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)

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

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Strategy for analyzing correlated electron systems

(cuprate superconductors, heavy fermion compounds ……..)

Standard paradigms of solid state physics (Bloch theory of metals, Landau Fermi liquid theory, BCS theory of electron pairing near Fermi surfaces) are very poor starting points.

So…….

Start from the point where the break down on Bloch theory is complete--- the Mott insulator.

Classify ground states of Mott insulators using conventional and topological order parameters.

Correlated electron systems are described by phases and quantum phase transitions associated with order parameters of Mott insulator and the "orders" of Landau/BCS theory. Expansion away from quantum critical points allows description of states in which the order of Mott insulator is "fluctuating".

<u>Outline</u>

I. **<u>Order in Mott insulators</u>**

<u>Magnetic order</u>

A. Collinear spins

B. Non-collinear spins

<u>Paramagnetic states</u>

A. Bond order and confined spinons

B. Topological order and deconfined spinons

II. Doping Mott insulators with collinear spins and bond order

A global phase diagram and applications to the cuprates

III. Doping Mott insulators with non-collinear spins and topological order

(A) A small Fermi surface state.

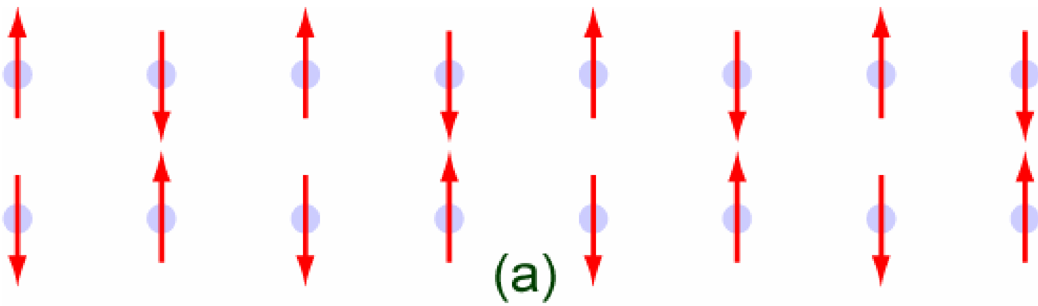
(B) Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-piercing arguments

IV. Conclusions

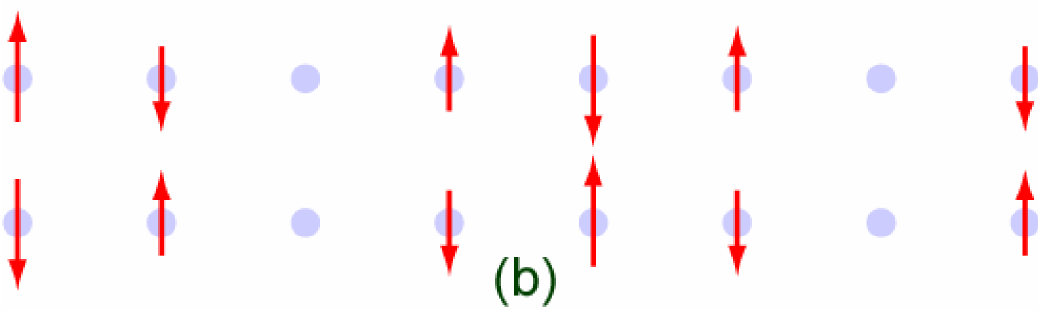
I. Order in Mott insulators

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

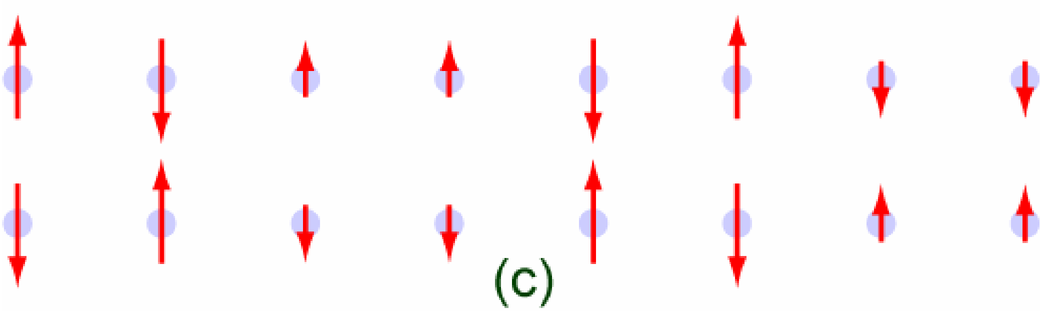
A. Collinear spins



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



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



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

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

I. Order in Mott insulators

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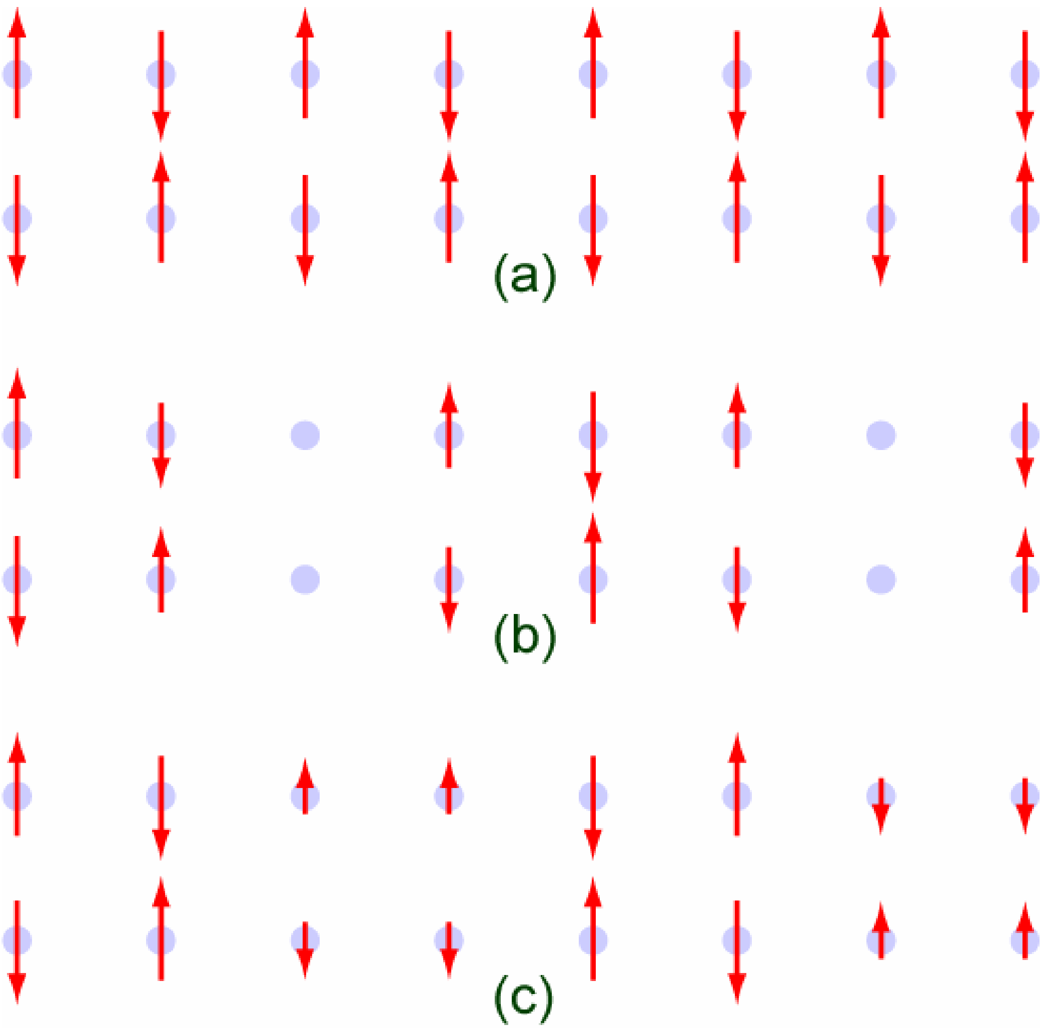
A. Collinear spins



