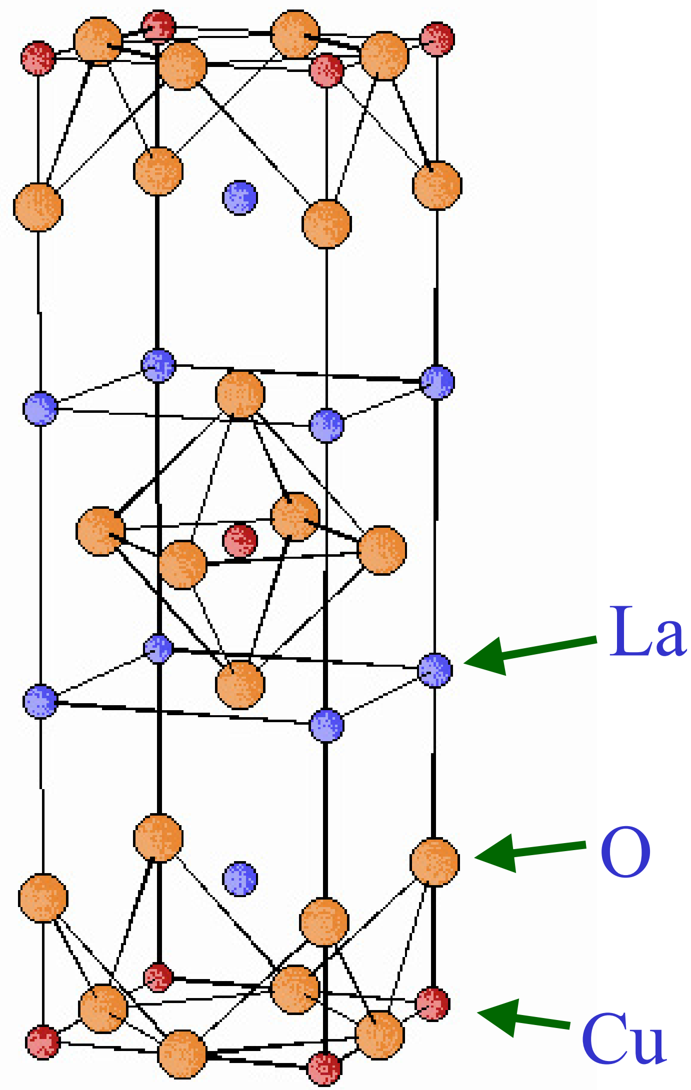
Understanding correlated electron systems by a classification of Mott insulators

Eugene Demler (Harvard)
Kwon Park (Maryland)
Anatoli Polkovnikov
Subir Sachdev
T. Senthil (MIT)
Matthias Vojta (Karlsruhe)
Ying Zhang (Maryland)

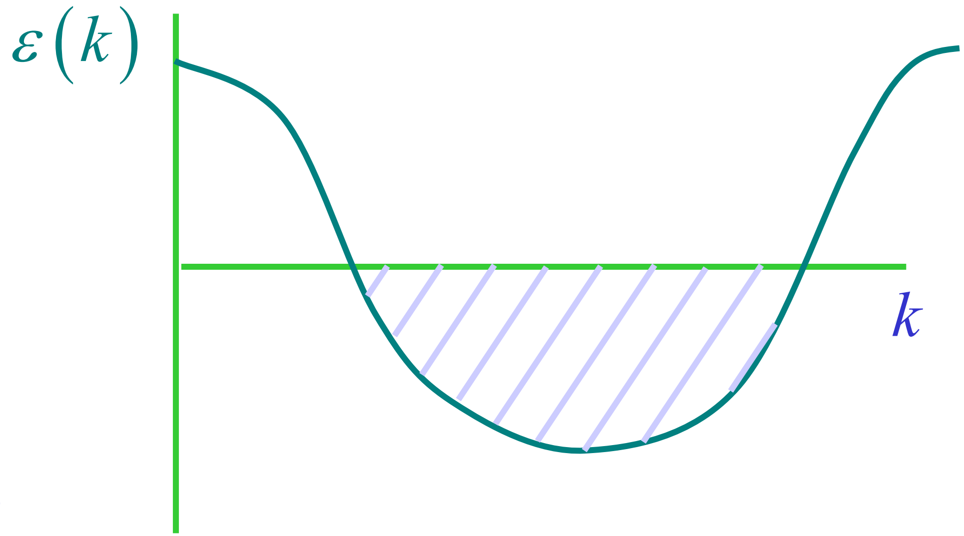
Colloquium article in *Reviews of Modern Physics*, July 2003, cond-mat/0211005.
Annals of Physics **303**, 226 (2003)

Talk online at
http://pantheon.yale.edu/~subir

Parent compound of the high temperature superconductors: La_2CuO_4



Band theory

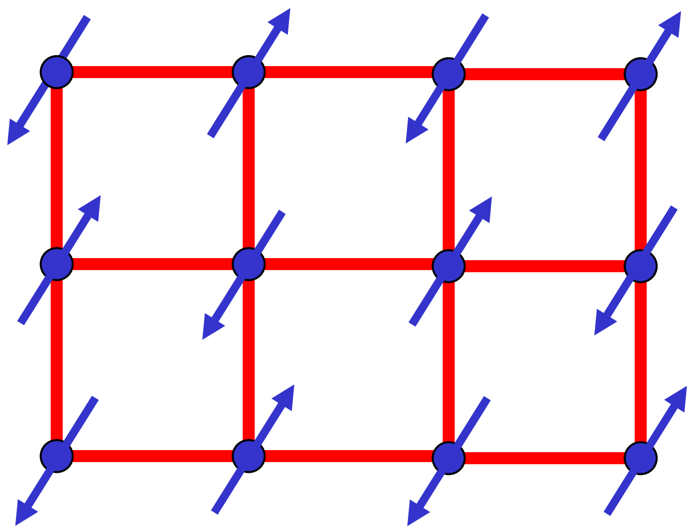


Half-filled band of Cu 3d orbitals – ground state is predicted to be a metal.

However, La_2CuO_4 is a very good insulator

Parent compound of the high temperature superconductors: La_2CuO_4

A Mott insulator



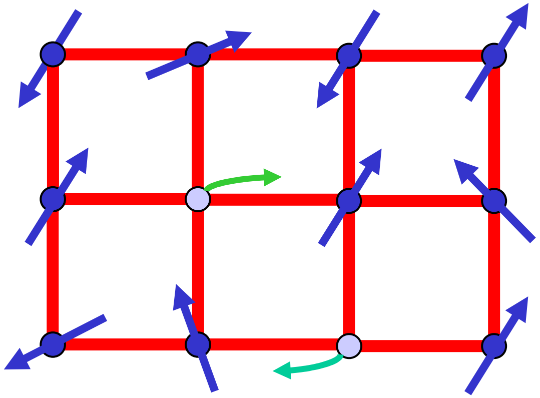
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

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

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

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

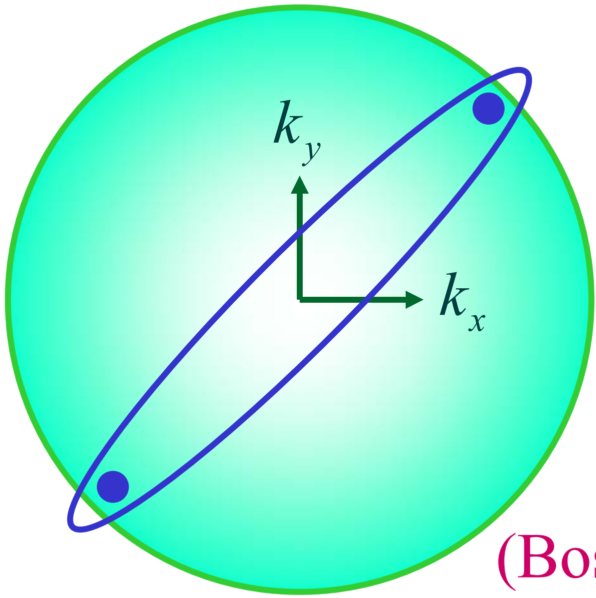


$$\left\langle \vec{S} \right\rangle = 0$$

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.

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, and are revealed in the presence of perturbations which locally destroy the BCS order (vortices, impurities, magnetic fields etc.)

The theory of quantum phase transitions, using expansions away from quantum critical points, allows a systematic description of states in which the order of Mott insulator is "fluctuating"

Outline

I. **Order in Mott insulators**

Magnetic order

A. Collinear spins

B. Non-collinear spins

Paramagnetic states

A. Compact U(1) gauge theory: bond order and confined spinons in d=2

B. Z_2 gauge theory: visons, topological order, and deconfined spinons

II. Class A in d=2

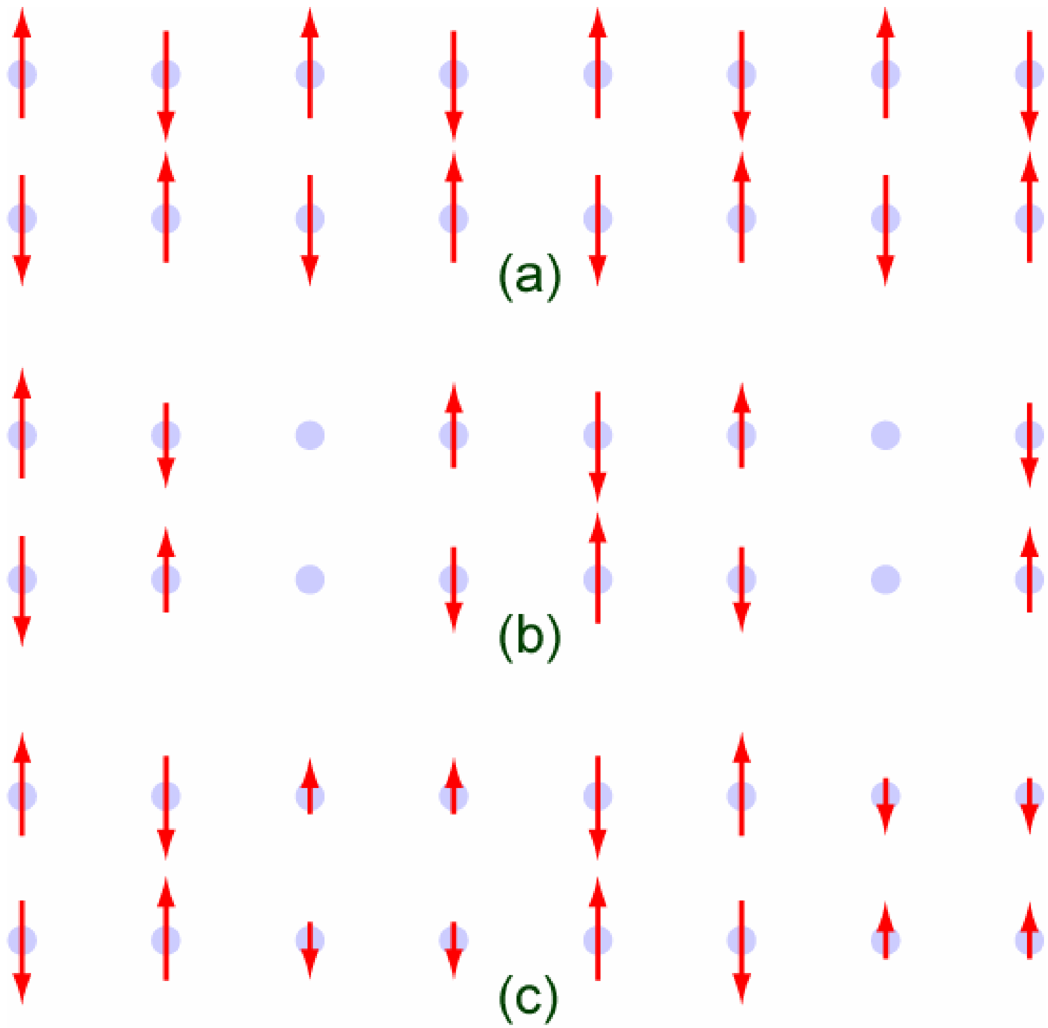
The cuprates

III. Conclusions

I. Order in Mott insulators

Magnetic order $\langle \mathbf{S}_j \rangle = \mathbf{N}_1 \cos\left(\vec{K} \cdot \vec{r}_j\right) + \mathbf{N}_2 \sin\left(\vec{K} \cdot \vec{r}_j\right)$

