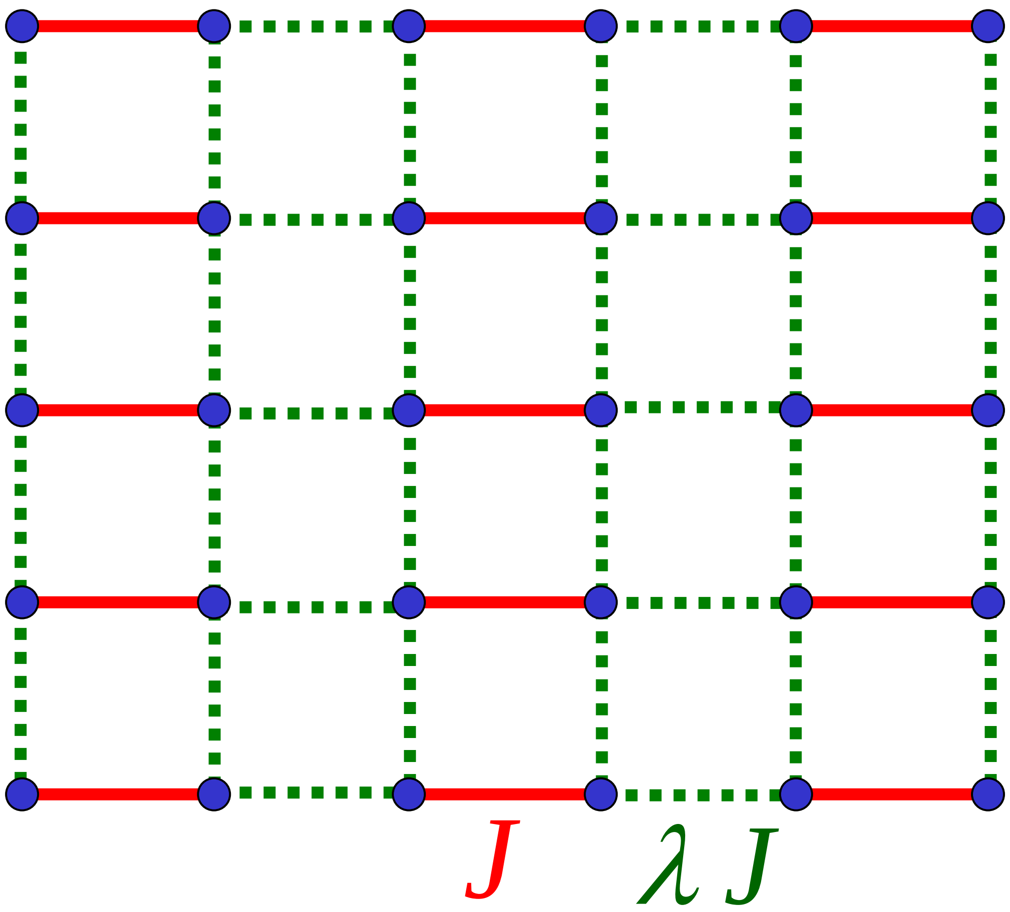


M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, cond-mat/0309440.

Coupled Dimer Antiferromagnet

M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).
N. Katoh and M. Imada, *J. Phys. Soc. Jpn.* **63**, 4529 (1994).
J. Tworzydlo, 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 dimers

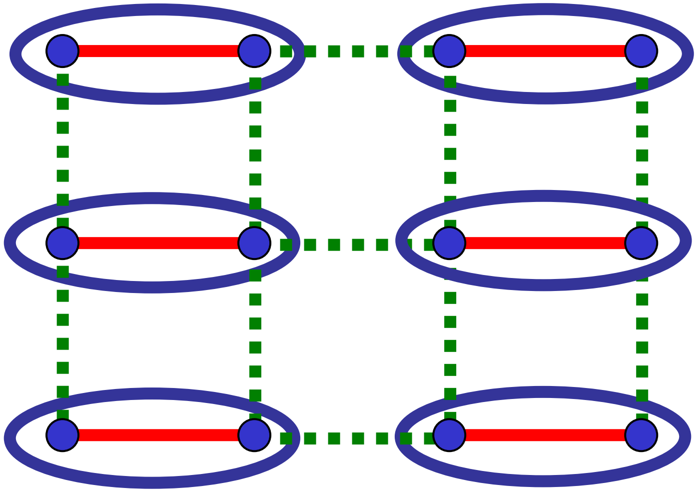


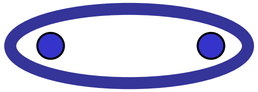
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$0 \le \lambda \le 1$$

λ close to 0

Weakly coupled dimers



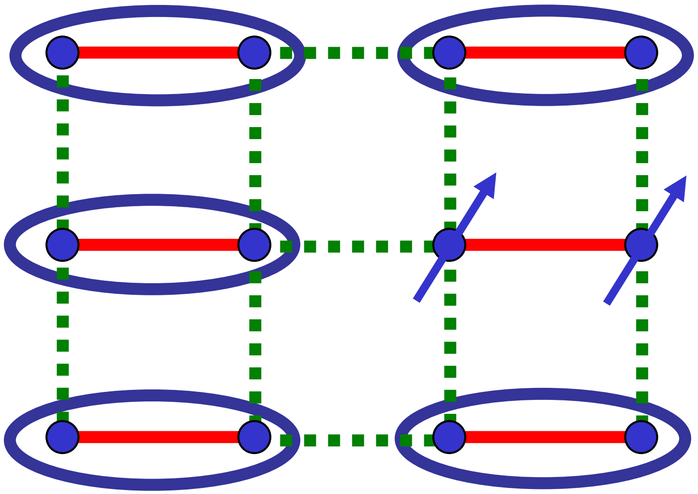
 $= \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

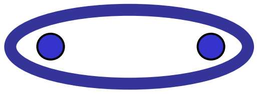
Paramagnetic ground state $\left\langle \vec{S}_i \right\rangle = 0$

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

λ close to 0

Weakly coupled dimers





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

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

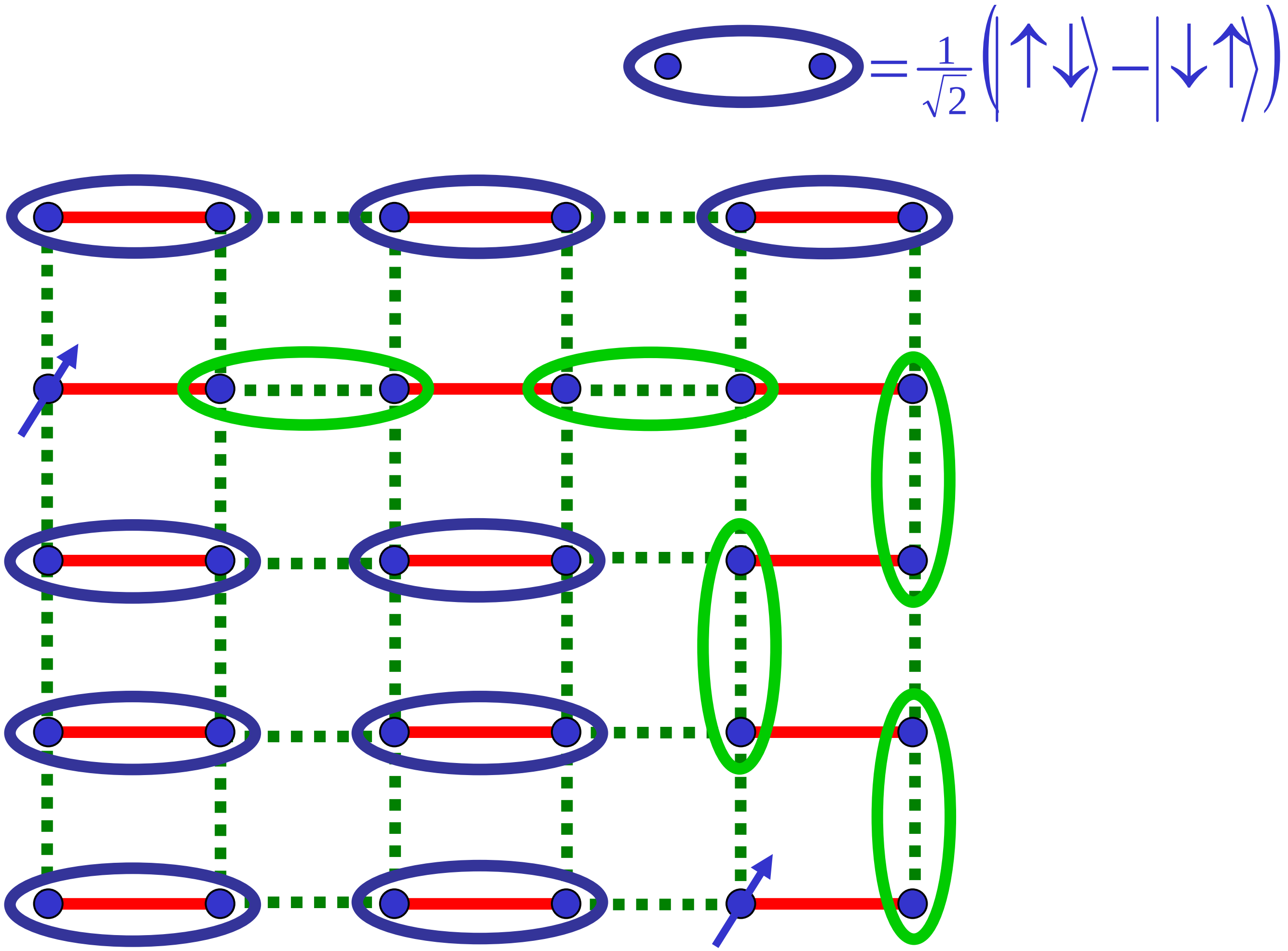
Energy dispersion away from antiferromagnetic wavevector