Key property

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

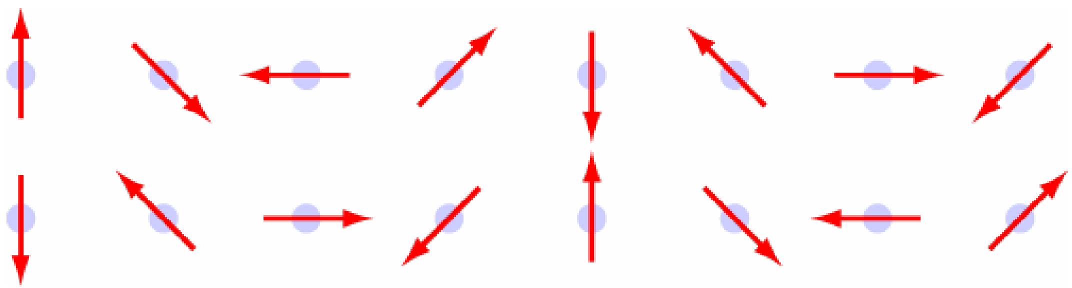
Quantum fluctuations leading to loss of magnetic order should produce a paramagnetic state with a vector (S=1) quasiparticle excitation.

I. Order in Mott insulators

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

B. Noncollinear spins

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



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

$\mathbf{N}_2^2 = \mathbf{N}_1^2 \, , \, \mathbf{N}_1 . \mathbf{N}_2 = 0$

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

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

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

This spinor could become a S=1/2 spinon in a quantum "disordered" state.

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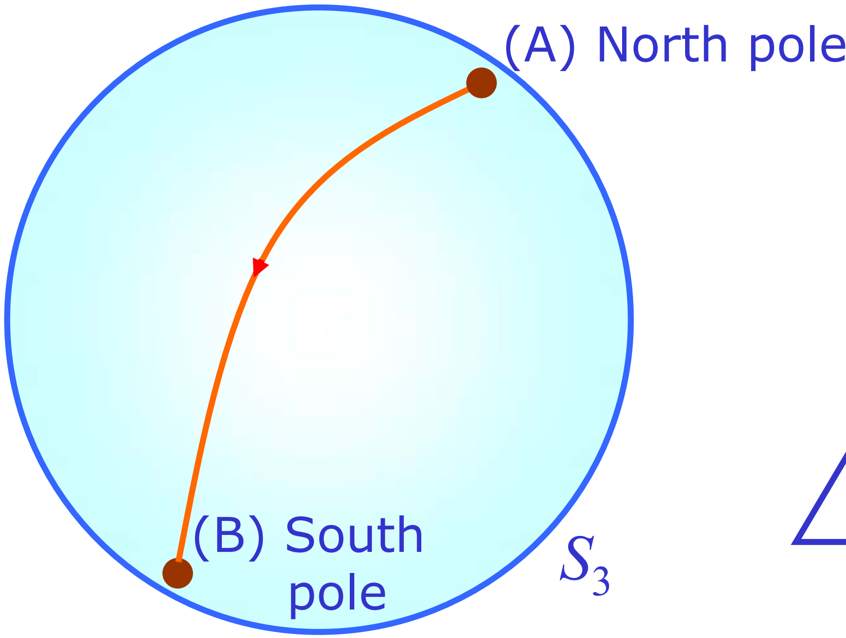
B. Noncollinear spins

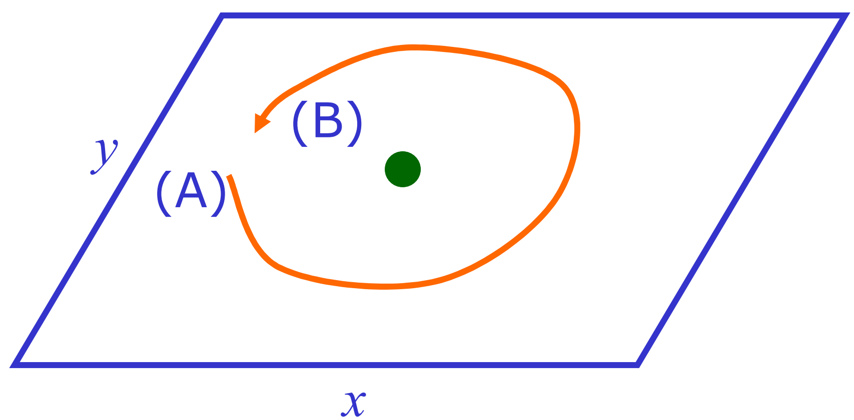
$$\mathbf{N}_1 + i\mathbf{N}_2 = \begin{pmatrix} z_\downarrow^2 - z_\uparrow^2 \\ i\left(z_\downarrow^2 + z_\uparrow^2\right) \\ 2 z_\uparrow z_\downarrow \end{pmatrix}$$

Order parameter space: S_3 / Z_2

Physical observables are invariant under the Z_2 gauge transformation $z_a \to \pm z_a$

Vortices associated with $\pi_1(S_3/Z_2)=Z_2$





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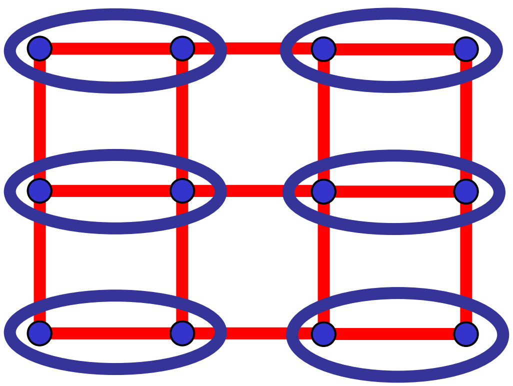
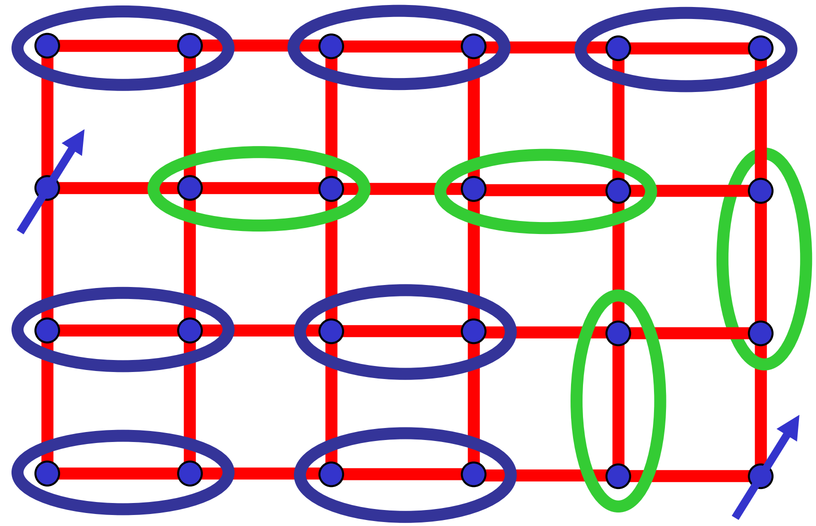
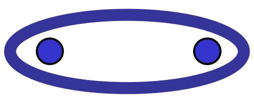
I. Order in Mott insulators