Class A. Collinear spins



$\vec{K} = (\pi, \pi)\ ;\ \mathbf{N}_2 = 0$

$\vec{K} = (3\pi/4, \pi)\ ;\ \mathbf{N}_2 = 0$

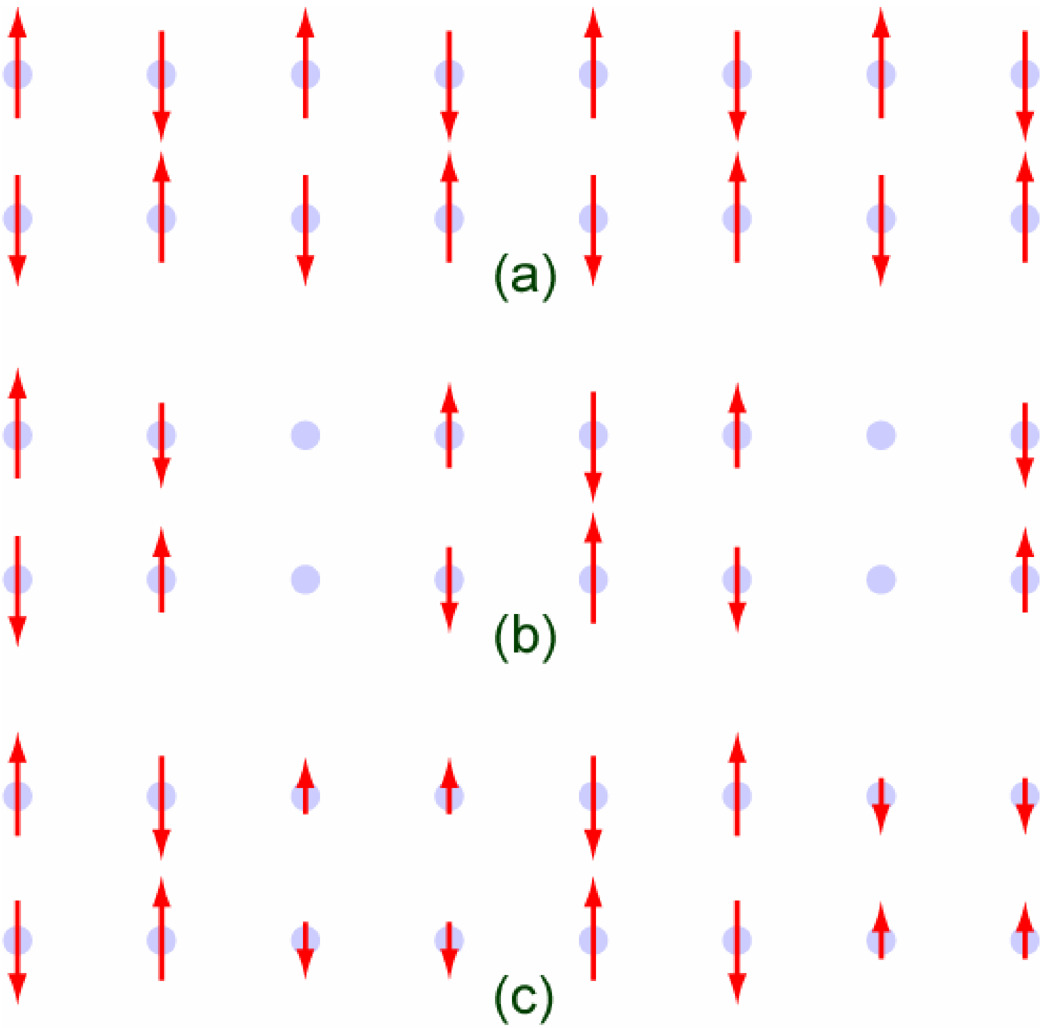
$\vec{K} = (3\pi/4, \pi)\ ;$

$\mathbf{N}_2 = \left(\sqrt{2} - 1\right) \mathbf{N}_1$

I. Order in Mott insulators

Magnetic order $\langle \boldsymbol{S}_j \rangle = \boldsymbol{N}_1 \cos\left(\vec{K} \cdot \vec{r}_j\right) + \boldsymbol{N}_2 \sin\left(\vec{K} \cdot \vec{r}_j\right)$

Class A. Collinear spins



Key property

Order specified by a single vector $\boldsymbol{N}$.

Quantum fluctuations leading to loss of magnetic order should produce a paramagnetic state with a vector (S=1) quasiparticle excitation.

Outline

I. **Order in Mott insulators**

Magnetic order

A. Collinear spins

B. Non-collinear spins

Paramagnetic states

A. Compact U(1) gauge theory: bond order and confined spinons in d=2

B. Z_2 gauge theory: visons, topological order, and deconfined spinons

II. Class A in d=2

The cuprates

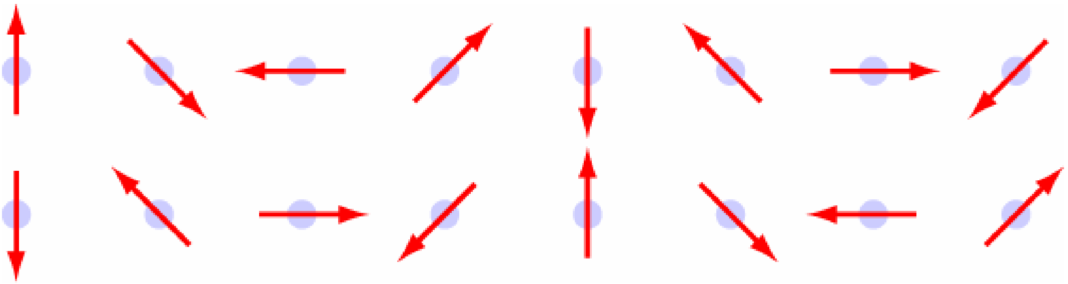
III. Conclusions

I. Order in Mott insulators

Magnetic order $\left\langle \boldsymbol{S}_j \right\rangle = \boldsymbol{N}_1 \cos\left(\vec{K} \cdot \vec{r}_j\right) + \boldsymbol{N}_2 \sin\left(\vec{K} \cdot \vec{r}_j\right)$

Class B. Noncollinear spins

(B.I. Shraiman and E.D. Siggia, *Phys. Rev. Lett.* **61**, 467 (1988))



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

$$\boldsymbol{N}_2^2 = \boldsymbol{N}_1^2 \,,\, \boldsymbol{N}_1 \cdot \boldsymbol{N}_2 = 0$$

Solve constraints by expressing $\boldsymbol{N}_{1,2}$ in terms of two complex numbers $z_\uparrow$, $z_\downarrow$

$$\boldsymbol{N}_1 + i\boldsymbol{N}_2 = \begin{pmatrix} z_\downarrow^2 - z_\uparrow^2 \\ i\left(z_\downarrow^2 + z_\uparrow^2\right) \\ 2z_\uparrow z_\downarrow \end{pmatrix}$$

Order in ground state specified by a spinor $\left(z_\uparrow, z_\downarrow\right)$ (modulo an overall sign).

This spinor can become a S=1/2 spinon in paramagnetic state.