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

$\Delta \rightarrow$ spin gap

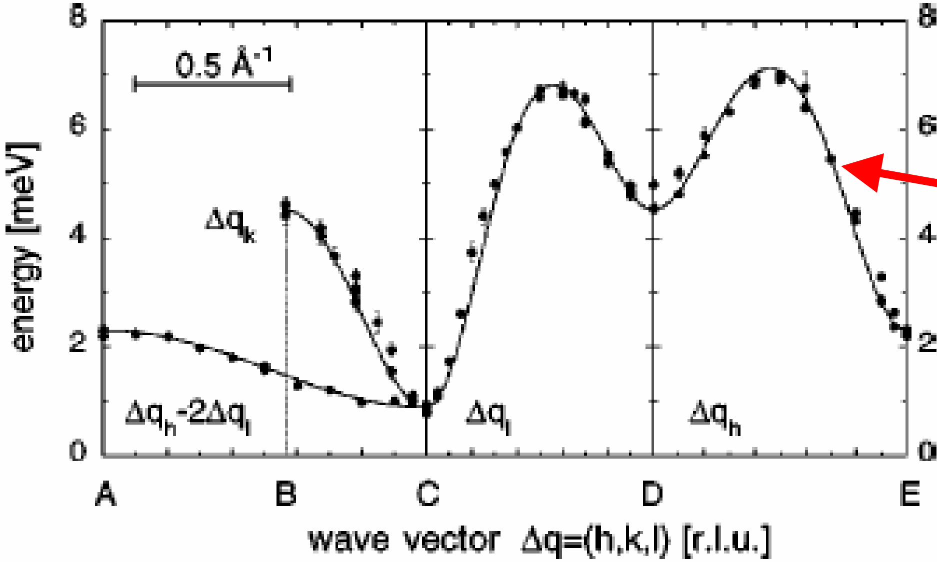
λ close to 0

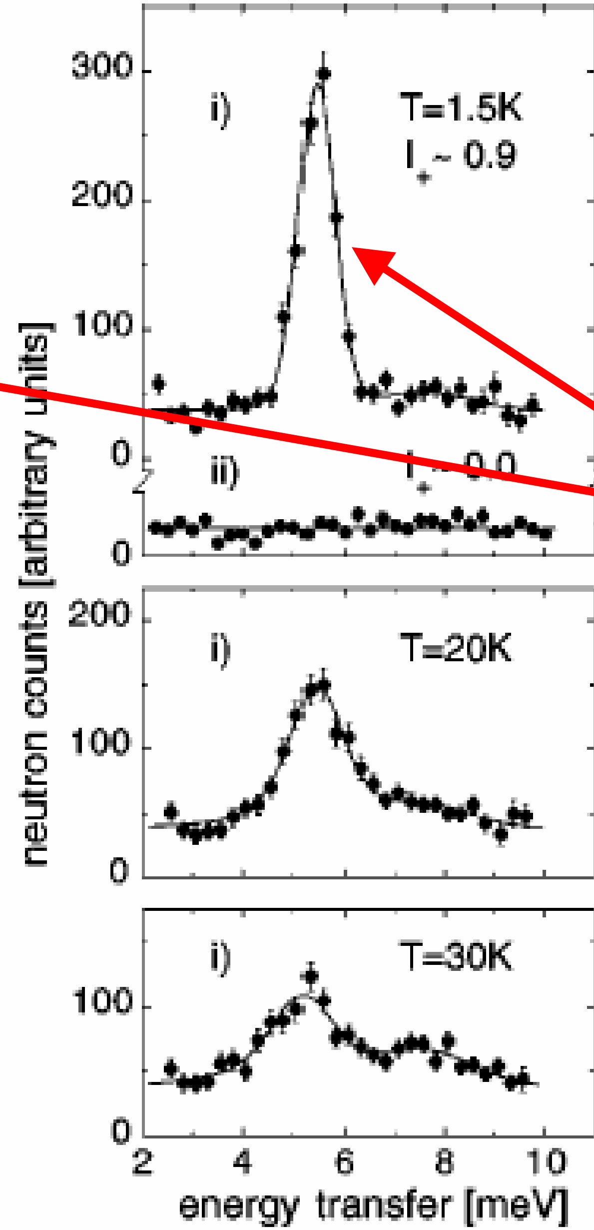
Weakly coupled dimers



S=1/2 ***spinons*** are <u>*confined*</u> by a linear potential into a *S*=1 ***triplon***

$TlCuCl_3$





"triplon" or spin exciton

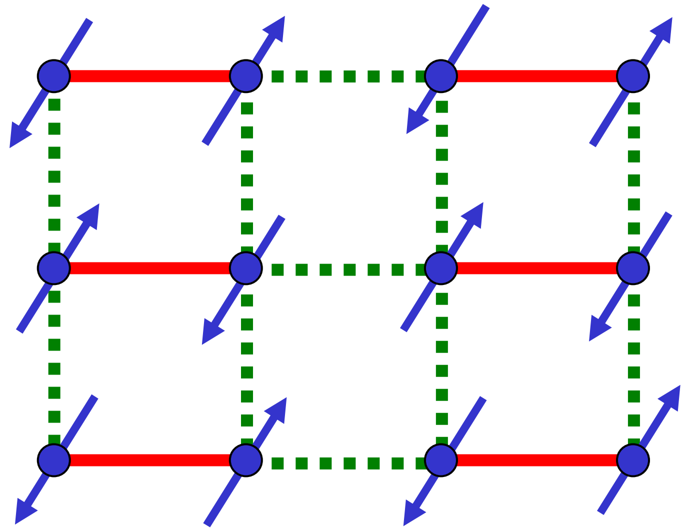
N. Cavadini, G. Heigold, W. Henggeler, A. Furrer, H.-U. Güdel, K. Krämer and H. Mutka, *Phys. Rev.* B 63 172414 (2001).

FIG. 1. Measured neutron profiles in the a^*c^* plane of $TlCuCl_3$ for $i=(1.35,0,0)$, $ii=(0,0,3.15)$ [r.l.u]. The spectrum at $T=1.5$ K

λ close to 1

Square lattice antiferromagnet

Experimental realization: La_2CuO_4



Ground state has long-range magnetic (Neel or spin density wave) order

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

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

$TlCuCl_3$

Neutron Diffraction Study of the Pressure-Induced Magnetic Ordering in the Spin Gap System $TlCuCl_3$

Akira OOSAWA*, Masashi FUJISAWA[1], Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA[2]

Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195
[1]*Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551*
[2]*Research Center for Low Temperature Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551*

(Received February 3, 2003)

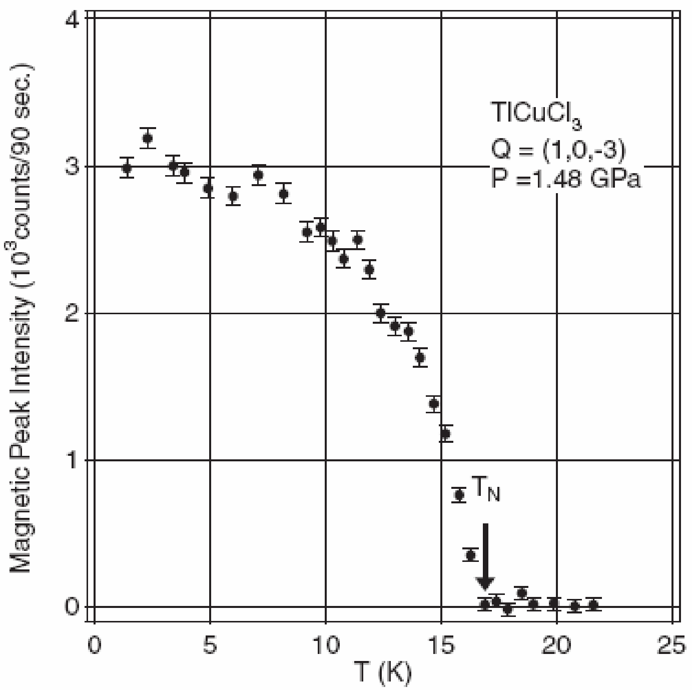


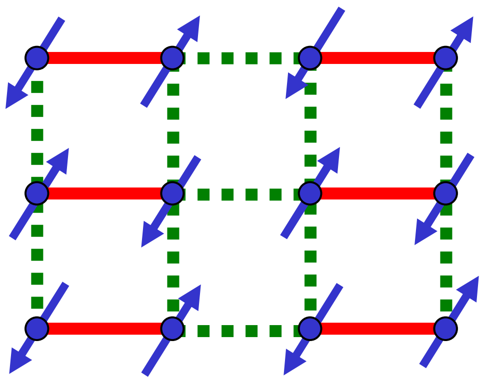
Fig. 3. Temperature dependence of the magnetic Bragg peak intensity for $Q = (1, 0, -3)$ reflection measured at $P = 1.48$ GPa in $TlCuCl_3$.