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

A. Bond order and spin excitons







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

S=1/2 spinons are ***confined***
by a linear potential into a
S=1 spin exciton

Such a state is obtained by quantum-``disordering" collinear state with $\vec{K} = (\pi, \pi)$:
fluctuating $\boldsymbol{N}$ becomes the S=1 spin exciton and Berry phases induce bond order

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

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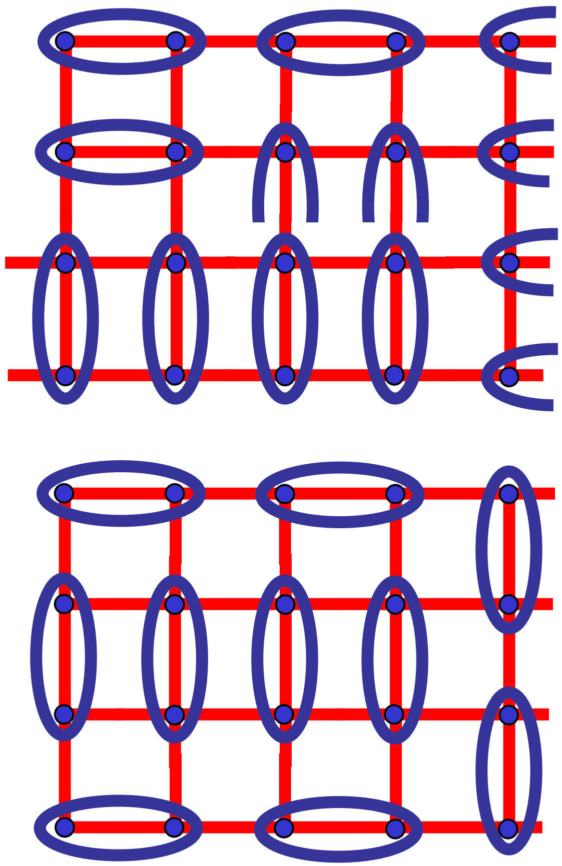
A. Bond order and spin excitons



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.

I. Order in Mott insulators

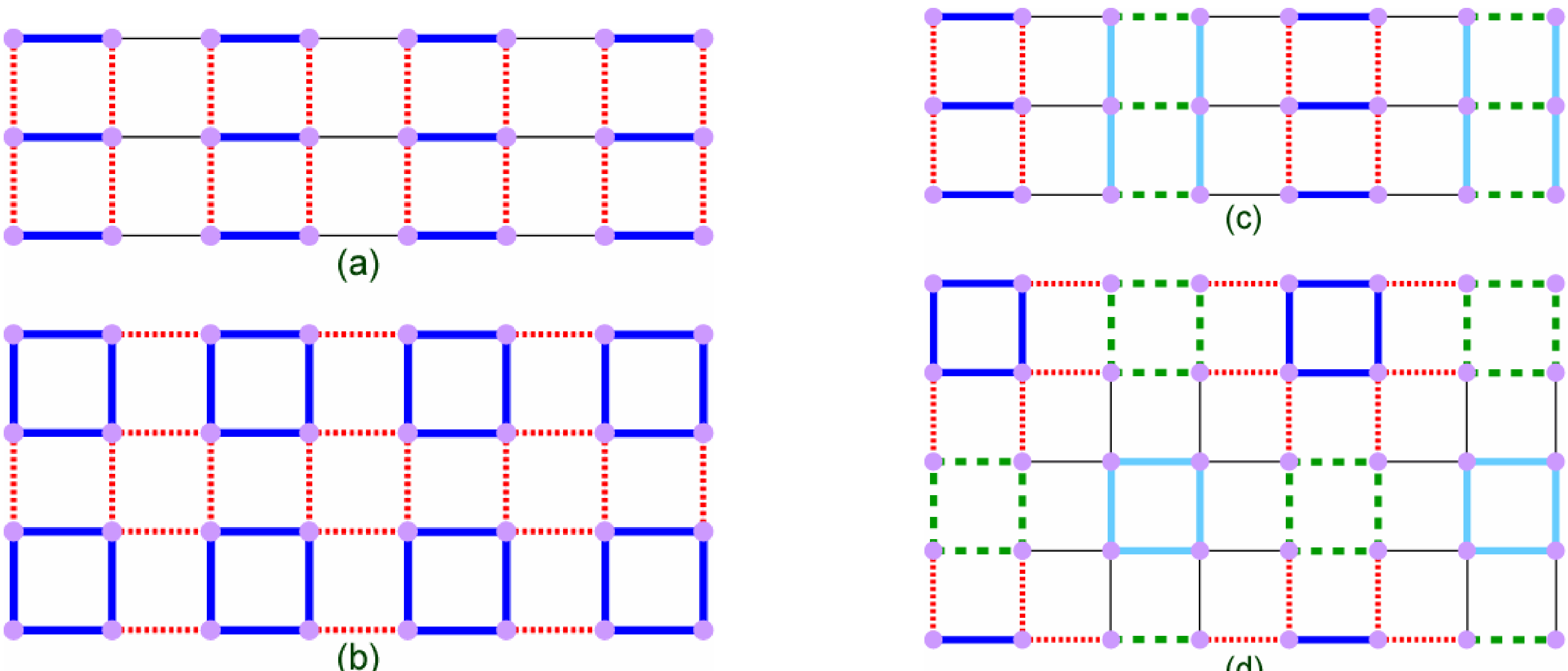
Paramagnetic states $\left\langle \boldsymbol{S}_j \right\rangle = 0$

A. Bond order and spin excitons

Bond order is defined as a modulation in $Q_a(\boldsymbol{r}_i) \equiv \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+a}$

Note that $\left\langle Q_0(\boldsymbol{r}) \right\rangle$ is a measure of site charge density.