Theory of spinons must obey the Z_2 gauge symmetry $z_a \to -z_a$

Outline

I. **Order in Mott insulators**

Magnetic order

A. Collinear spins

B. Non-collinear spins

Paramagnetic states

A. Compact U(1) gauge theory: bond order and confined spinons in *d*=2

B. Z_2 gauge theory: visons, topological order, and deconfined spinons

II. Class A in *d*=2

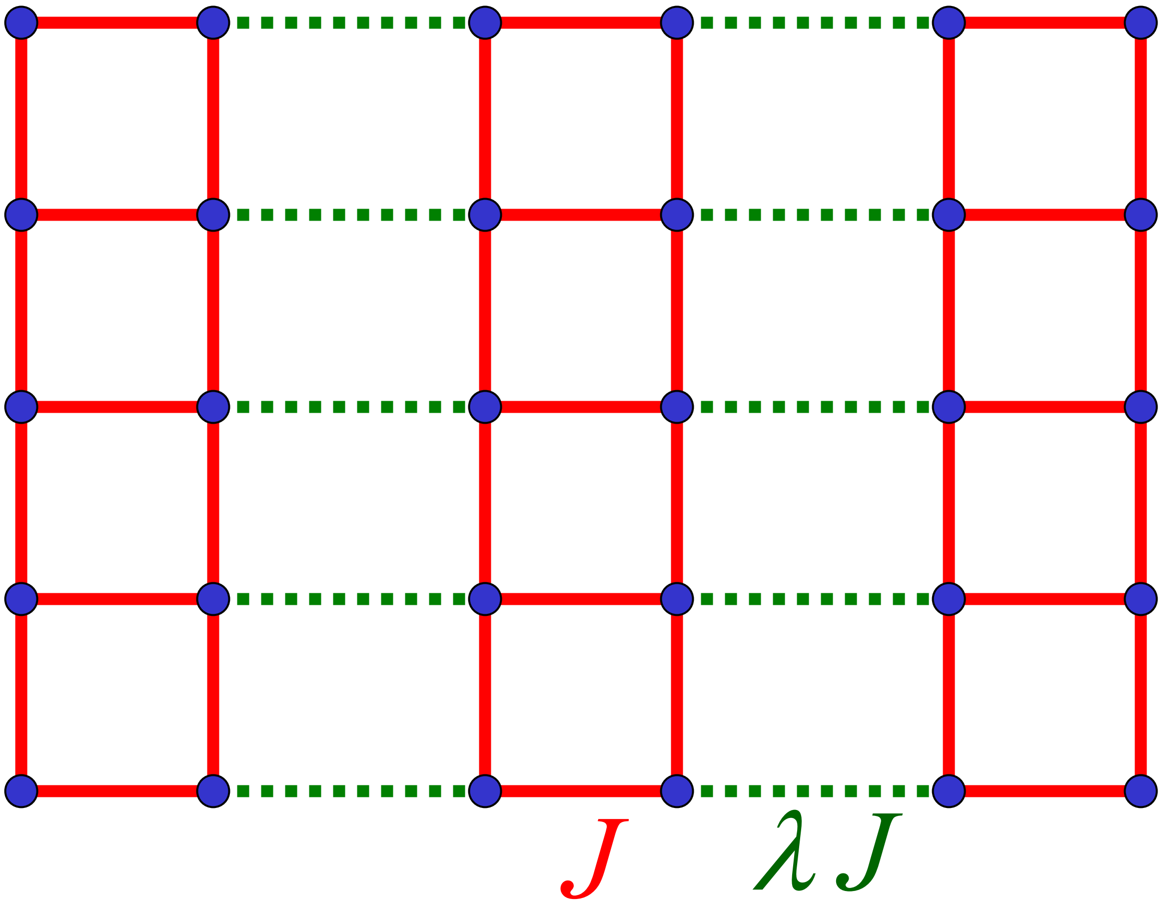
The cuprates

III. Conclusions

Coupled ladder antiferromagnet

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 2-leg ladders



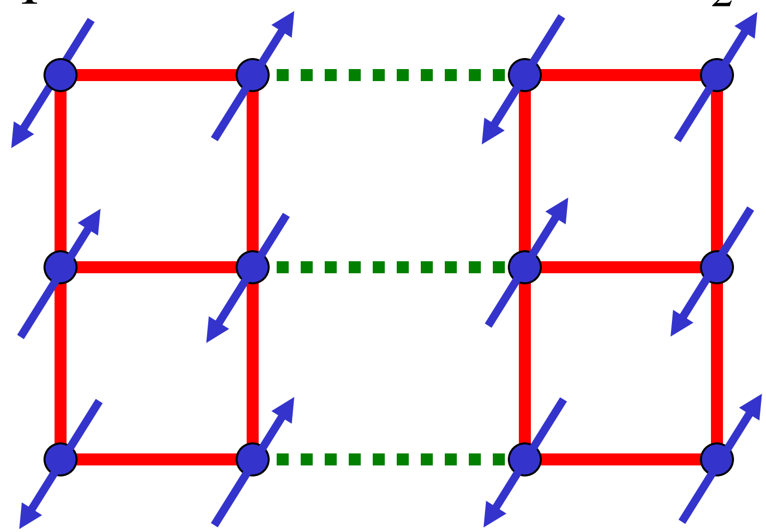
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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

λ close to 1

Square lattice antiferromagnet

Experimental realization: La_2CuO_4



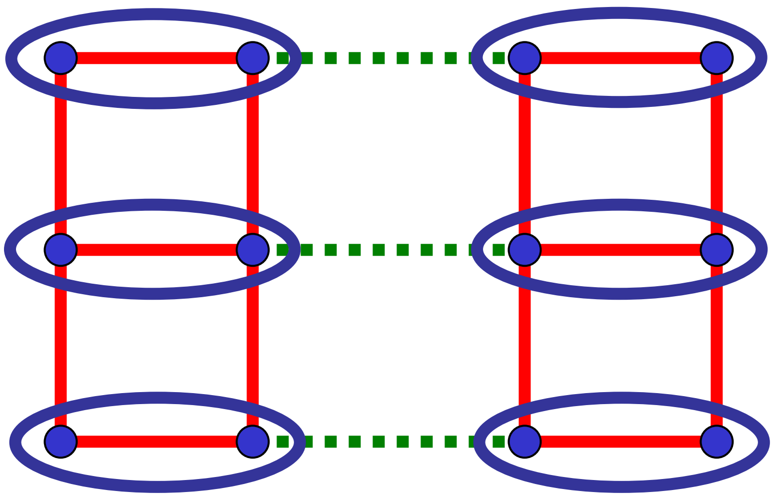
Ground state has long-range collinear magnetic (Neel) order

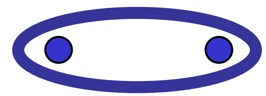
$$\left\langle \vec{S}_i \right\rangle = \left(-1\right)^{i_x+i_y} N_0 \neq 0$$

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

λ close to 0

Weakly coupled ladders



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

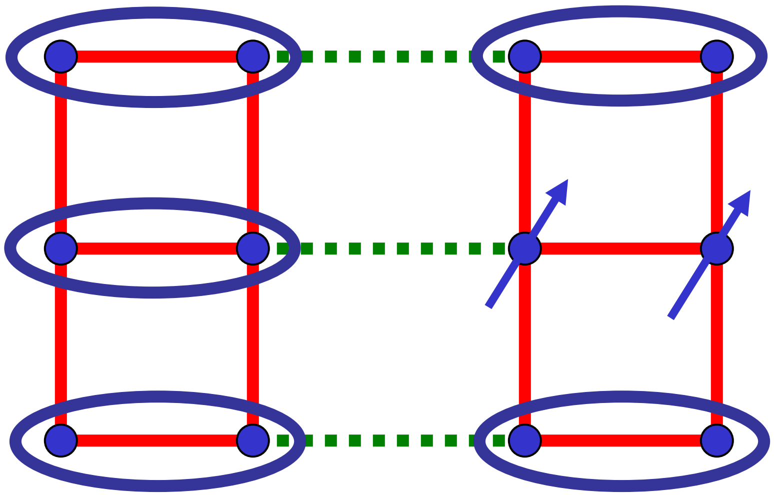
Real space Cooper pairs with their charge localized. Upon doping, motion and condensation of Cooper pairs leads to superconductivity

Paramagnetic ground state

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

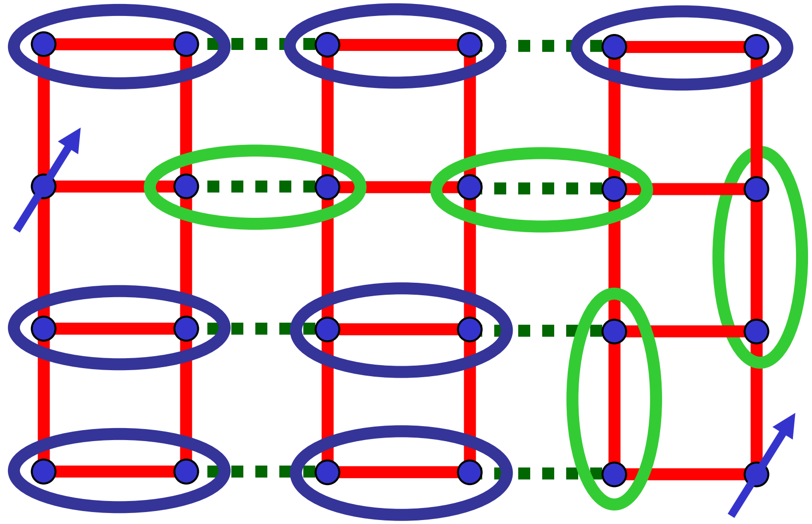
λ close to 0

Excitations



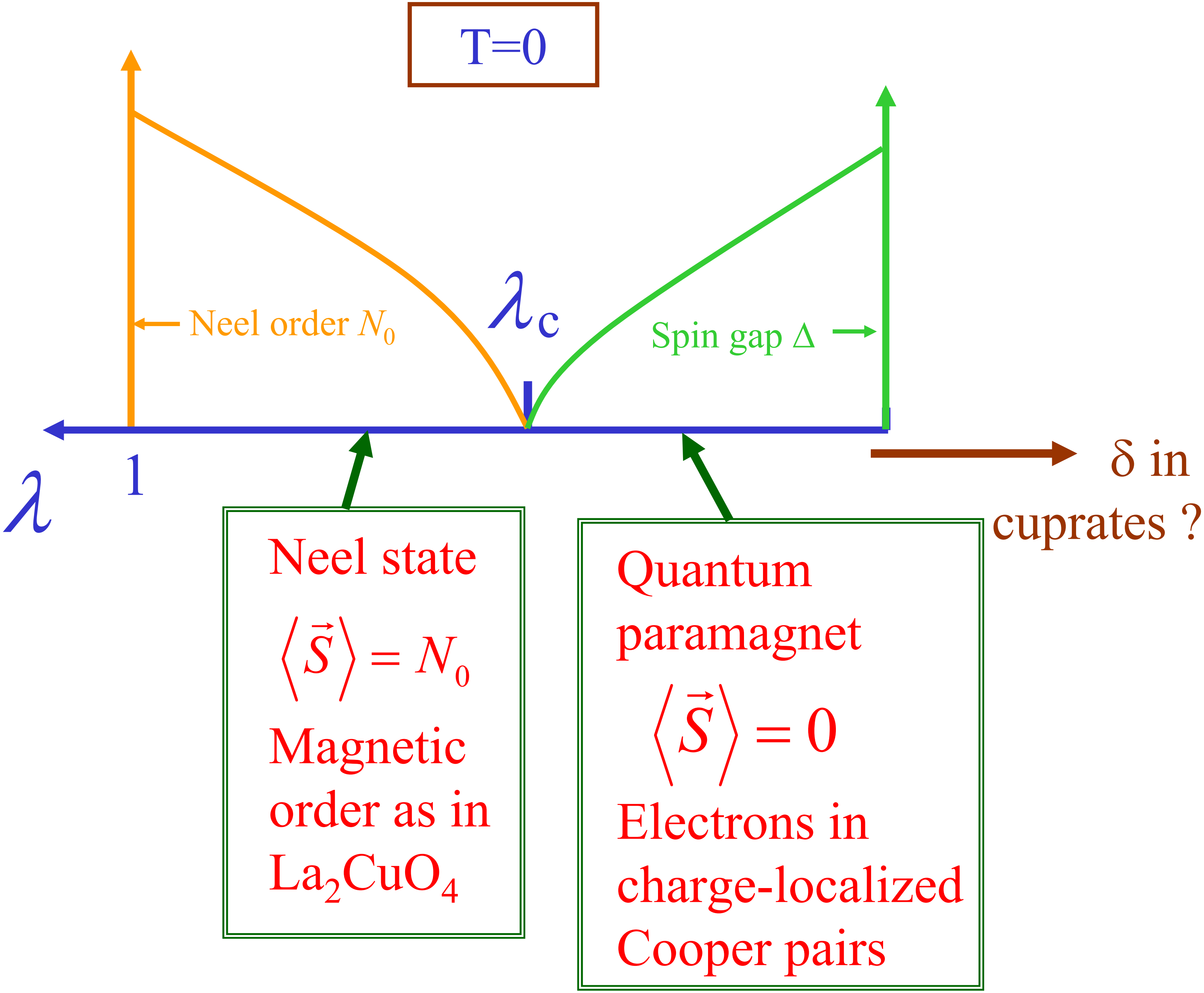
Excitation: S=1 ***exciton***

(vector ***N*** particle of paramagnetic state)