J. Phys. Soc. Jpn **72**, 1026 (2003)

T=0

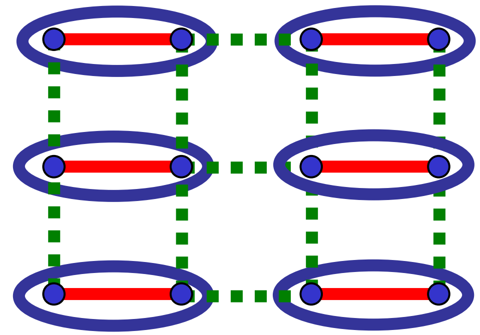
$\lambda_c = 0.52337(3)$

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



Neel state

$\left\langle \vec{S} \right\rangle = N_0$



Quantum paramagnet

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

Magnetic order as in La_2CuO_4

Electrons in charge-localized Cooper pairs

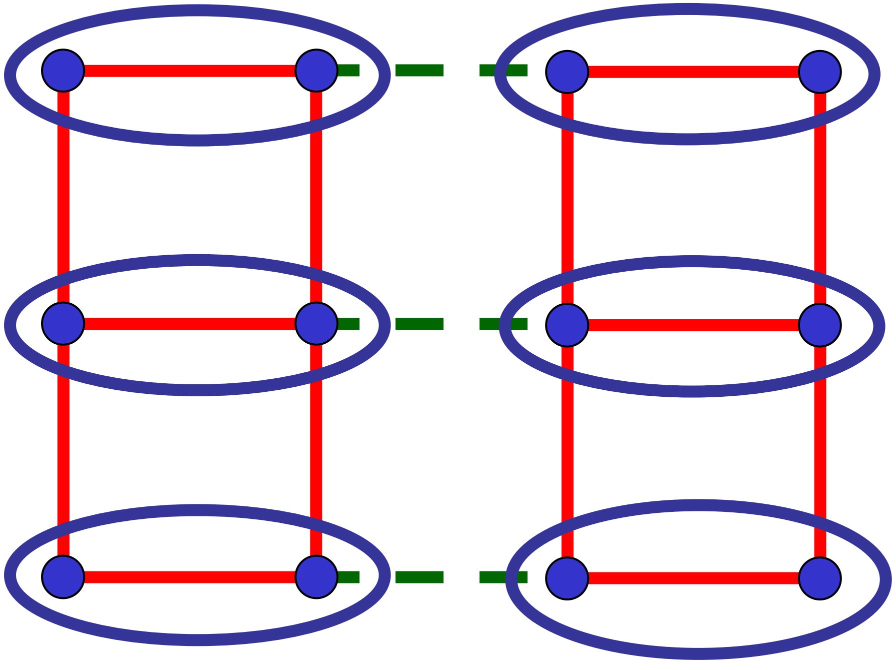
λ 1 λ_c

δ in cuprates ?

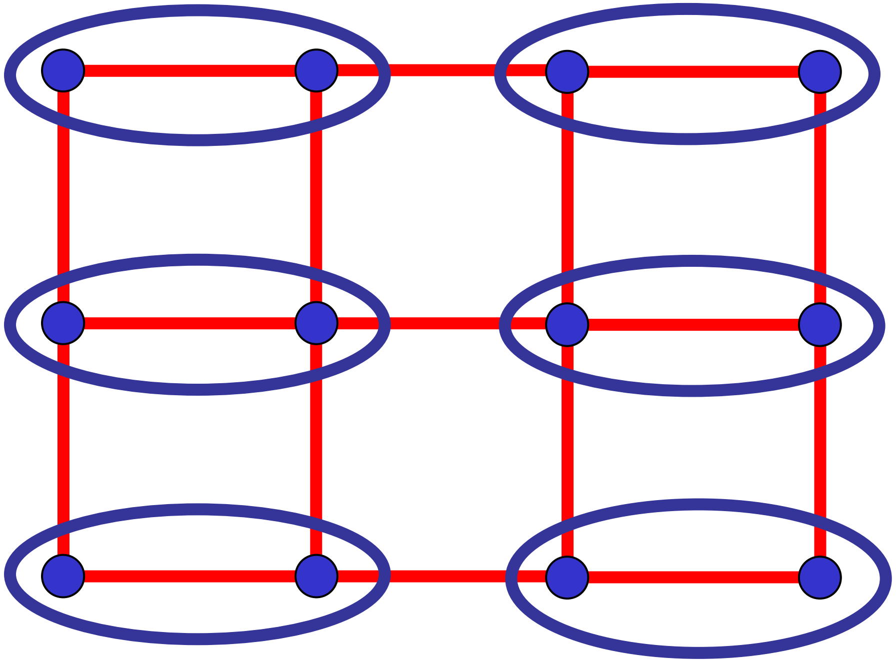
Pressure in $TlCuCl_3$

Bond order in a Mott insulator

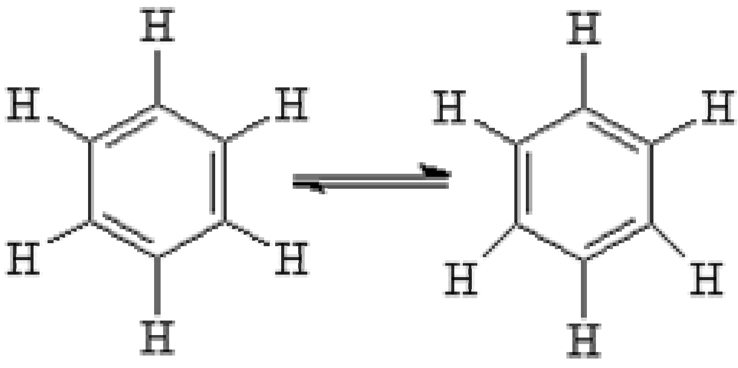
Paramagnetic ground state of coupled ladder model

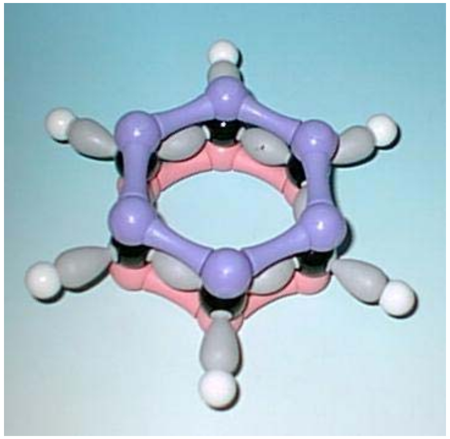


Can such a state with ***bond order*** be the ground state of a system with full square lattice symmetry ?

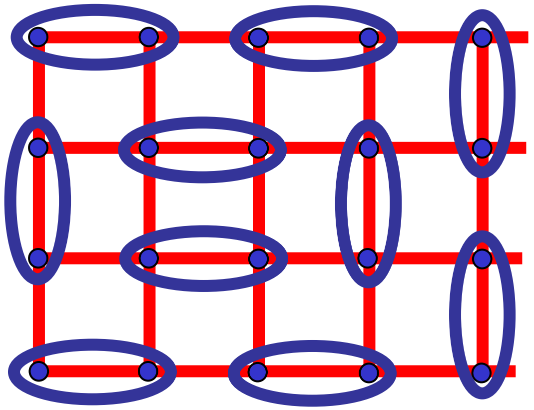


Resonating valence bonds



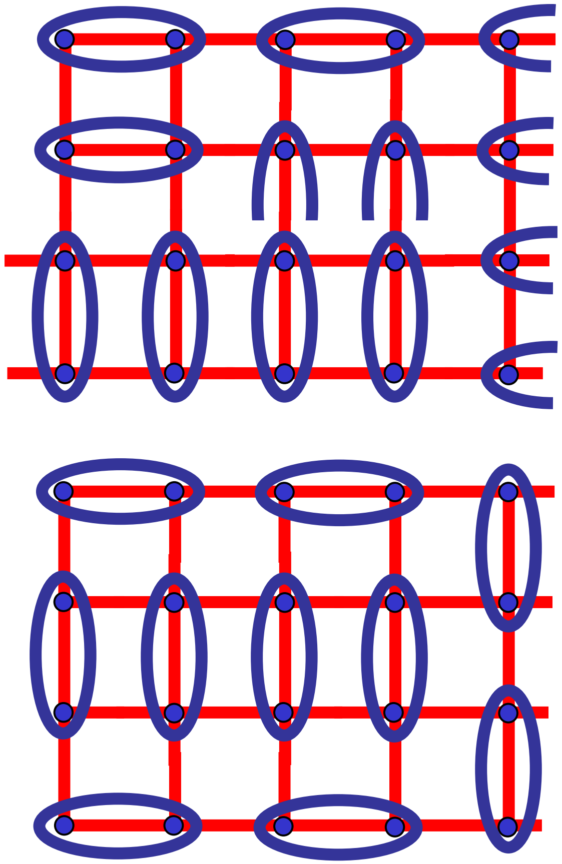


Resonance in benzene leads to a symmetric configuration of valence bonds
(*F. Kekulé, L. Pauling*)



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*)