Bond order patterns with coexisting *d*-wave-like superconductivity:

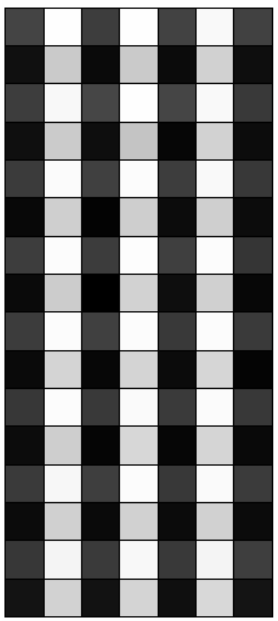


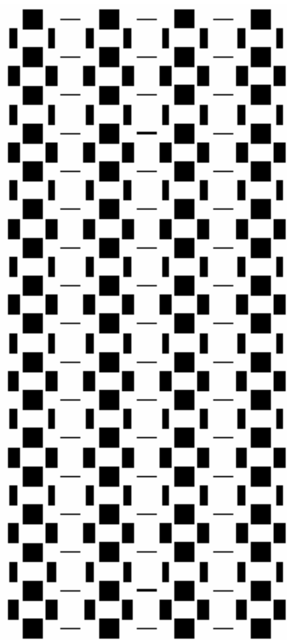
S. Sachdev and N. Read, *Int. J. Mod. Phys.* B **5**, 219 (1991).
M. Vojta and S. Sachdev, *Phys. Rev. Lett.* **83**, 3916 (1999); M. Vojta, *Phys. Rev.* B **66**, 104505 (2002)

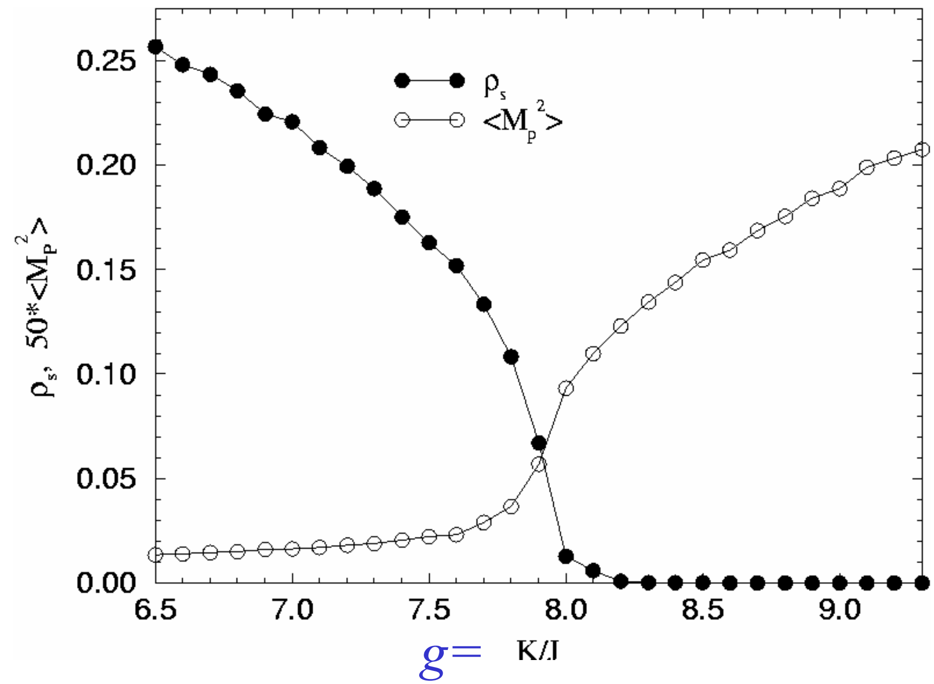
Bond order in a frustrated *S=1/2* XY magnet

A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, cond-mat/0205270

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







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

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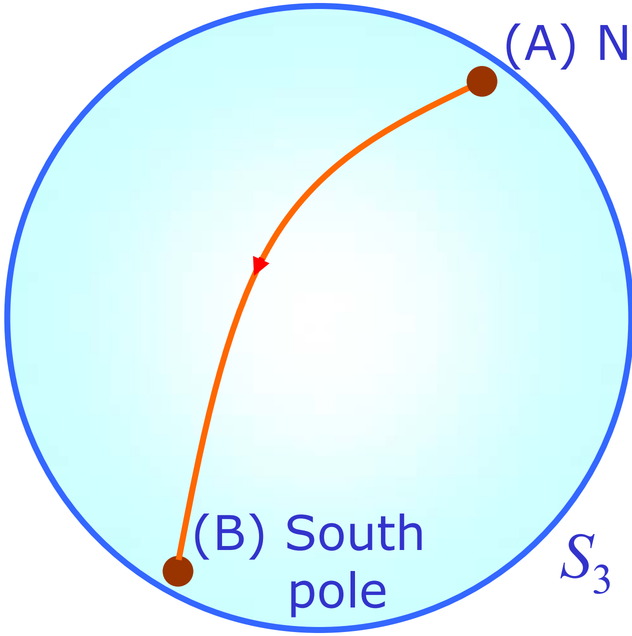
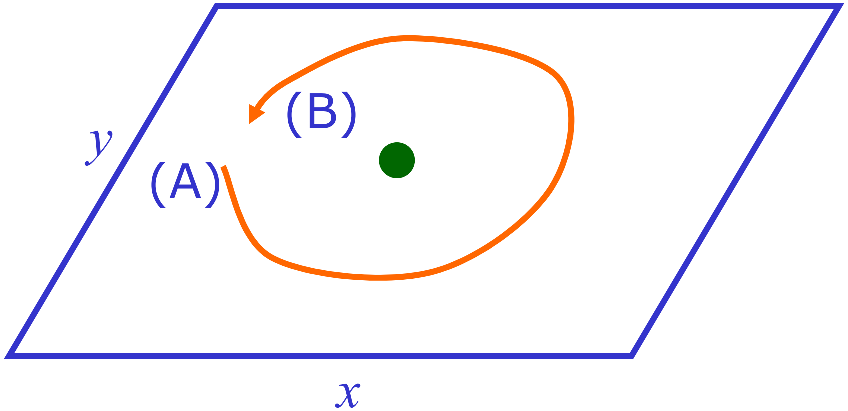
Paramagnetic states $\langle \boldsymbol{S}_j \rangle = 0$

B. Topological order and deconfined spinons

Vortices associated with $\pi_1(S_3/Z_2)=Z_2$ (*visons*)





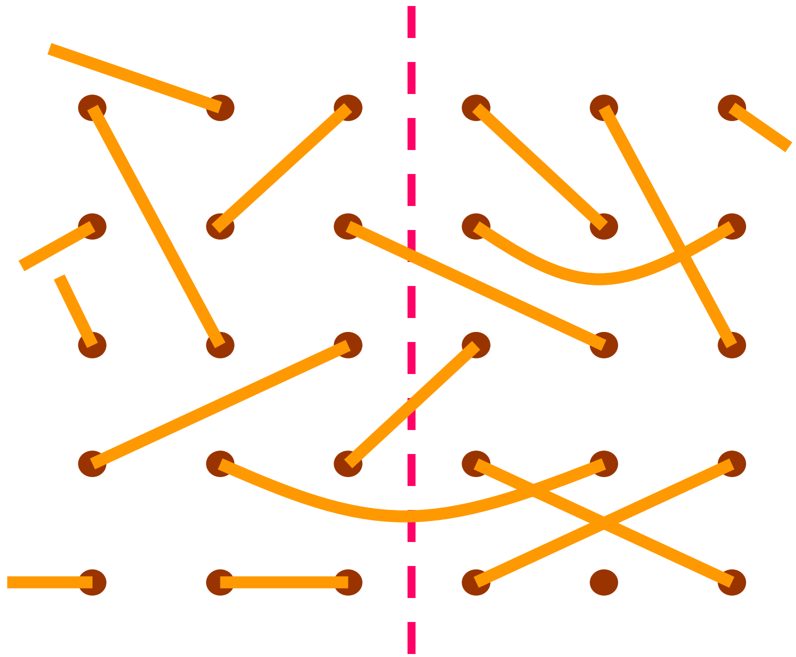
Such vortices (visons) can also be defined in the phase in which spins are "quantum disordered". A vison gap implies that sign of z_a can be globally defined: this is the RVB state with S=1/2 spinons,