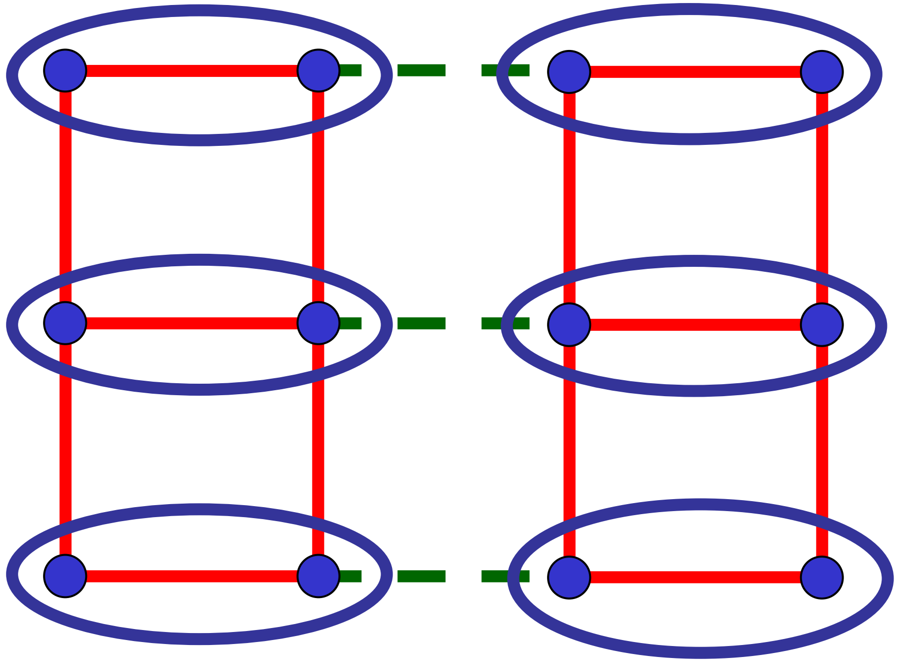


S=1/2 spinons are ***confined*** by a linear potential.

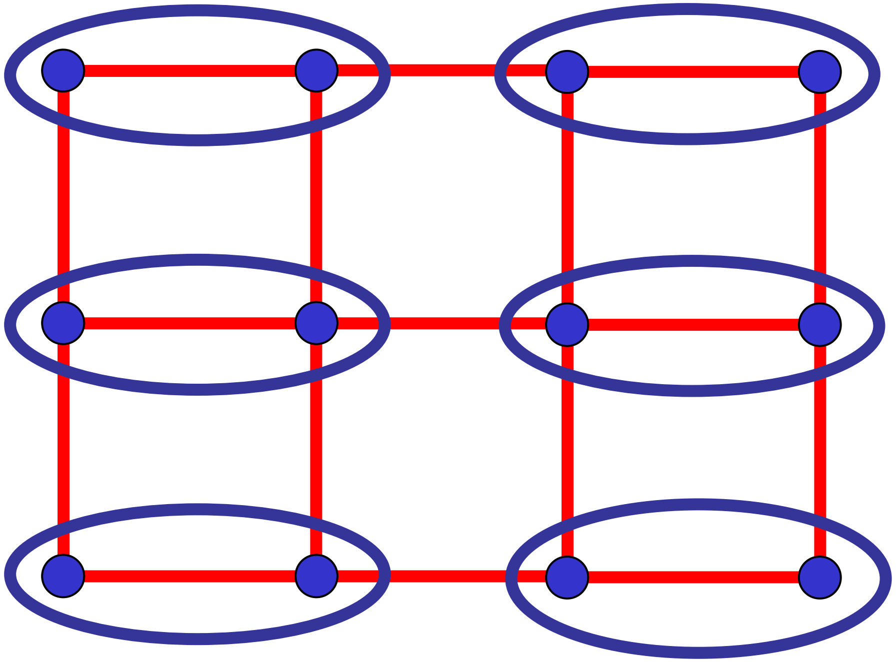
Energy dispersion away from antiferromagnetic wavevector $\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$


T=0
Neel order N_0
λ_c
Spin gap Δ
λ
1
δ in
cuprates ?
Neel state
$\langle \vec{S} \rangle = N_0$
Magnetic
order as in
La_2CuO_4
Quantum
paramagnet
$\langle \vec{S} \rangle = 0$
Electrons in
charge-localized
Cooper pairs

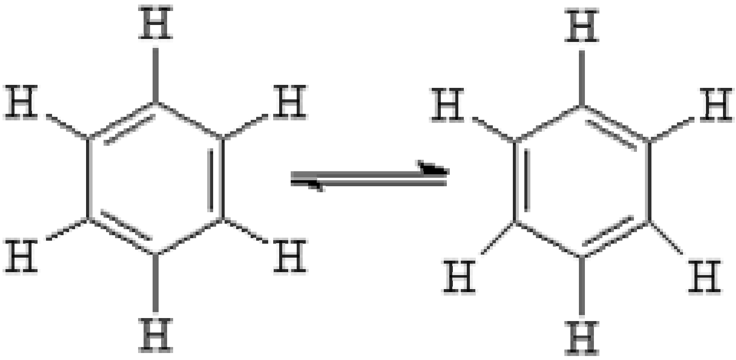
Paramagnetic ground state of coupled ladder model

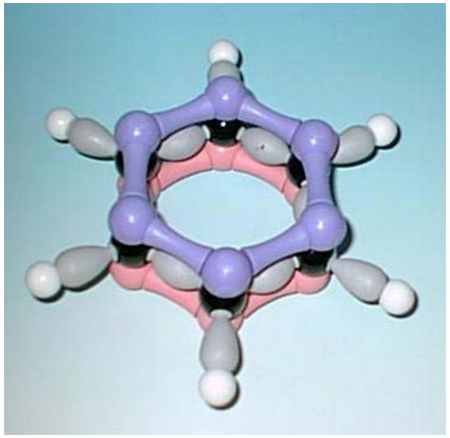


Can such a state with ***bond order*** be the ground state of a system with full square lattice symmetry ?



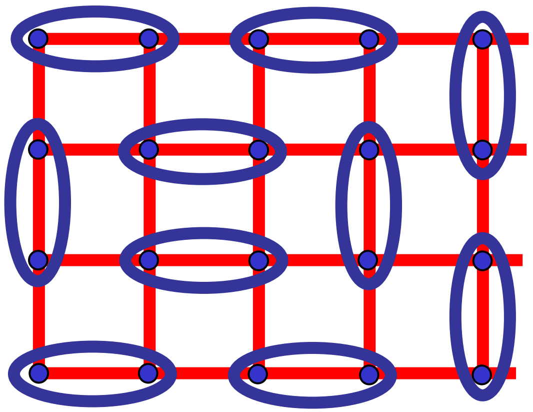
Resonating valence bonds





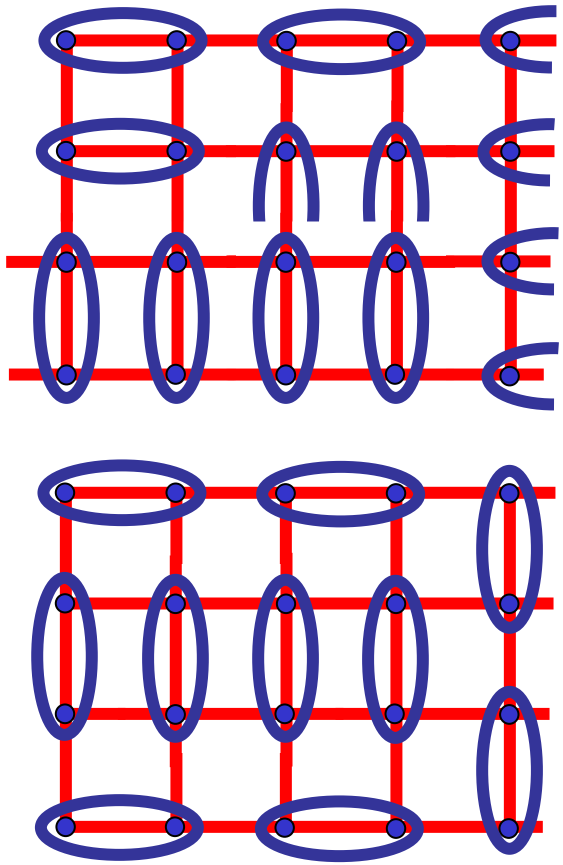
Resonance in benzene leads to a symmetric configuration of valence bonds

(*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*)



Possible 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.

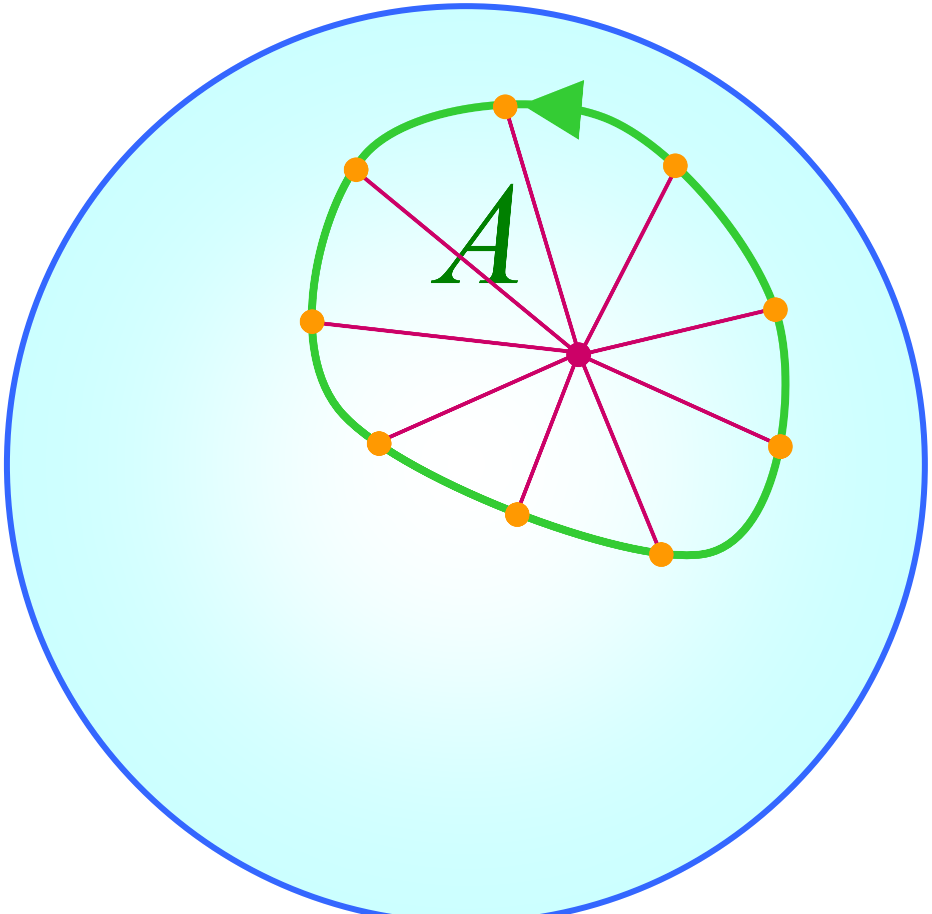
A precise description of this physics is obtained by a compact U(1) gauge theory of the paramagnetic Mott insulator