Resonating valence bonds



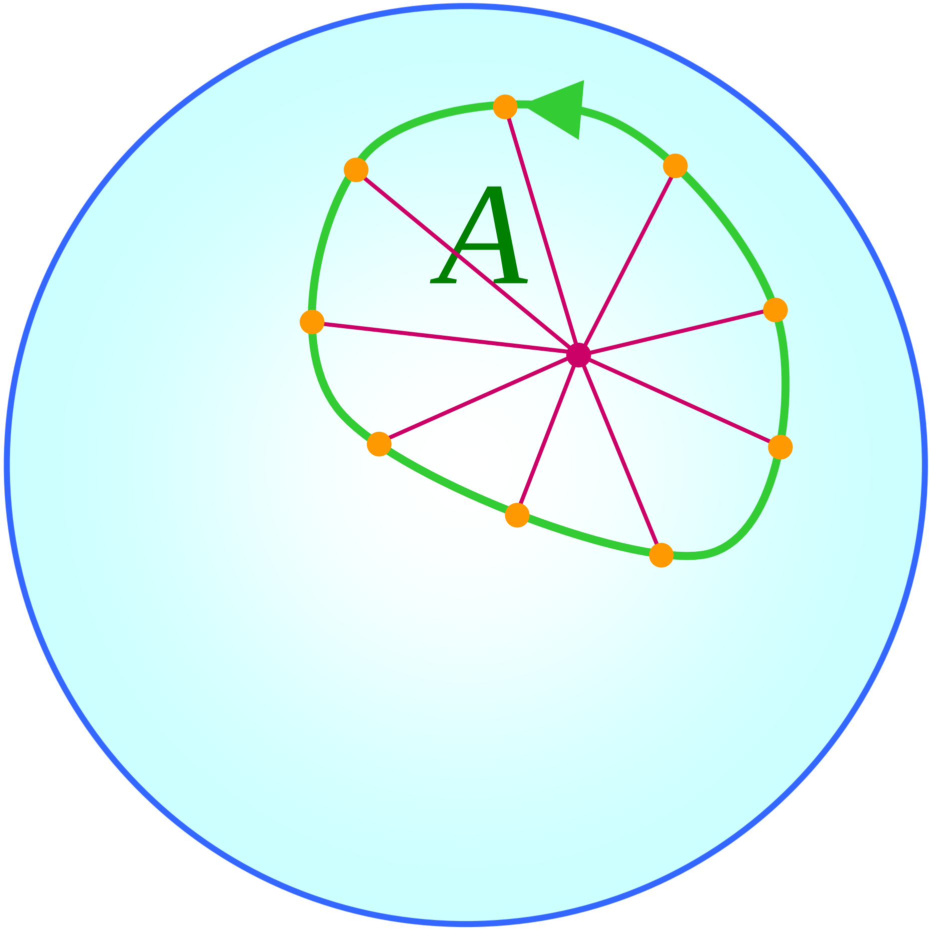
Resonances on different plaquettes are strongly correlated with each other.
Theoretical description: compact U(1) gauge theory

N. Read and S. Sachdev, *Phys.Rev. Lett*. **62**, 1694 (1989)
E. Fradkin and S. A. Kivelson, *Mod. Phys. Lett*. B **4**, 225 (1990)

(Slightly) Technical interlude:

Quantum theory for bond order

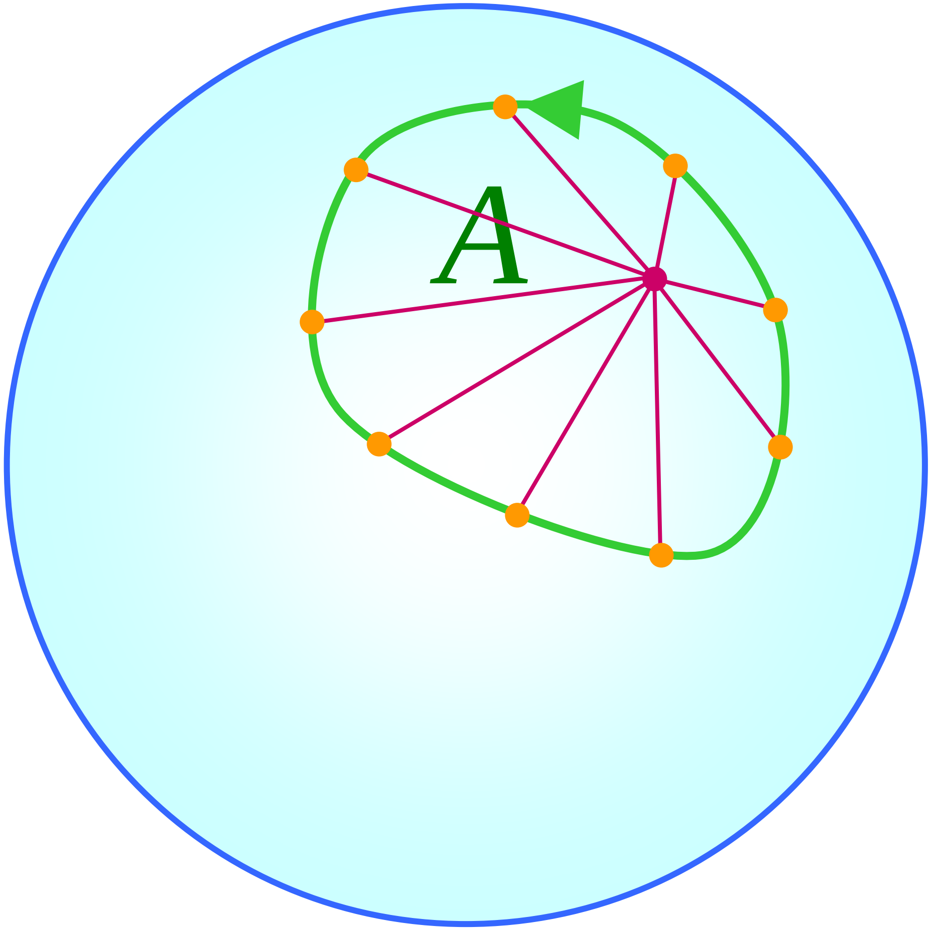
Key ingredient: Spin Berry Phases



$$e^{iSA}$$

(Slightly) Technical interlude:
Quantum theory for bond order

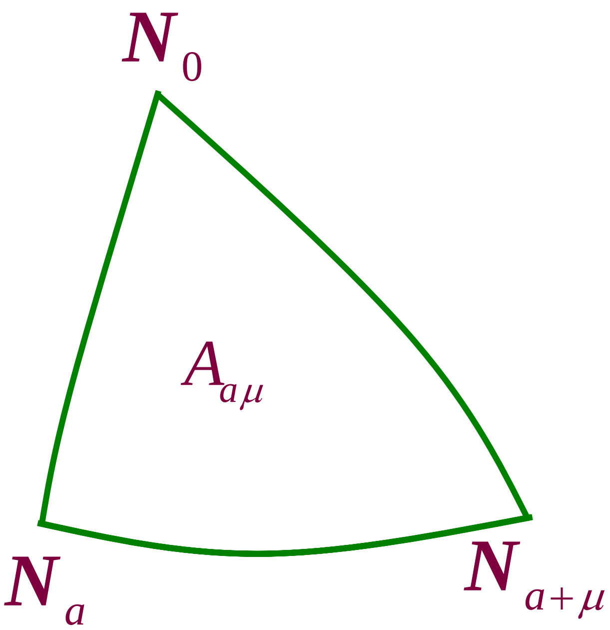
Key ingredient: Spin Berry Phases



$$e^{iSA}$$

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

formed by $\boldsymbol{N}_a$, $\boldsymbol{N}_{a+\mu}$, and an arbitrary reference point $\boldsymbol{N}_0$

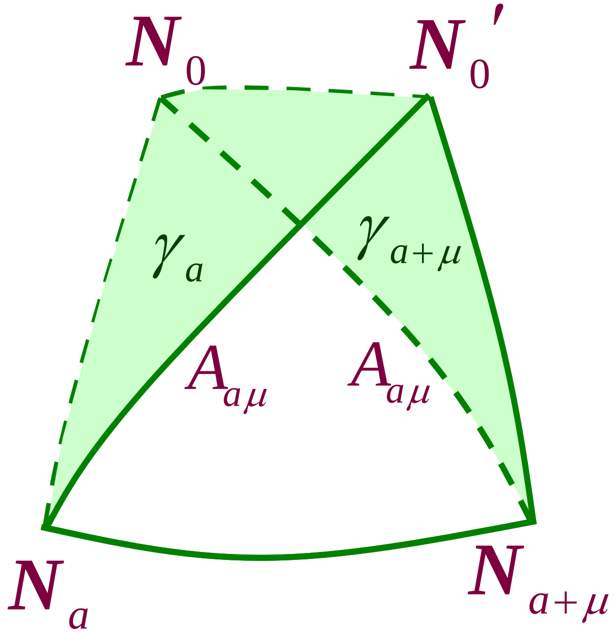


$A_{a\mu} \rightarrow$ oriented area of spherical triangle
formed by $\boldsymbol{N}_a$, $\boldsymbol{N}_{a+\mu}$, and an arbitrary reference point $\boldsymbol{N}_0$

Change in choice of $\boldsymbol{n}_0$ is like a "gauge transformation"

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

(γ_a is the oriented area of the spherical triangle formed by $\boldsymbol{N}_a$ and the two choices for $\boldsymbol{N}_0$).



The area of the triangle is uncertain modulo 4π, 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

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

$\eta_{\mathrm{a}} \rightarrow \pm 1$ on two square sublattices.

This is compact QED in $d+1$ dimensions with static charges ± 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.

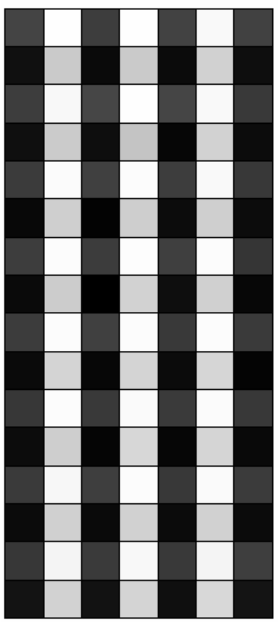
***d*=3**: A deconfined phase with a gapless "photon" is possible.