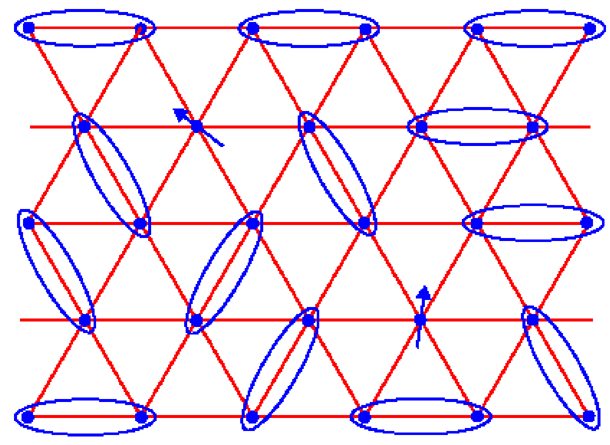
N. Read and S. Sachdev, *Phys. Rev. Lett.* **66**, 1773 (1991)

I. Order in Mott insulators

Paramagnetic states $\left\langle \boldsymbol{S}_j \right\rangle = 0$

B. Topological order and deconfined spinons





RVB state with free spinons

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

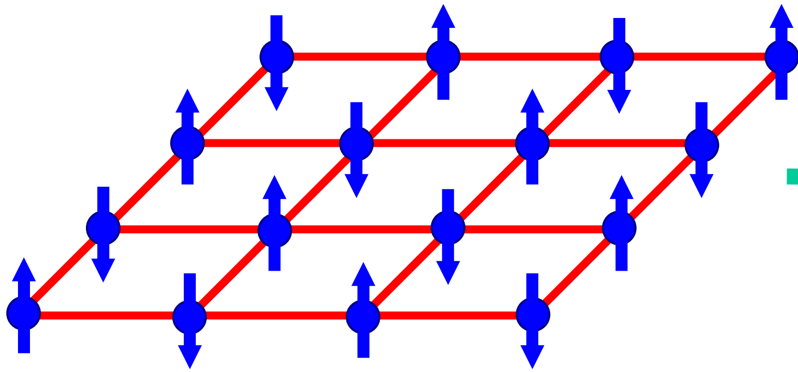
Number of valence bonds cutting line is conserved modulo 2 – this is described by the same Z_2 gauge theory as non-collinear spins

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).

Orders of Mott insulators in two dimensions

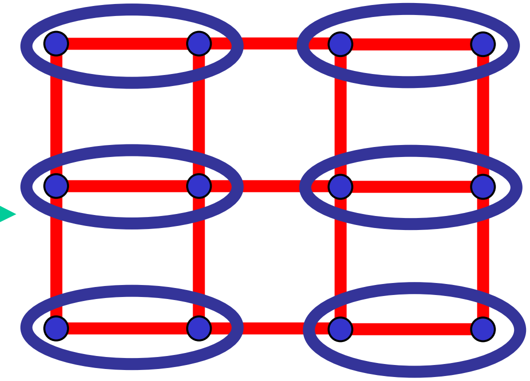
N. Read and S. Sachdev, *Phys. Rev. Lett.* **66**, 1773 (1991); S.S. and N.R. *Int. J. Mod. Phys.* B **5**, 219 (1991).

A. Collinear spins, Berry phases, and bond order



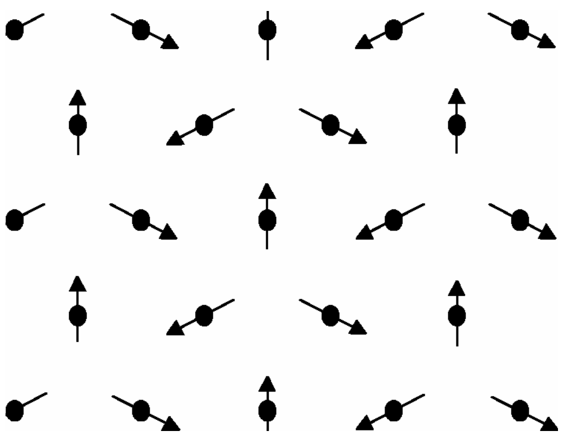
Néel ordered state

Quantum transition restoring spin rotation invariance



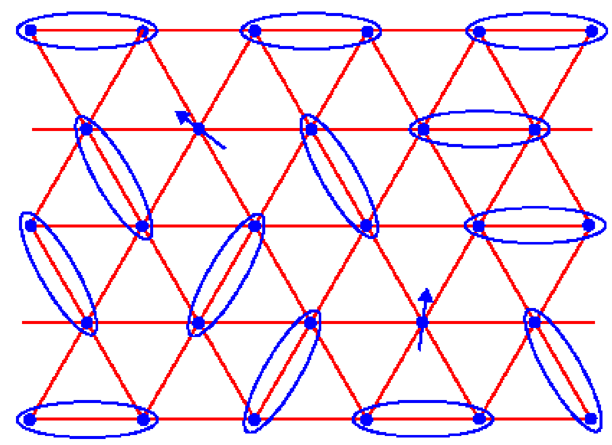
Bond order and $S=1$ spin exciton

B. Non-collinear spins and deconfined spinons.



Non-collinear ordered antiferromagnet

Quantum transition restoring spin rotation invariance



Topological order: RVB state with Z_2 gauge visons, $S=1/2$ spinons

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(A) A small Fermi surface state.

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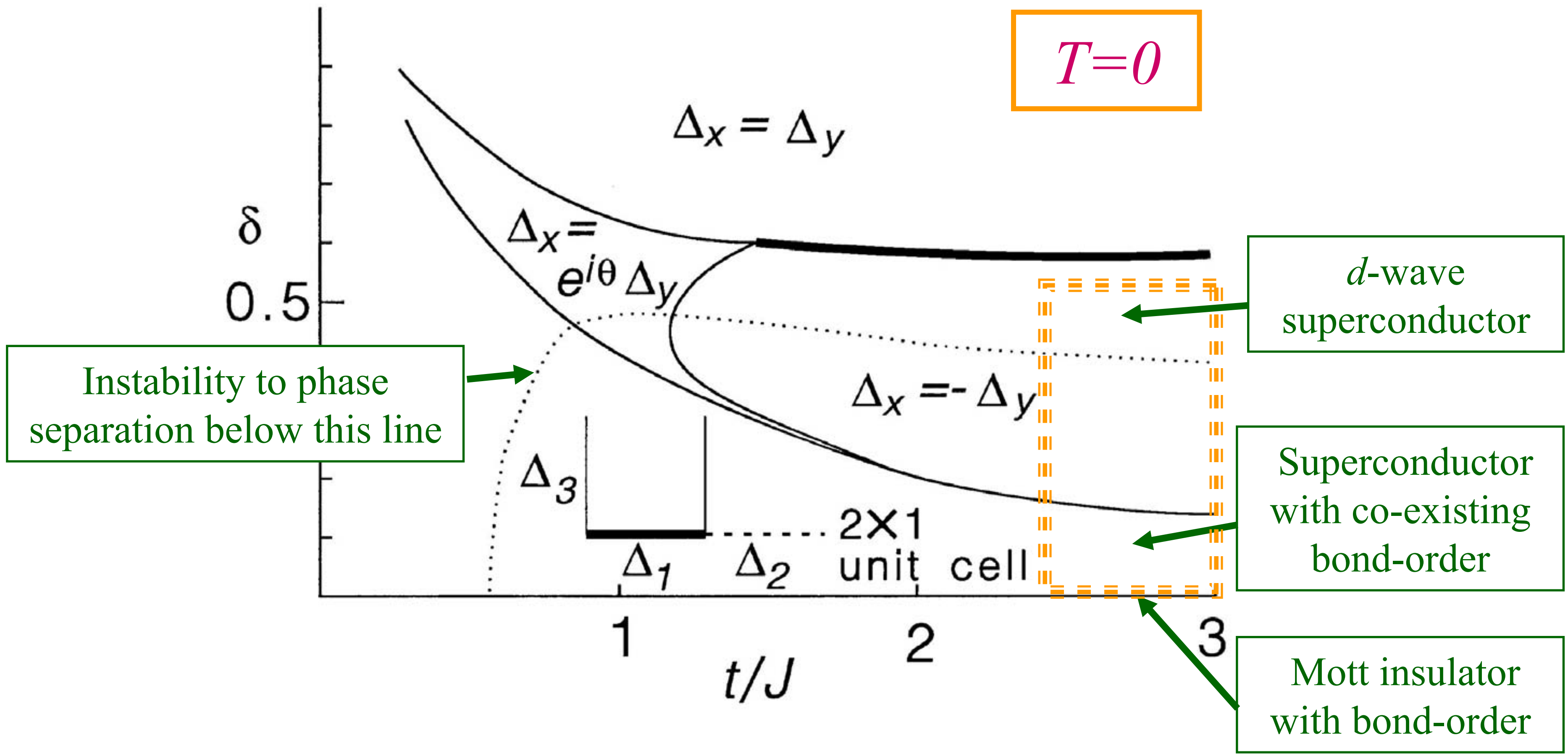
II. Doping Mott insulators with collinear spins and bons order