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

Class A: Collinear spins and compact U(1) gauge theory

Write down path integral for quantum spin fluctuations

Key ingredient: Spin Berry Phases

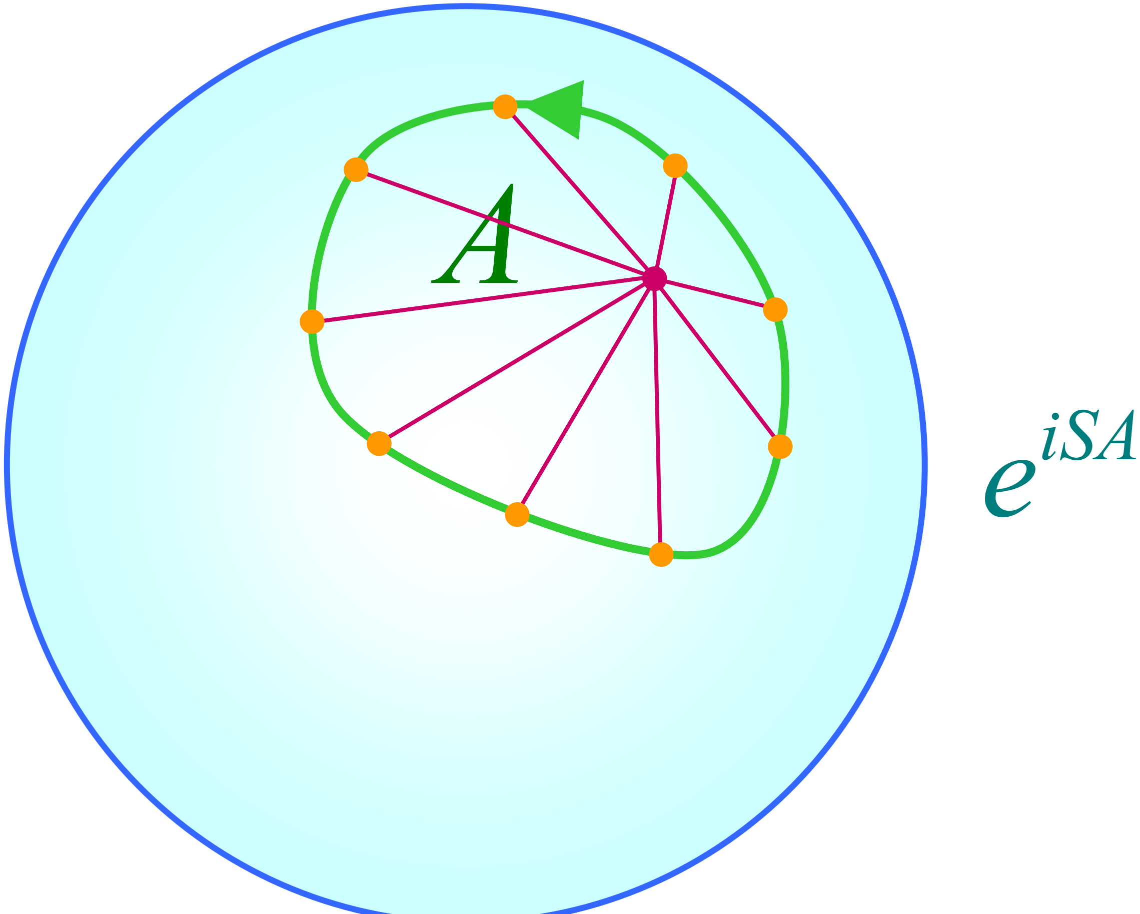


$$e^{iSA}$$

Class A: Collinear spins and compact U(1) gauge theory

Write down path integral for quantum spin fluctuations

Key ingredient: Spin Berry Phases



Class A: Collinear spins and compact U(1) gauge theory

S=1/2 square lattice antiferromagnet with non-nearest neighbor exchange

$$H = \sum_{i<j} J_{ij} \; \vec{S}_i \cdot \vec{S}_j$$

Include Berry phases after discretizing coherent state path integral on a cubic lattice in spacetime

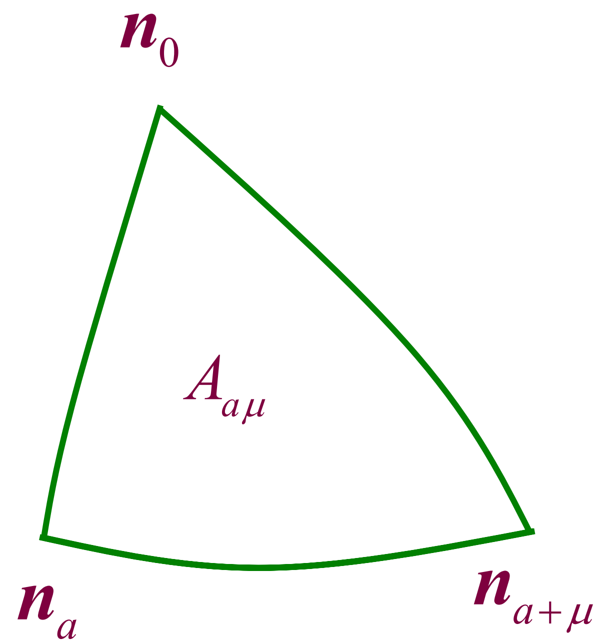
$$Z = \prod_a \int d\boldsymbol{n}_a \delta\left(\boldsymbol{n}_a^2 - 1\right) \exp\left(\frac{1}{g} \sum_{a,\mu} \boldsymbol{n}_a \cdot \boldsymbol{n}_{a+\mu} - \frac{i}{2} \sum_a \eta_a A_{a\tau} \right)$$

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

$\boldsymbol{n}_a \sim \eta_a \vec{S}_a \rightarrow$ Neel order parameter;

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

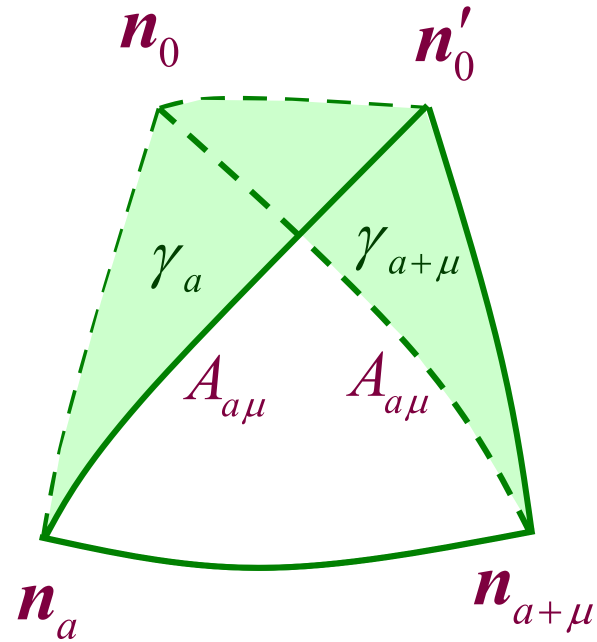
formed by $\boldsymbol{n}_a$, $\boldsymbol{n}_{a+\mu}$, and an arbitrary reference point $\boldsymbol{n}_0$


$\boldsymbol{n}_0$
$A_{a\mu}$
$\boldsymbol{n}_a$
$\boldsymbol{n}_{a+\mu}$

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 large g phase

Simplest large g effective action for the $A_{a\mu}$

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

with $e^2 \sim g^2$

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.

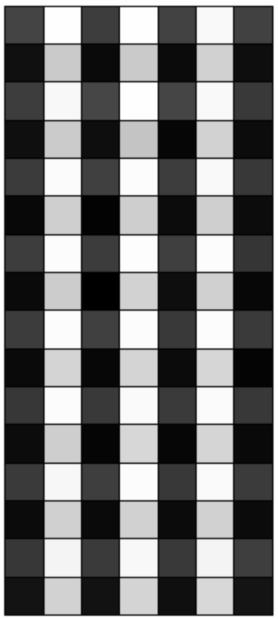
***d*=3**: A deconfined phase with a gapless "photon" is possible.

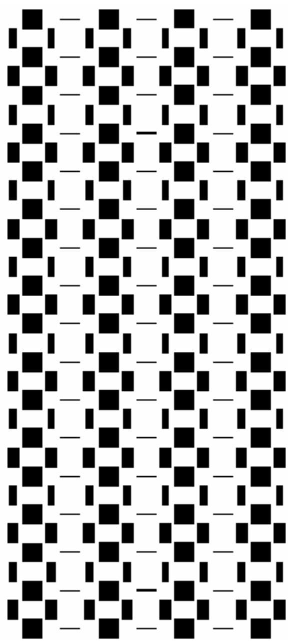
N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).
S. Sachdev and R. Jalabert, *Mod. Phys. Lett.* B **4**, 1043 (1990).
K. Park and S. Sachdev, *Phys. Rev.* B **65**, 220405 (2002).

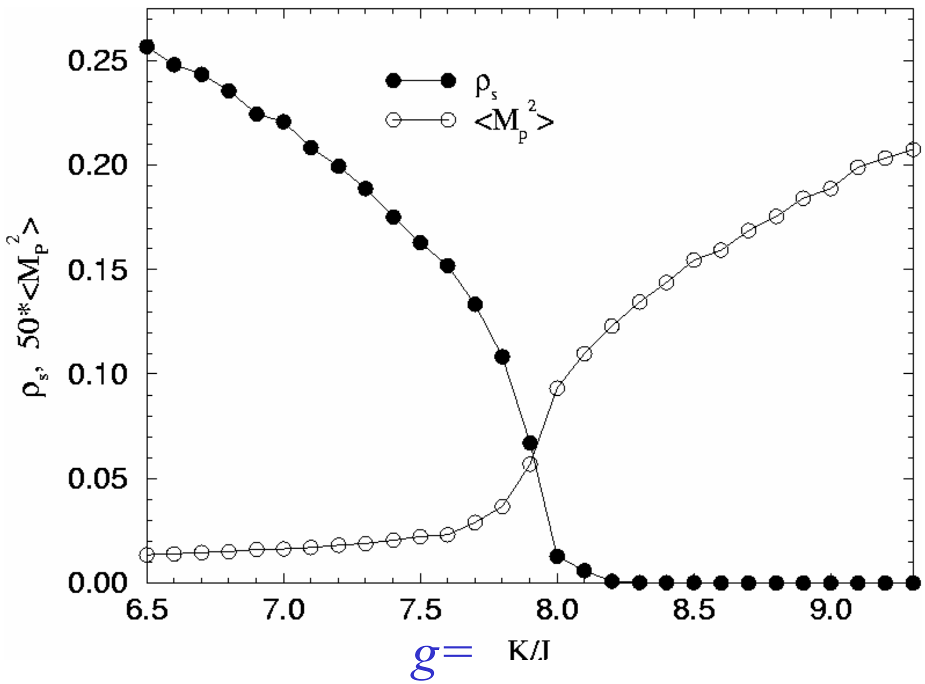
Bond order in a frustrated *S=1/2* XY magnet