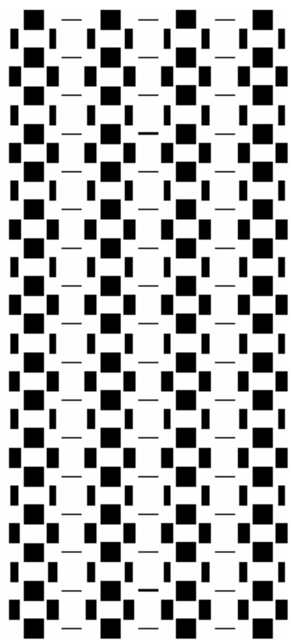
N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).
S. Sachdev and R. Jalabert, *Mod. Phys. Lett.* B **4**, 1043 (1990).
K. Park and S. Sachdev, *Phys. Rev.* B **65**, 220405 (2002).

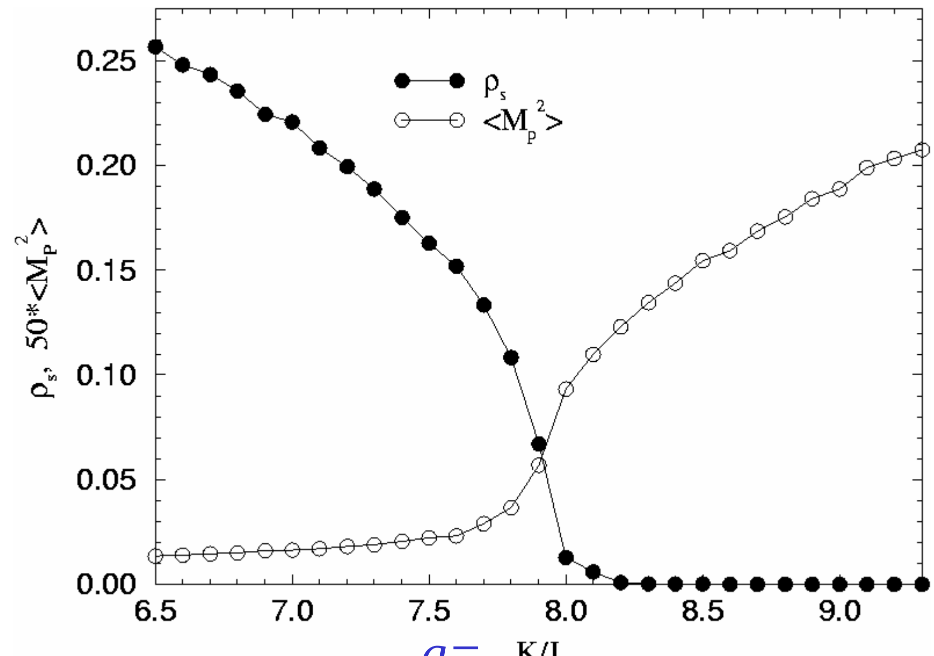
Bond order in a frustrated *S=1/2* XY magnet

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

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







g=

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

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

Competing order parameters in the cuprate superconductors

1. Pairing order of BCS theory (SC)

(Bose-Einstein) condensation of *d*-wave Cooper pairs

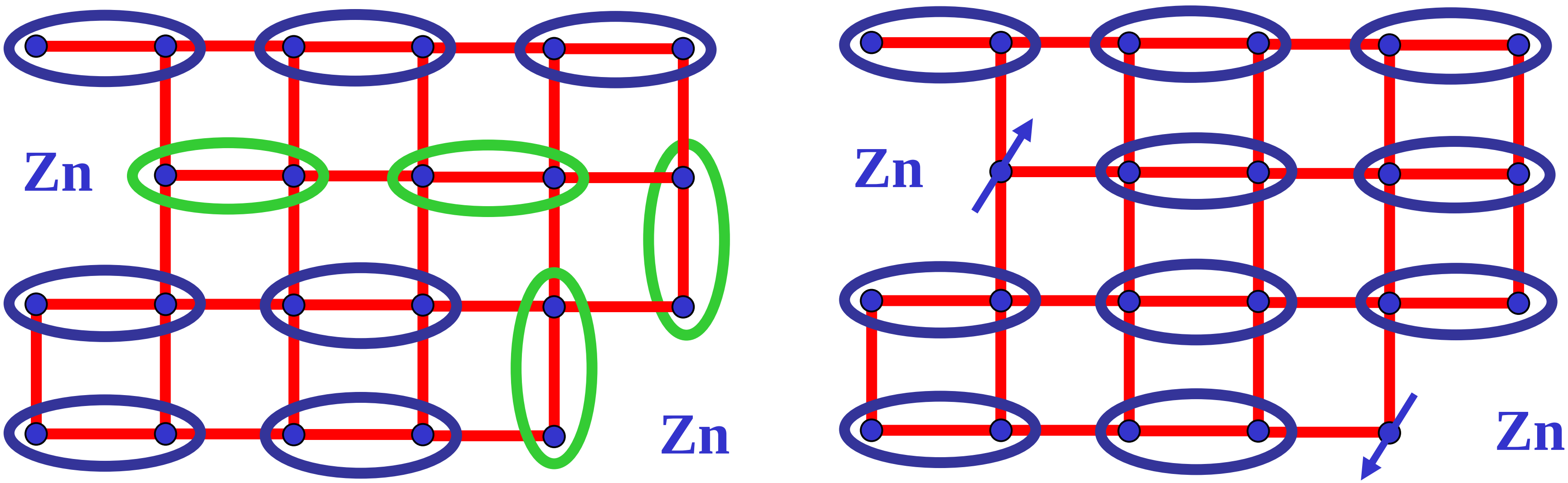
Orders associated with proximate Mott insulator

2. Collinear magnetic order (CM)

3. Bond order

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).

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

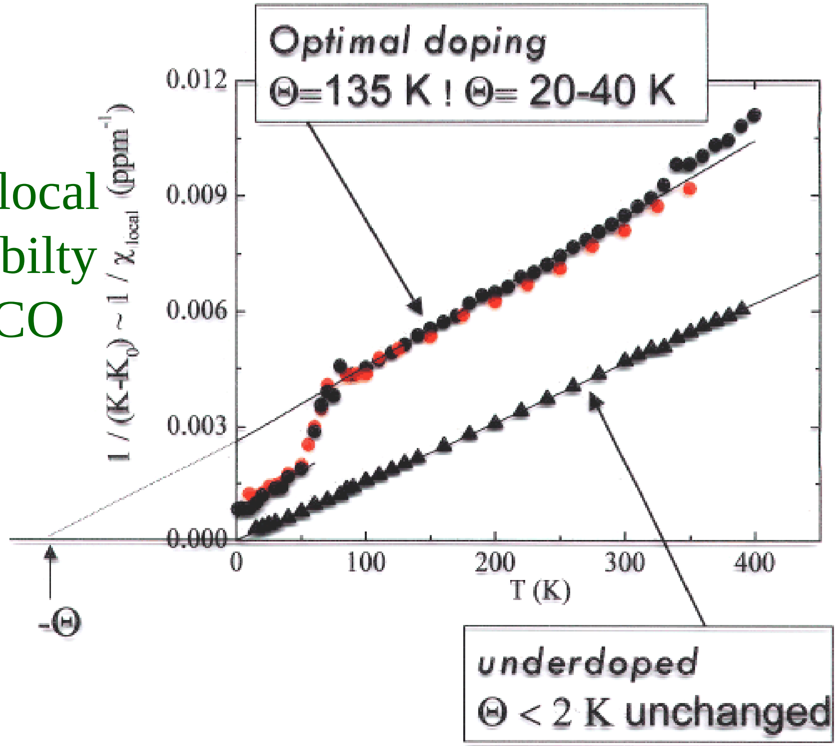


Spinon confinement implies that free S=1/2 moments form near each impurity

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

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

Inverse local susceptibilty in YBCO



^{7}Li NMR below T_c

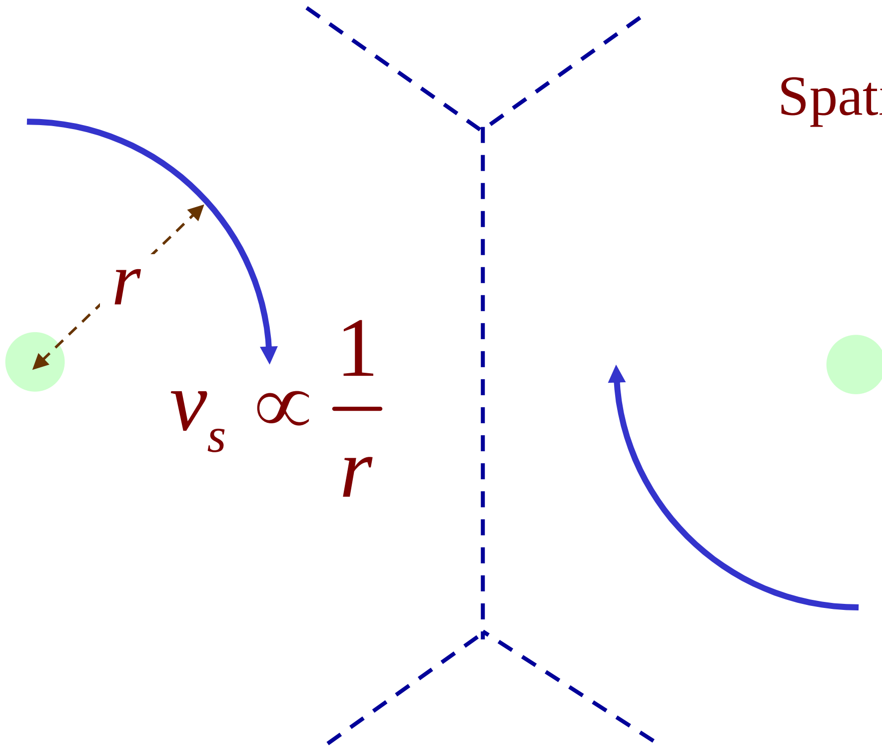
J. Bobroff, H. Alloul, W.A. MacFarlane, P. Mendels, N. Blanchard, G. Collin, and J.-F. Marucco, *Phys. Rev. Lett*. **86**, 4116 (2001).