Doping a paramagnetic bond-ordered Mott insulator

systematic Sp(*N*) theory of translational symmetry breaking, while preserving spin rotation invariance.

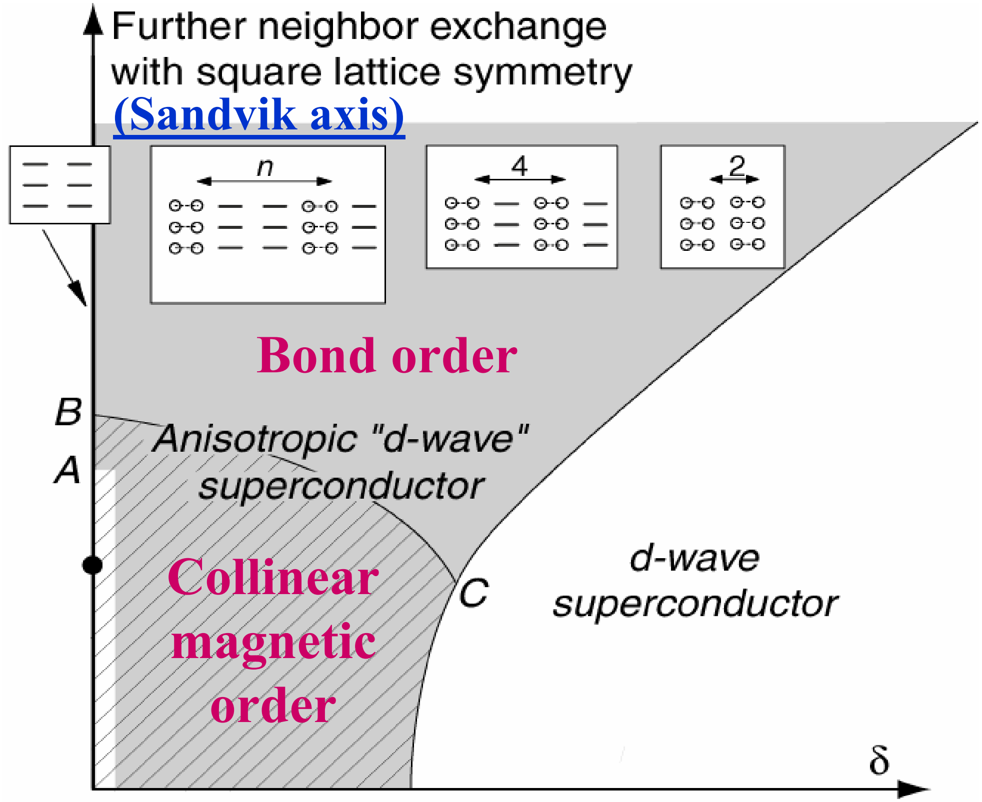


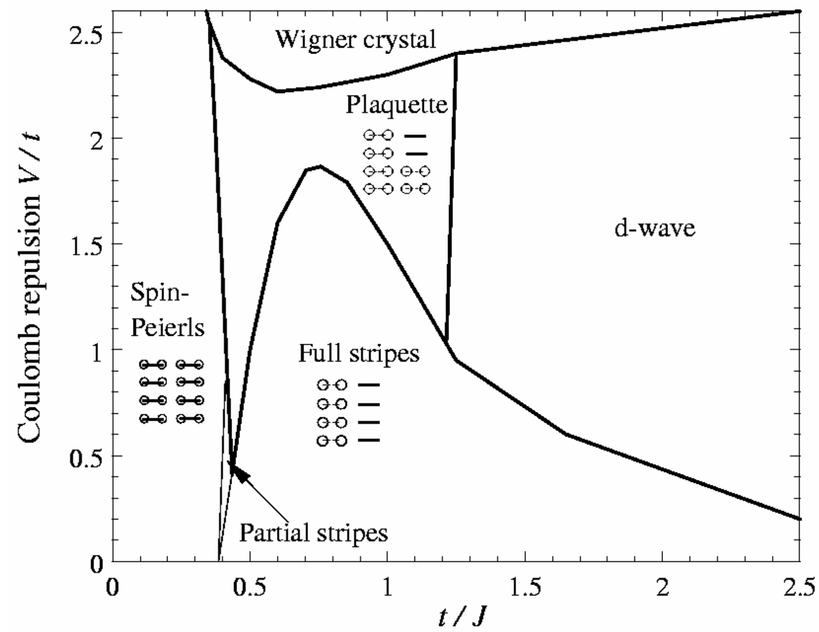
S. Sachdev and N. Read, *Int. J. Mod. Phys.* B **5**, 219 (1991).

II.Global phase diagram

Include long-range Coulomb interactions: frustrated phase separation

V.J. Emery, S.A. Kivelson, and H.Q. Lin, *Phys. Rev. Lett*. **64**, 475 (1990).