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

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







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

Outline

I. Order in Mott insulators

Magnetic order

A. Collinear spins

B. Non-collinear spins

Paramagnetic states

A. Compact U(1) gauge theory: bond order and confined spinons in d=2

B. Z_2 gauge theory: visons, topological order, and deconfined spinons

II. Class A in d=2

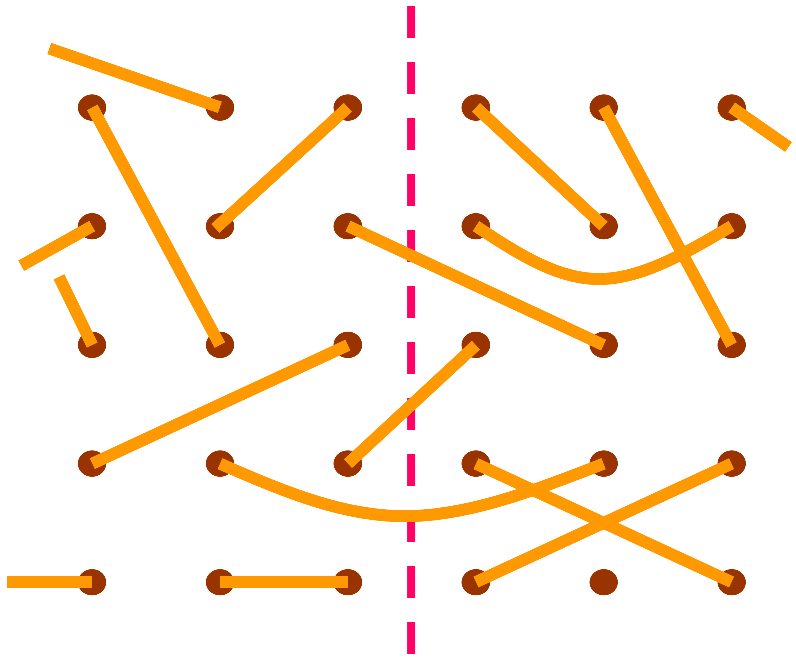
The cuprates

III. Conclusions

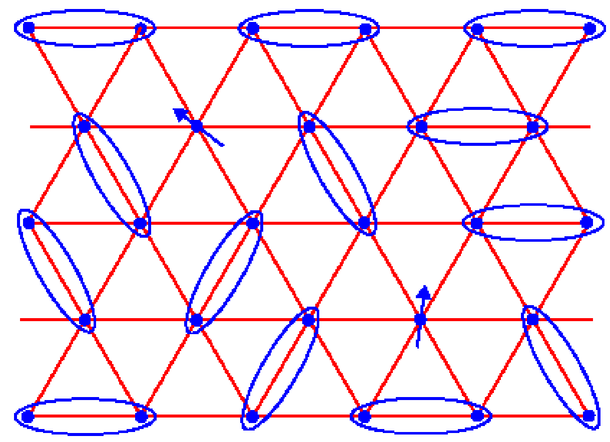
I. Order in Mott insulators

Paramagnetic states $\langle \mathbf{S}_j \rangle = 0$

Class B. Topological order and deconfined spinons



Number of valence bonds cutting line is conserved modulo 2 – this is described by the same Z_2 gauge theory as non-collinear spins



RVB state with free spinons

P. Fazekas and P.W. Anderson, *Phil Mag* **30**, 23 (1974).

D.S. Rokhsar and S. Kivelson, *Phys. Rev. Lett*. **61**, 2376 (1988)
N. Read and S. Sachdev, *Phys. Rev. Lett*. **66**, 1773 (1991);
R. Jalabert and S. Sachdev, *Phys. Rev*. B **44**, 686 (1991);
X. G. Wen, *Phys. Rev*. B **44**, 2664 (1991).
T. Senthil and M.P.A. Fisher, *Phys. Rev*. B **62**, 7850 (2000).

<u>Outline</u>

I. Order in Mott insulators

<u>*Magnetic order*</u>

A. Collinear spins

B. Non-collinear spins

<u>*Paramagnetic states*</u>

A. Compact U(1) gauge theory: bond order and confined spinons in $d=2$

B. Z_2 gauge theory: visons, topological order, and deconfined spinons

II. <u>Class A in d=2</u>

The cuprates

III. Conclusions

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 in class A

2. Collinear magnetic order (CM)

3. Bond order (B)

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

Evidence cuprates are in class A

Evidence cuprates are in class A

- Neutron scattering shows collinear magnetic order co-existing with superconductivity

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

Evidence cuprates are in class A

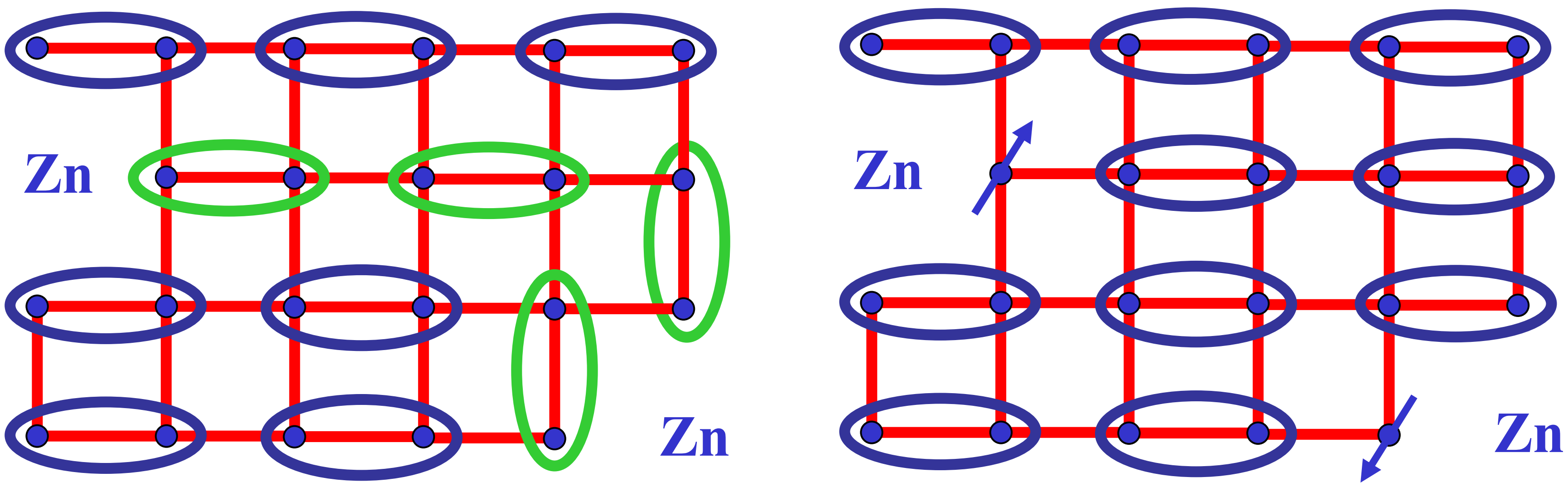
- Neutron scattering shows collinear magnetic order co-existing with superconductivity
- Proximity of Z_2 Mott insulators requires stable *hc/e* vortices, vison gap, and Senthil flux memory effect

S. Sachdev, *Physical Review* B **45**, 389 (1992)
N. Nagaosa and P.A. Lee, *Physical Review* B **45**, 966 (1992)
T. Senthil and M. P. A. Fisher, *Phys. Rev. Lett.* **86**, 292 (2001).
D. A. Bonn, J. C. Wynn, B. W. Gardner, Y.-J. Lin, R. Liang, W. N. Hardy, J. R. Kirtley, and K. A. Moler, *Nature* **414**, 887 (2001).
J. C. Wynn, D. A. Bonn, B. W. Gardner, Y.-J. Lin, R. Liang, W. N. Hardy, J. R. Kirtley, and K. A. Moler, *Phys. Rev. Lett.* **87**, 197002 (2001).

Evidence cuprates are in class A

- Neutron scattering shows collinear magnetic order co-existing with superconductivity
- Proximity of Z_2 Mott insulators requires stable *hc/e* vortices, vison gap, and Senthil flux memory effect
- Non-magnetic impurities in underdoped cuprates acquire a S=1/2 moment

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

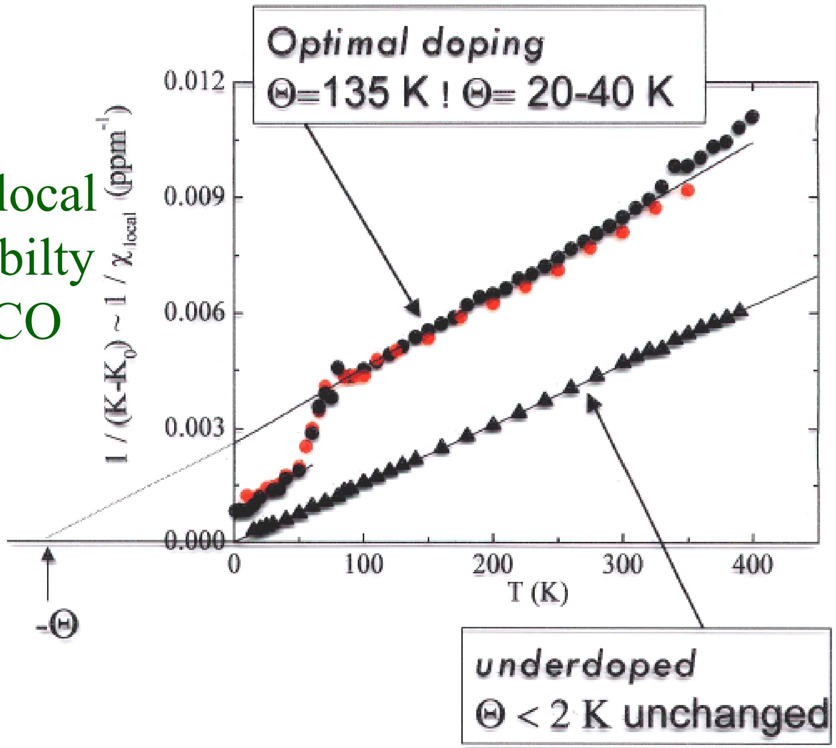


Spinon confinement implies that free S=1/2 moments form near each impurity

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

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

Evidence cuprates are in class A

- Neutron scattering shows collinear magnetic order co-existing with superconductivity
- Proximity of Z_2 Mott insulators requires stable *hc/e* vortices, vison gap, and Senthil flux memory effect
- Non-magnetic impurities in underdoped cuprates acquire a S=1/2 moment