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

This behavior does not emerge out of BCS theory.

A.M Finkelstein, V.E. Kataev, E.F. Kukovitskii, G.B. Teitel'baum, *Physica* C **168**, 370 (1990).

Phase diagram of superconducting (SC) and magnetic (CM) order in a magnetic field



Spatially averaged superflow kinetic energy

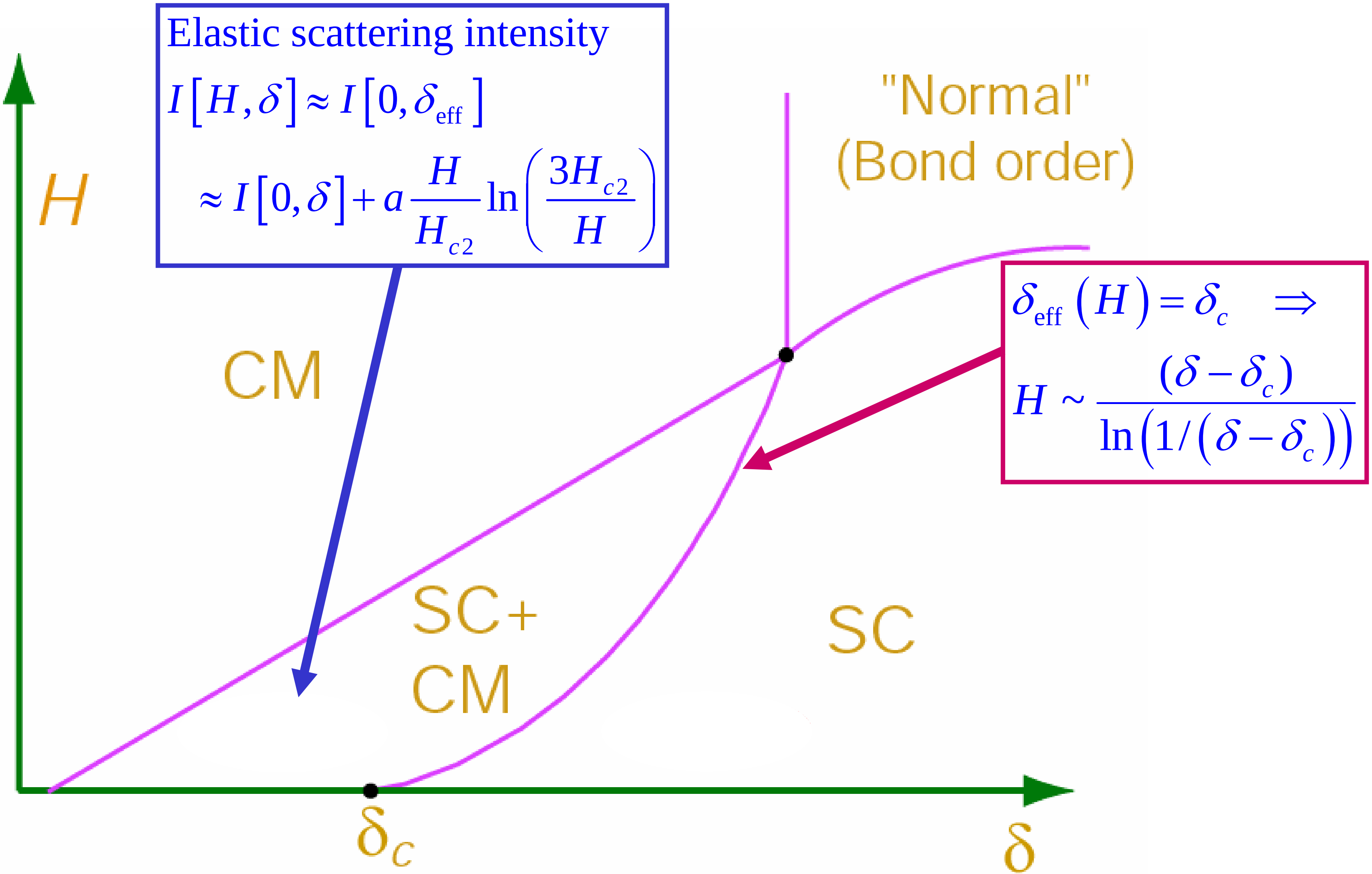
$$\left\langle v_s^2 \right\rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H}$$

The suppression of SC order appears to the CM order as an effective "doping" δ:

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

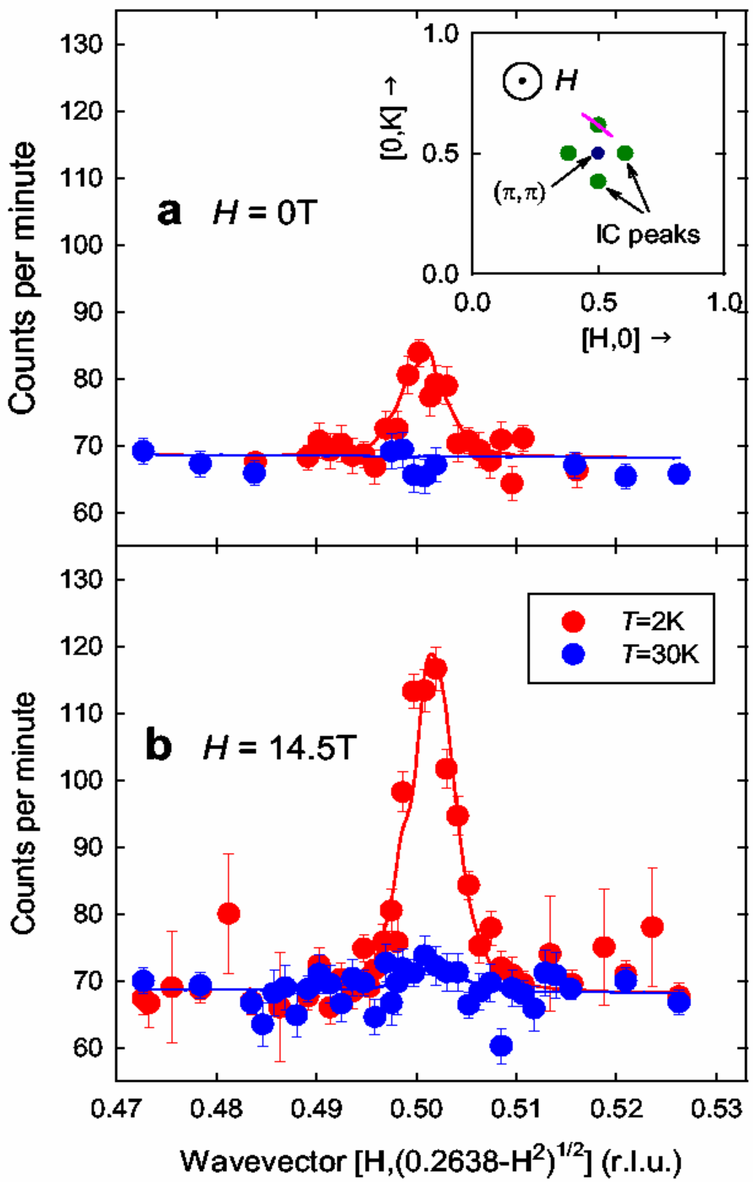
E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

Phase diagram of a superconductor in a magnetic field

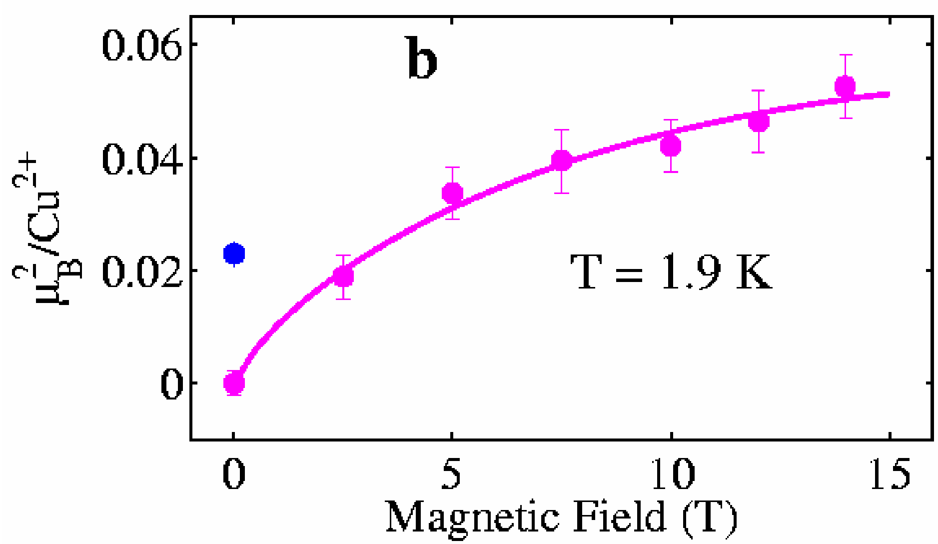


E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

Neutron scattering of $La_{2-x}Sr_xCuO_4$ 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).