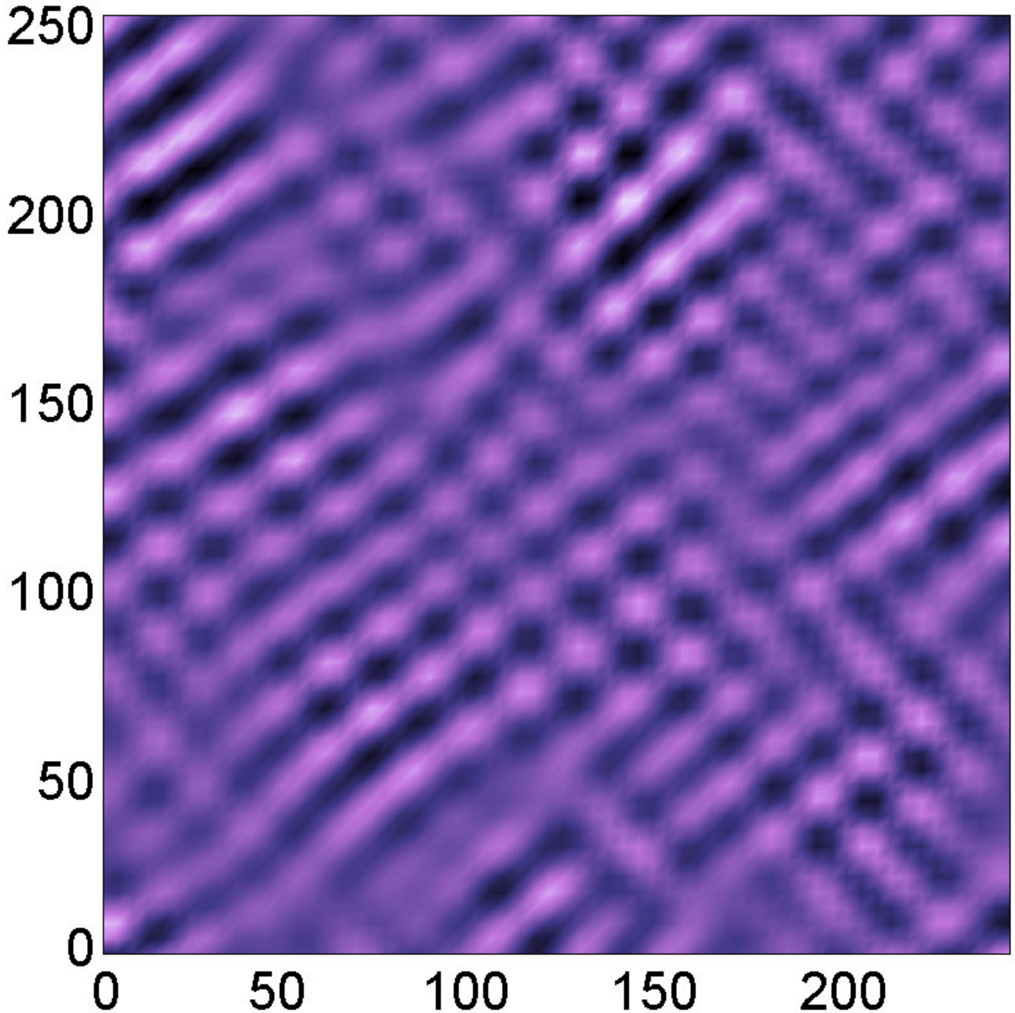


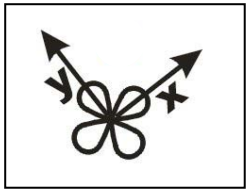
Hatched region --- static spin order
Shaded region ---- static bond/charge order

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

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

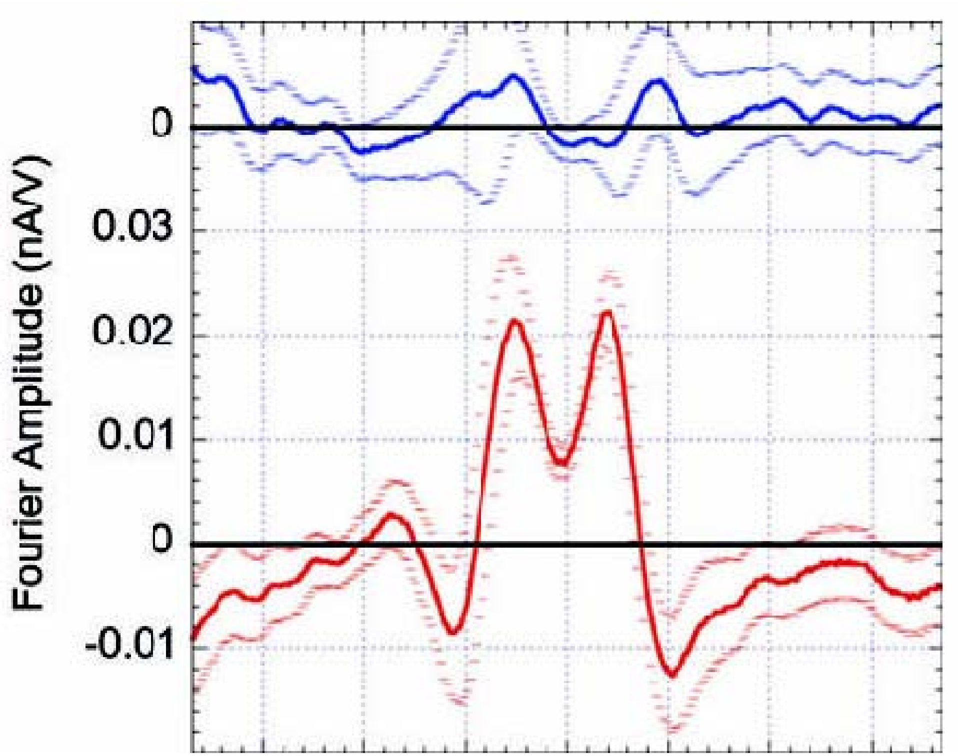




Period = 4 lattice spacings

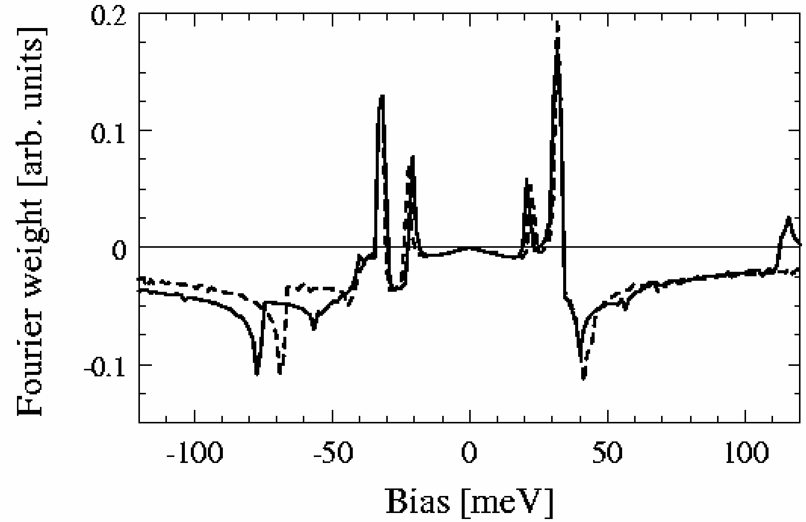
C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, cond-mat/0201546