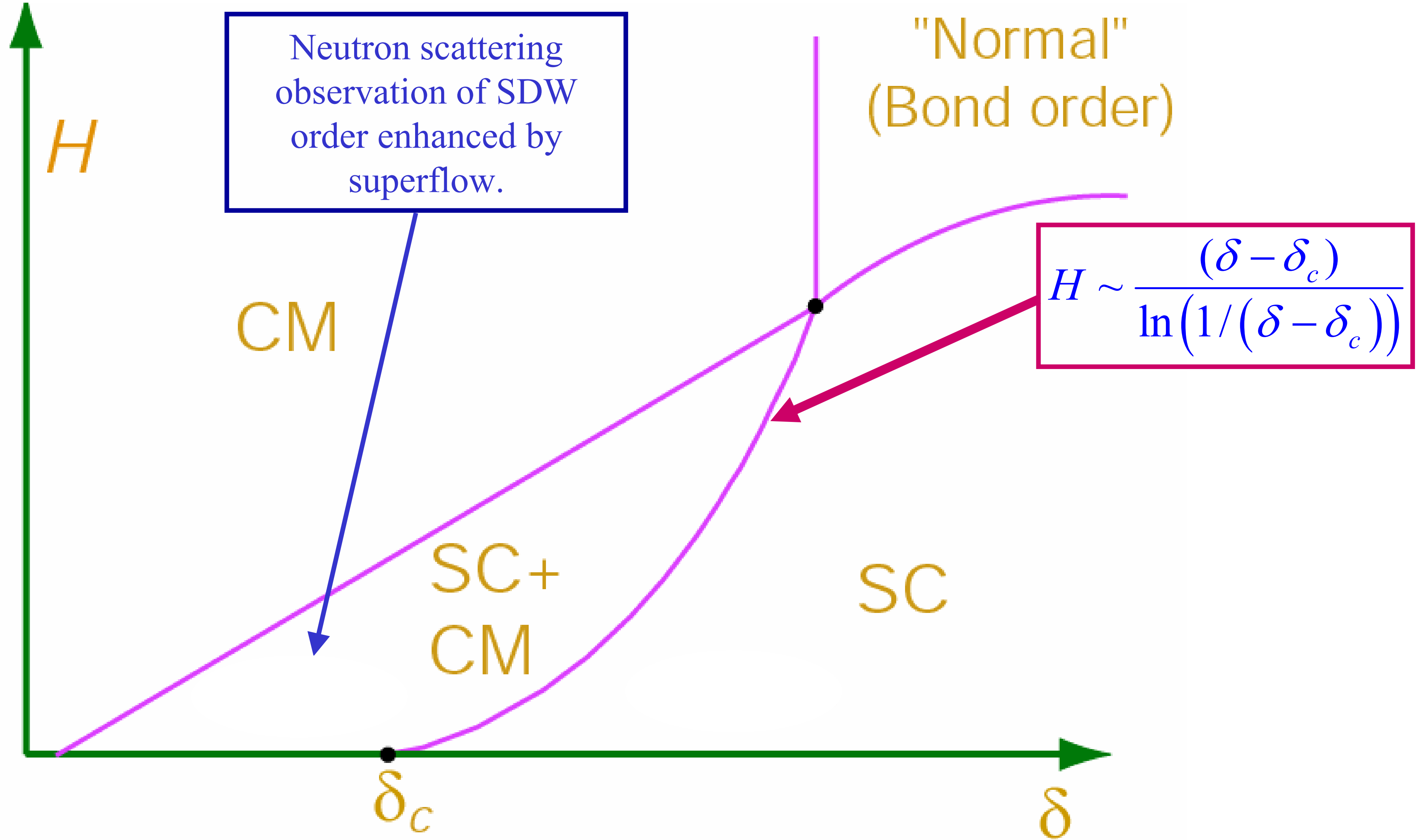
Evidence cuprates are in class A

- Neutron scattering shows collinear magnetic order co-existing with superconductivity
- Proximity of Z_2 Mott insulators requires stable *hc/e* vortices, vison gap, and Senthil flux memory effect
- Non-magnetic impurities in underdoped cuprates acquire a $S=1/2$ moment
- Tests of phase diagram in a magnetic field

Superflow kinetic energy $\left\langle v_s^2 \right\rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H} \Rightarrow \delta_{\text{eff}}\left(H\right) = \delta - C \frac{H}{H_{c2}} \ln\left(\frac{3H_{c2}}{H}\right)$

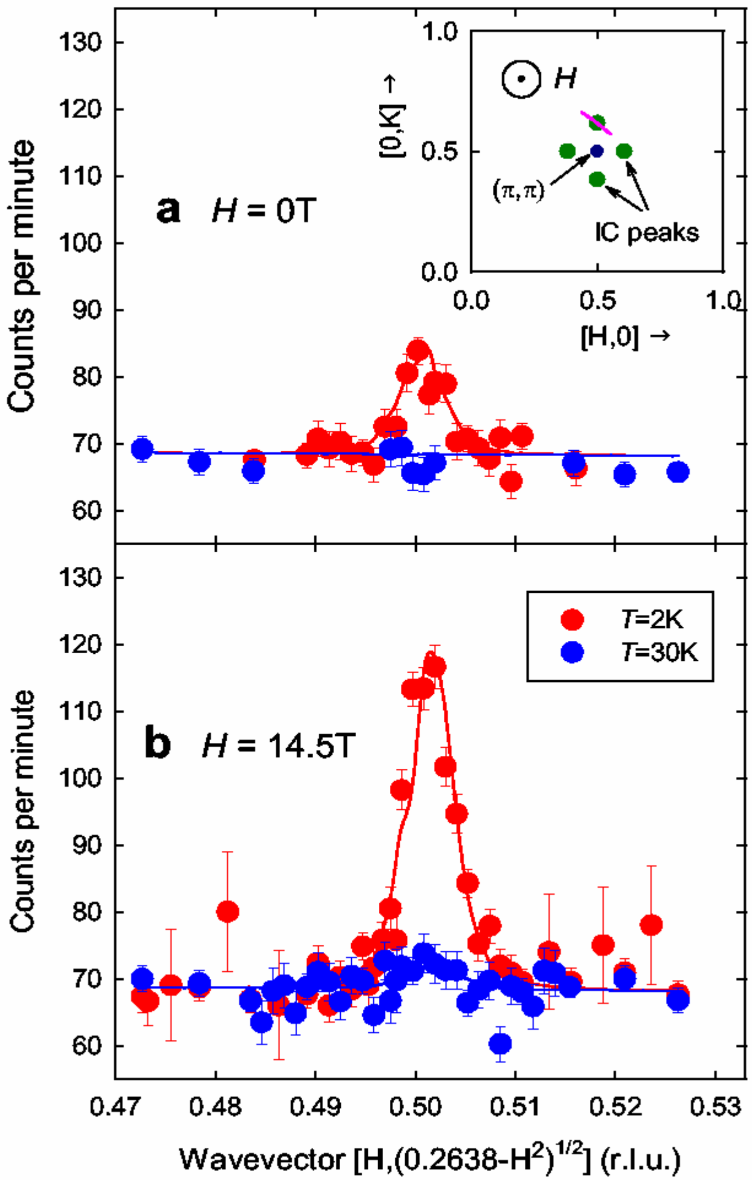
E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

Superflow kinetic energy $\left\langle v_s^2 \right\rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H} \Rightarrow \delta_{\text{eff}}(H) = \delta - C \frac{H}{H_{c2}} \ln\left(\frac{3H_{c2}}{H}\right)$