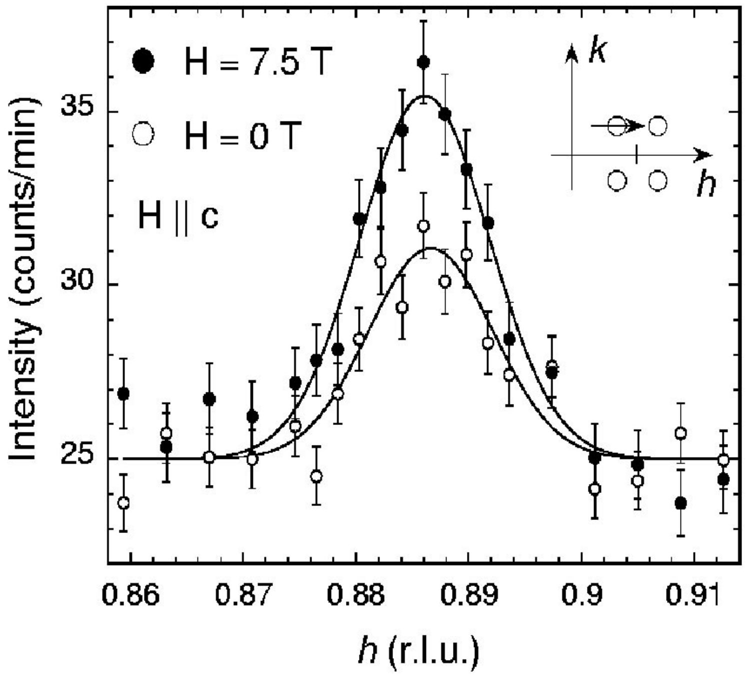
Solid line - fit to : $I(H) = a\dfrac{H}{H_{c2}}\ln\left(\dfrac{H_{c2}}{H}\right)$

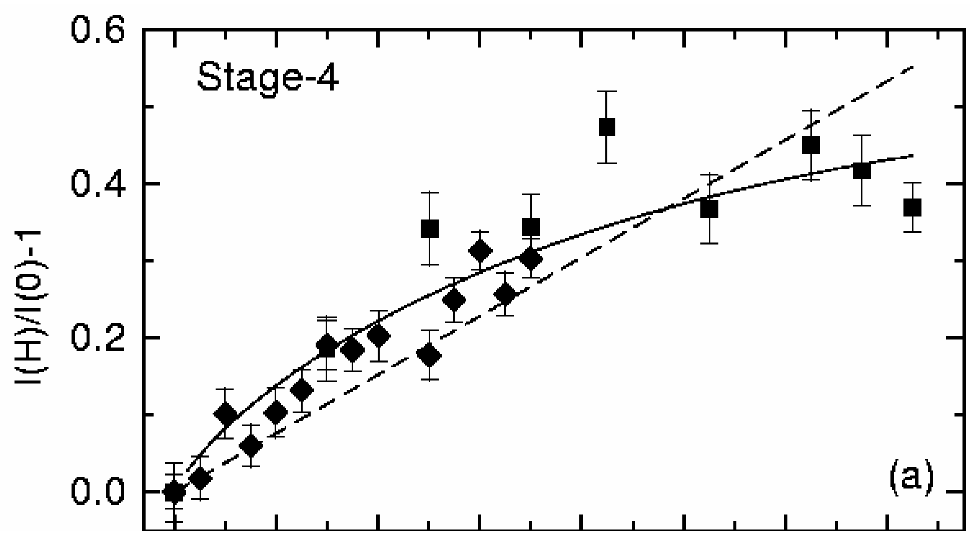
See also S. Katano, M. Sato, K. Yamada, T. Suzuki, and T. Fukase, *Phys. Rev.* B **62**, R14677 (2000).

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

Elastic neutron scattering off La_2CuO_{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).





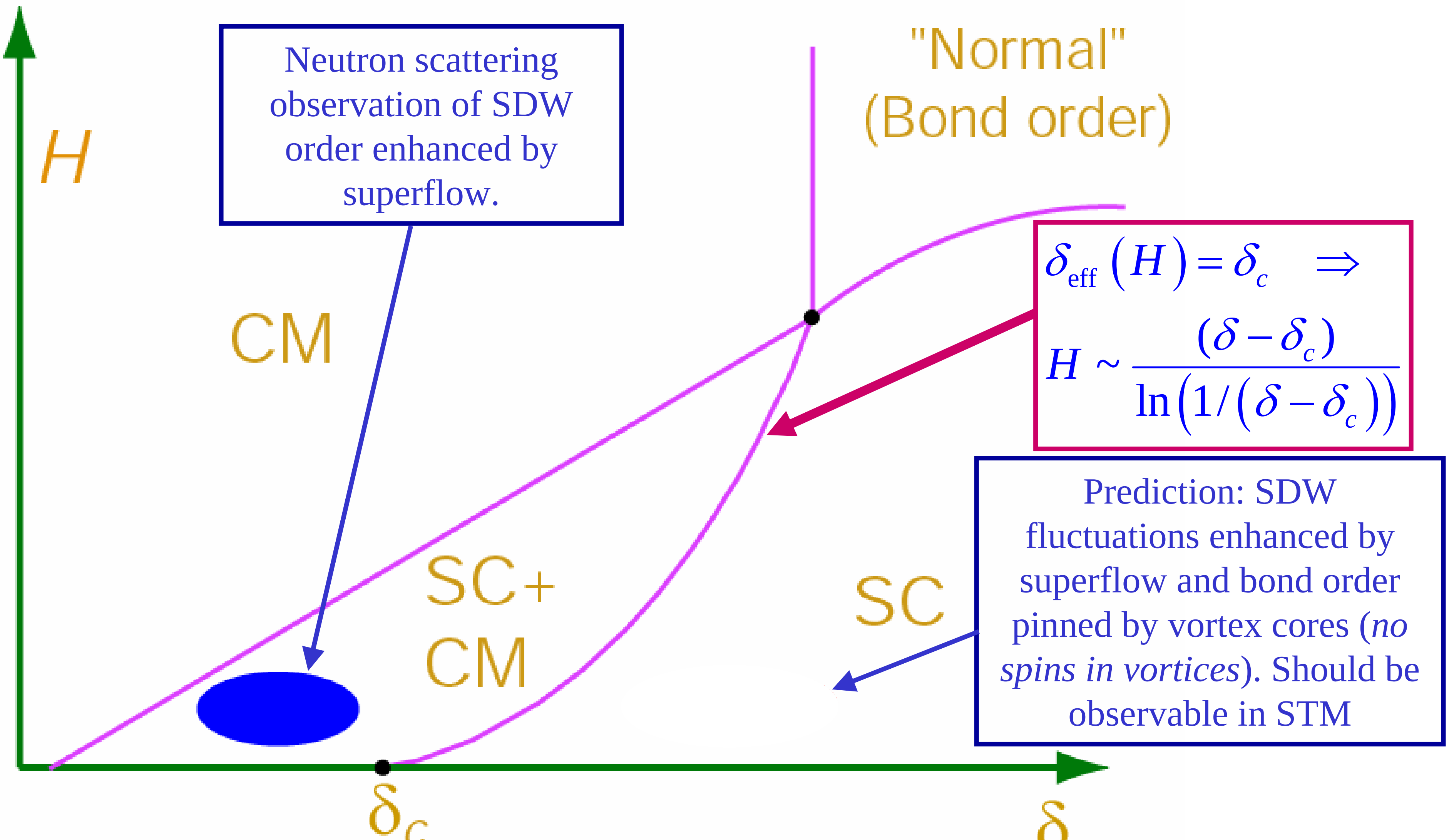
H (Tesla)