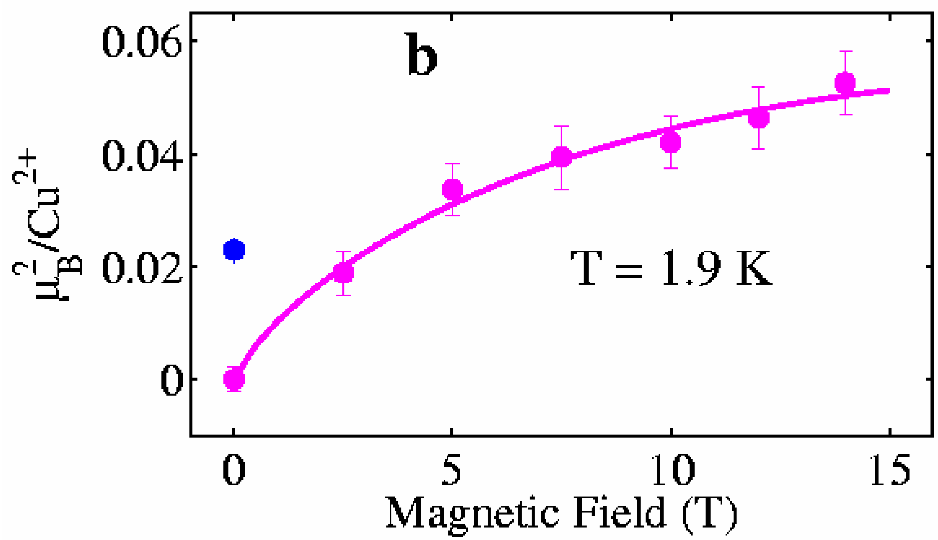


E. Demler, S. Sachdev, and Ying Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).

Neutron scattering of $La_{2-x}Sr_xCuO_4$ at x=0.1



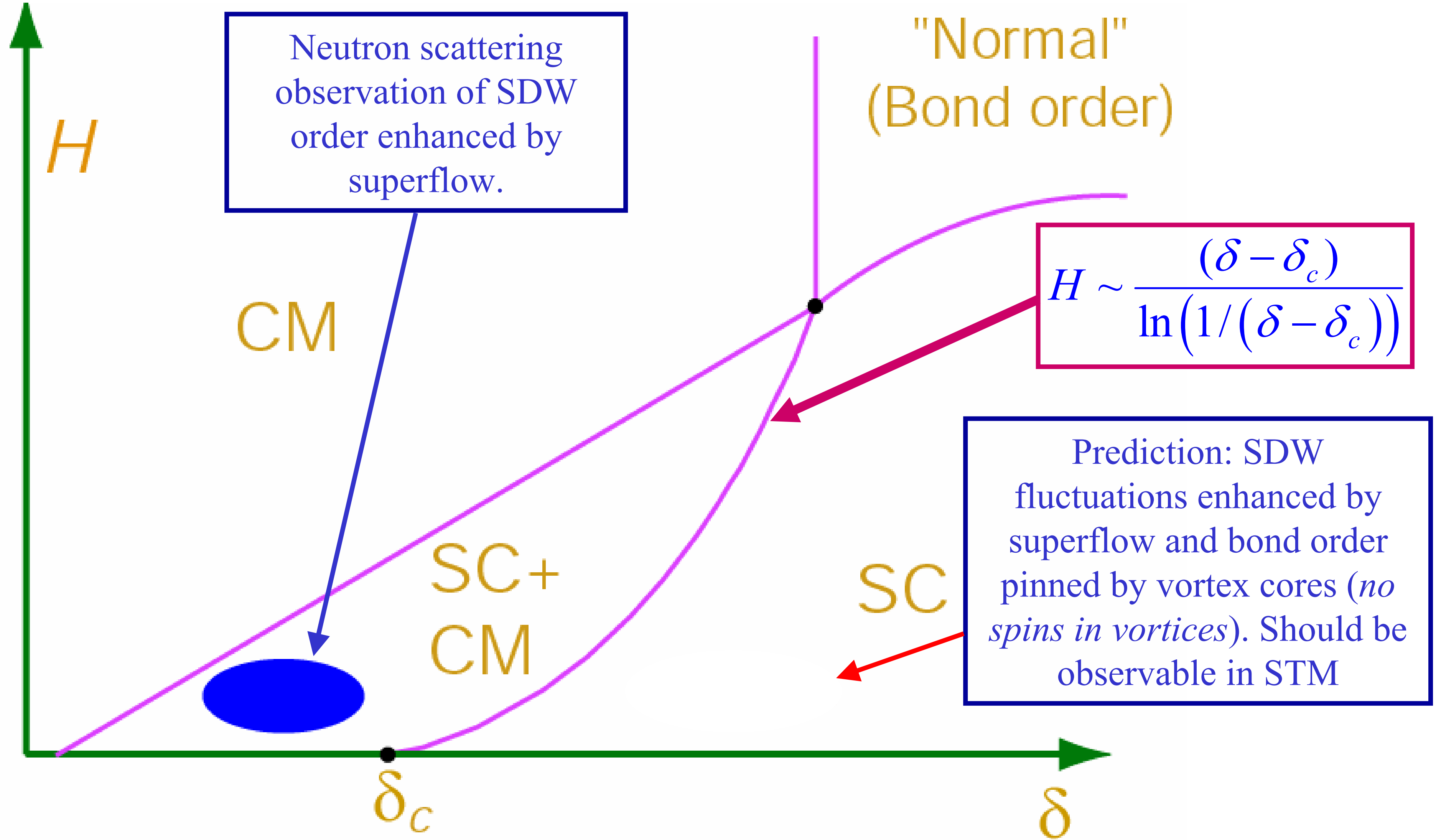
B. Lake, H. M. Rønnow, N. B. Christensen, G. Aeppli, K. Lefmann, D. F. McMorrow, P. Vorderwisch, P. Smeibidl, N. Mangkorntong, T. Sasagawa, M. Nohara, H. Takagi, T. E. Mason, *Nature*, **415**, 299 (2002).



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

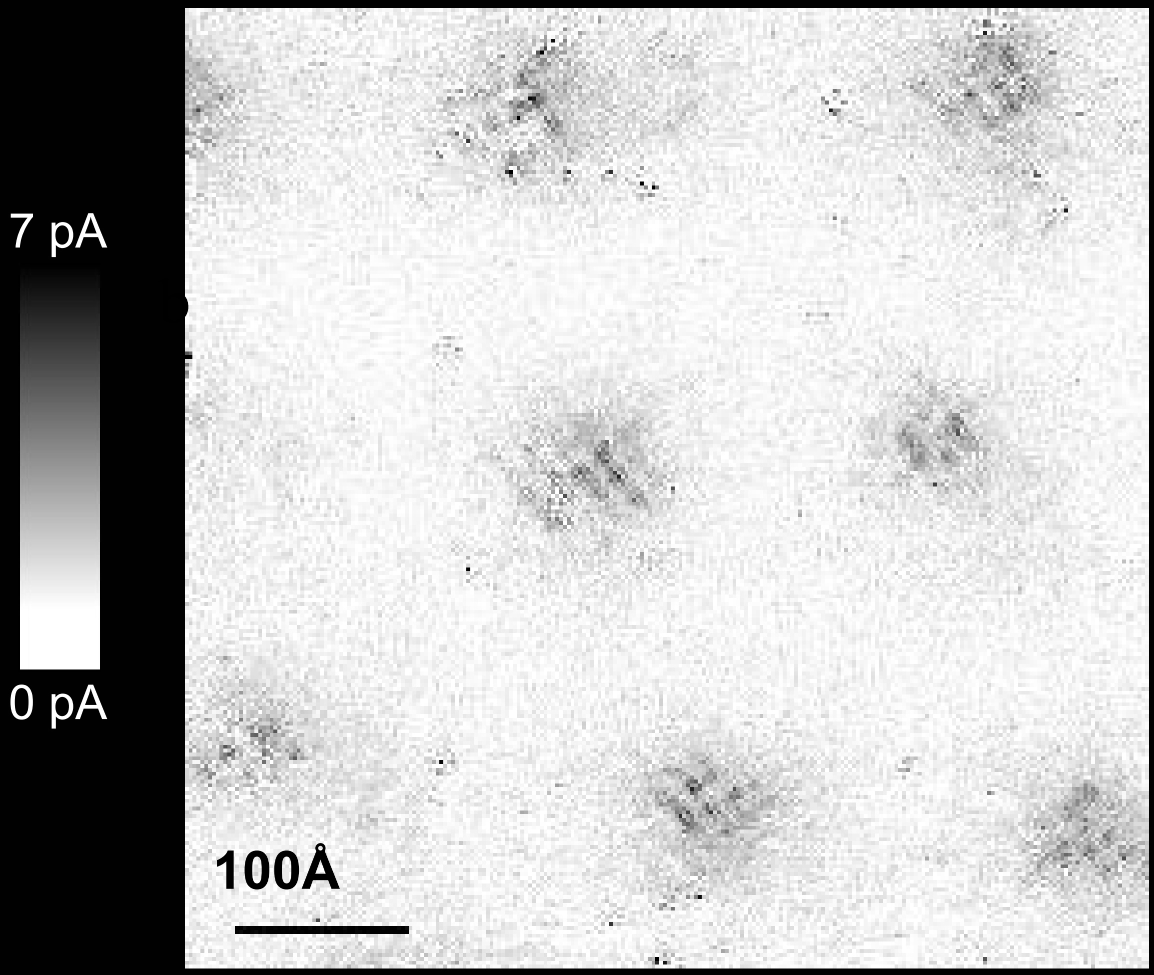
See also S. Katano, M. Sato, K. Yamada, T. Suzuki, and T. Fukase, *Phys. Rev*. B **62**, R14677 (2000).

Superflow kinetic energy $\left\langle v_s^2 \right\rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H} \Rightarrow \delta_{\text{eff}}(H) = \delta - C \frac{H}{H_{c2}} \ln\left(\frac{3H_{c2}}{H}\right)$



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

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

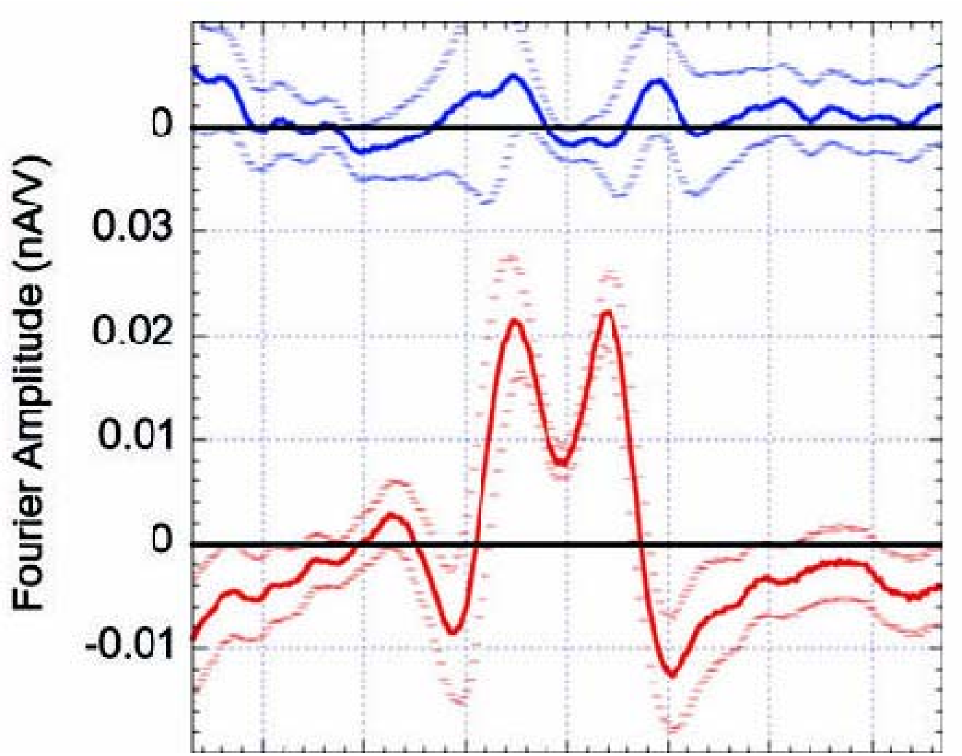


J. Hoffman E. W. Hudson, K. M. Lang,
V. Madhavan, S. H. Pan, H. Eisaki, S. Uchida,
and J. C. Davis, *Science* 295, 466 (2002).

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

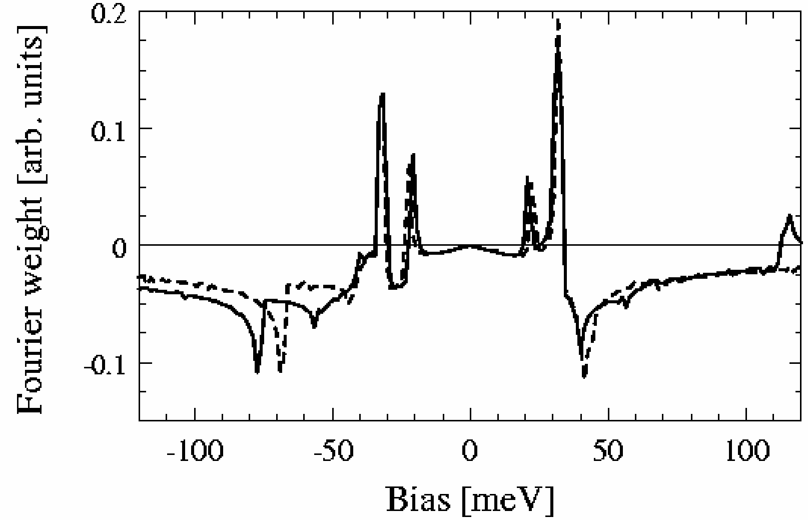
See also:
S. A. Kivelson, E. Fradkin,
V. Oganesyan, I. P. Bindloss,
J. M. Tranquada,
A. Kapitulnik, and
C. Howald,
cond-mat/0210683.

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



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).



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

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

Conclusions

I. Two classes of Mott insulators:

(A) Collinear spins, compact U(1) gauge theory;
bond order and confinements of spinons in d=2

(B) Non-collinear spins, Z_2 gauge theory

II. Doping Class A in d=2

Magnetic/bond order co-exist with superconductivity at low doping

Cuprates most likely in this class.

Theory of quantum phase transitions provides a description of "fluctuating order" in the superconductor.