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

a is the only fitting parameter

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

Phase diagram of a superconductor in a magnetic field



K. Park and S. Sachdev *Physical Review* B **64**, 184510 (2001);

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

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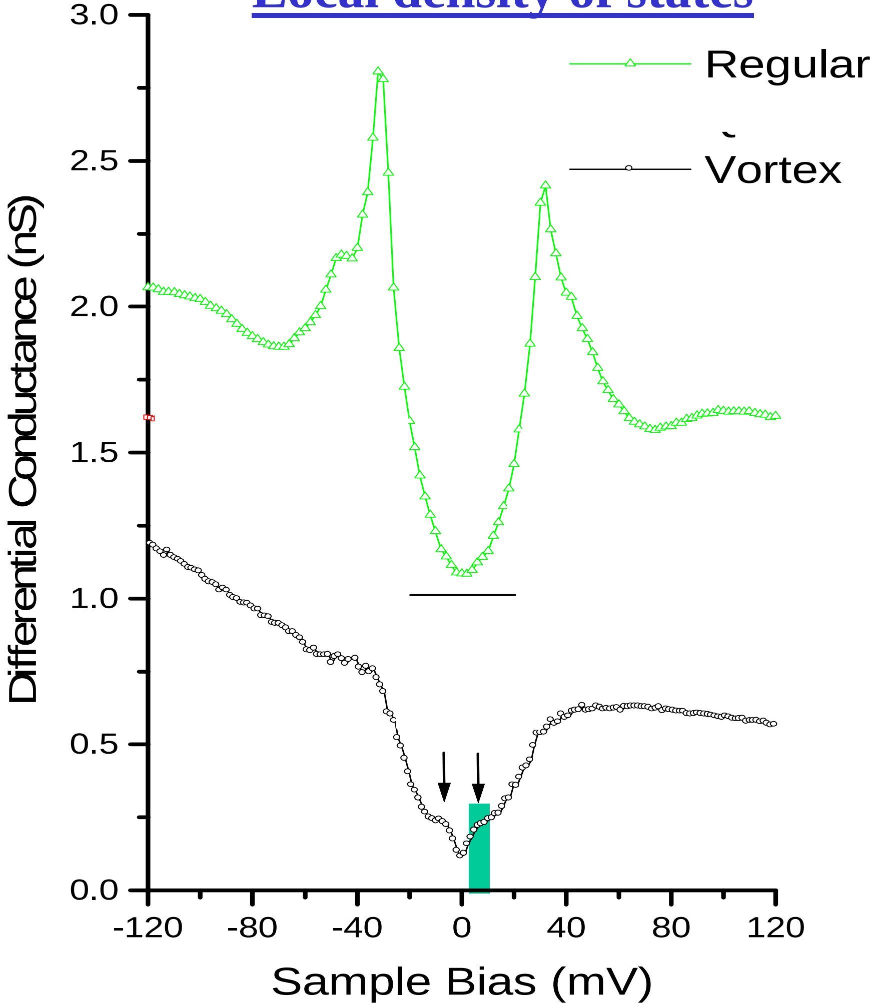
STM around vortices induced by a magnetic field in the superconducting state

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).

Local density of states

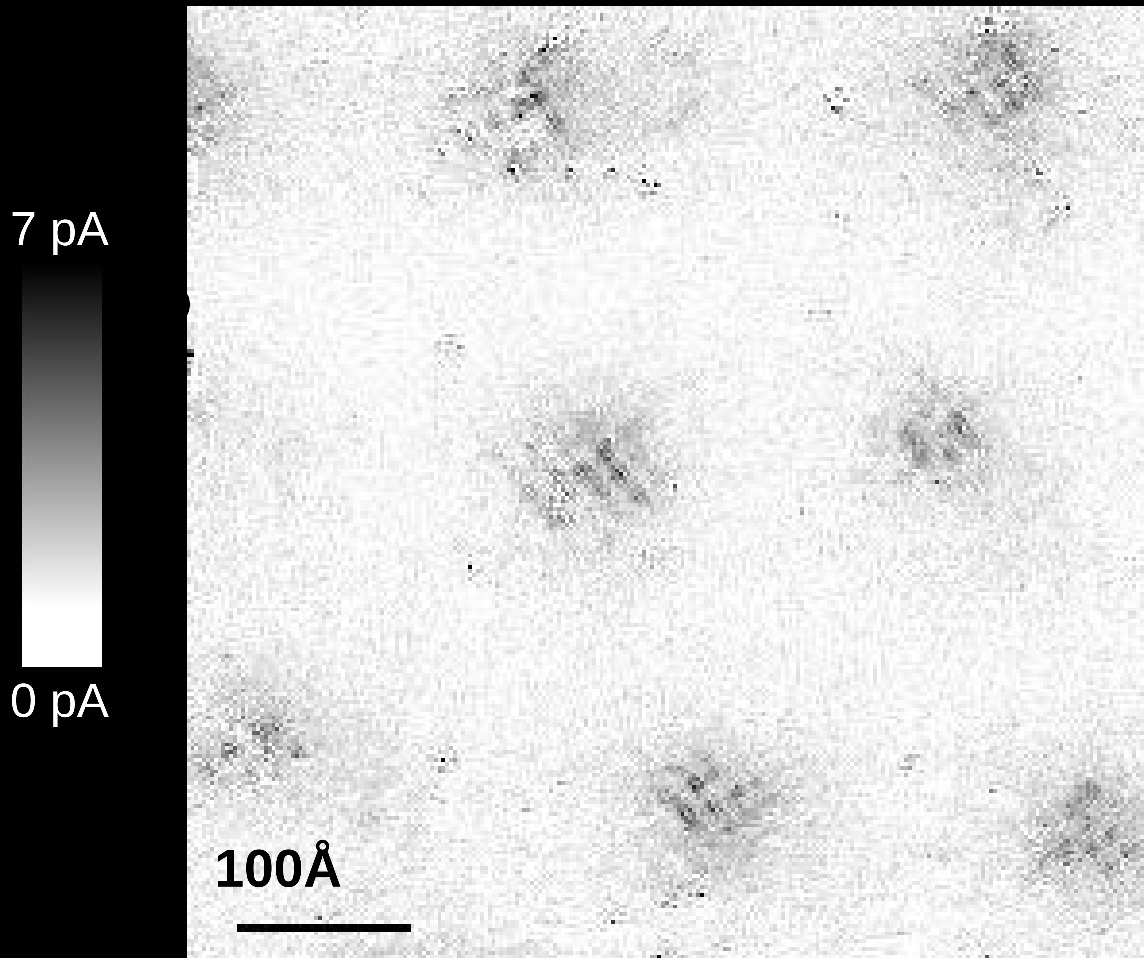


S.H. Pan *et al. Phys. Rev. Lett.* **85**, 1536 (2000).

1Å spatial resolution image of integrated LDOS of $Bi_2Sr_2CaCu_2O_{8+\delta}$

(1meV to 12 meV) at B=5 Tesla.

Vortex-induced LDOS of $Bi_2Sr_2CaCu_2O_{8+\delta}$ integrated from 1meV to 12meV

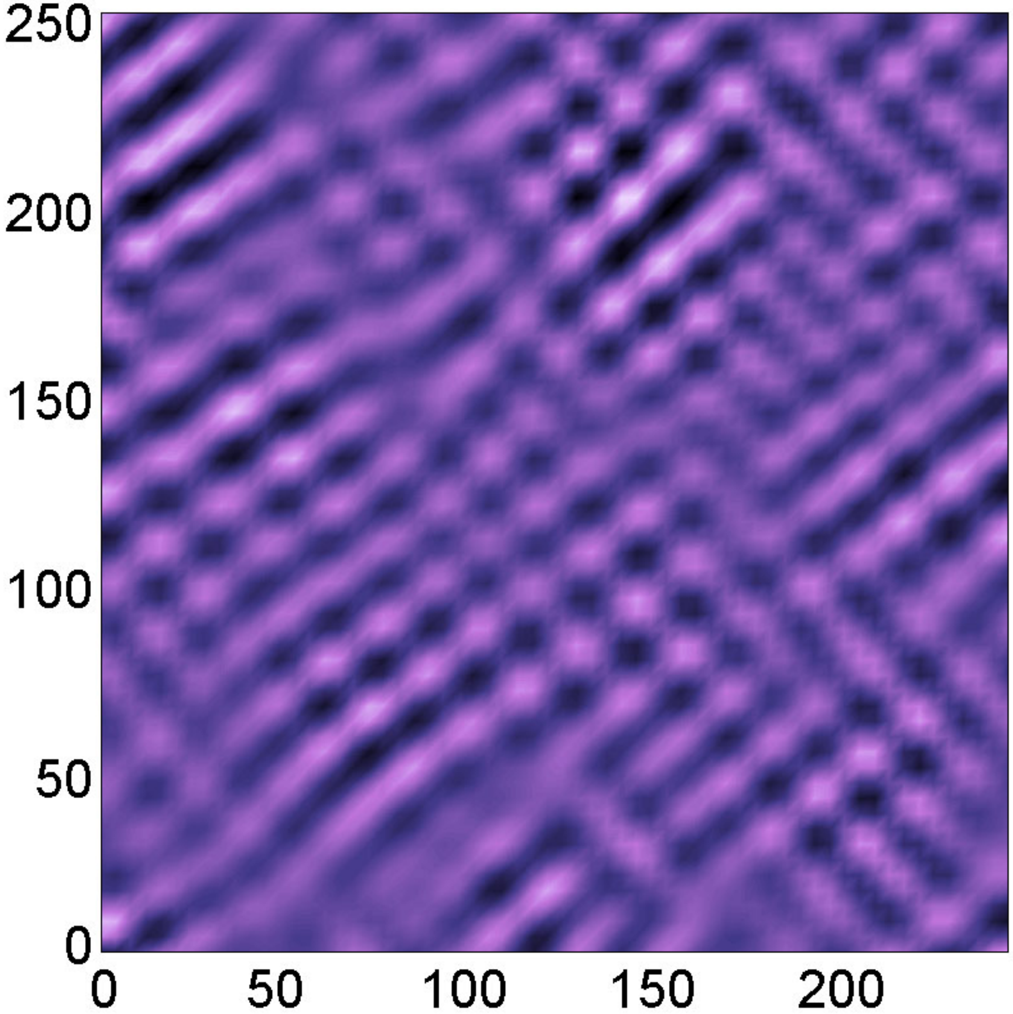


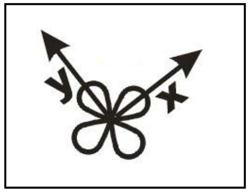
Our interpretation:
LDOS modulations are signals of bond order of period 4 revealed in vortex halo

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).

III. STM image of LDOS modulations in $Bi_2Sr_2CaCu_2O_{8+\delta}$ in zero magnetic field





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

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.