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

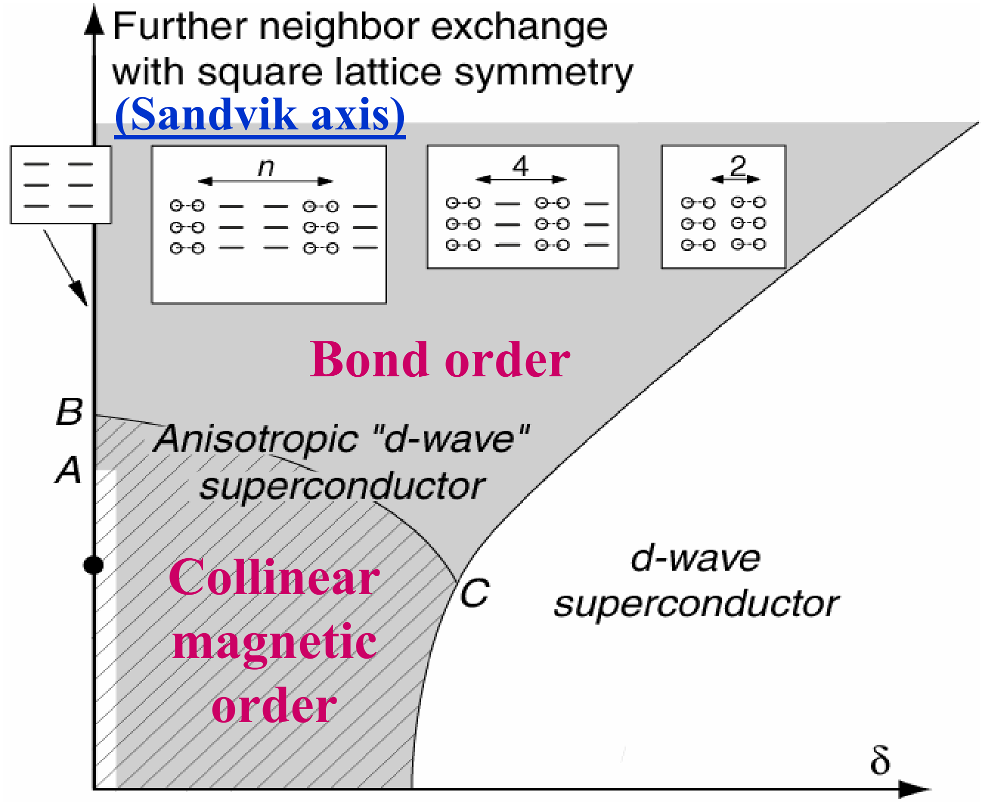
C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, cond-mat/0201546



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, cond-mat/0204011;
D. Zhang cond-mat/0210386

II.Global phase diagram

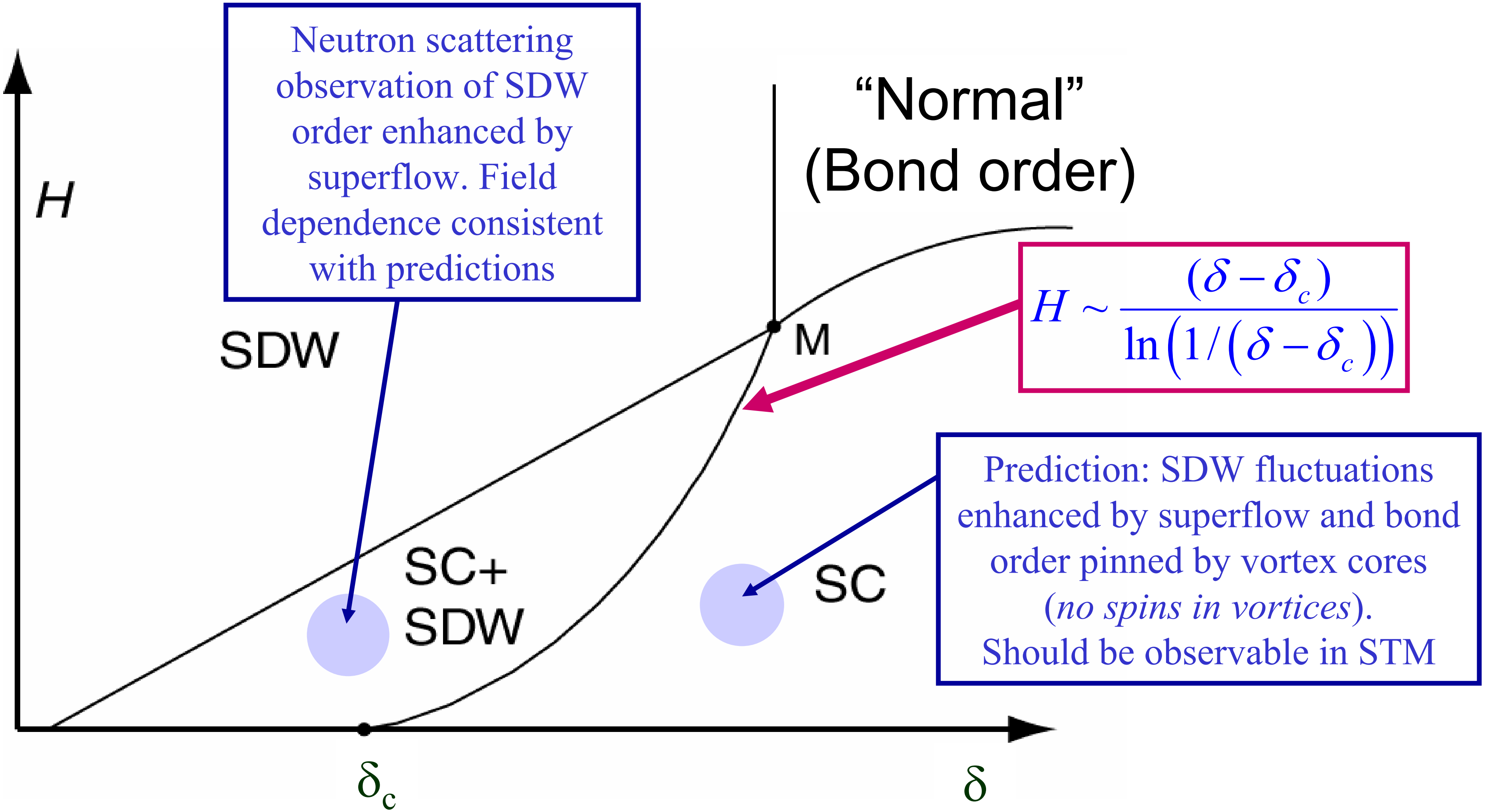


An applied magnetic field suppresses superconductivity

$$\propto \frac{H}{H_{c2}} \ln\left(\frac{H_{c2}}{H}\right)$$

Vertical axis can be tuned by varying *H*

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



K. Park and S. Sachdev *Phys. Rev.* B **64**, 184510 (2001).
E. Demler, S. Sachdev, and Y. Zhang, *Phys. Rev. Lett.* **87**, 067202 (2001).
Y. Zhang, E. Demler and S. Sachdev, *Phys. Rev.* B **66,** 094501 (2002).

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IV. Conclusions

III. Doping topologically ordered Mott insulators (RVB)

A likely possibility:

Added electrons do *not* fractionalize, but retain their bare quantum numbers.
Spinons and vison states of the insulator survive unscathed.
There is a Fermi surface of *sharp electron-like* quasiparticles, enclosing a volume determined by the dopant electron alone.

This is a "Fermi liquid" state which violates Luttinger's theorem

A "small" Fermi surface

T. Senthil, S. Sachdev, and M. Vojta, cond-mat/0209144

Luttinger's theorem on a d-dimensional lattice

For simplicity, we consider systems with SU(2) spin rotation invariance, which is preserved in the ground state.

Let v_0 be the volume of the unit cell of the ground state,
n_T be the total number density of electrons per volume v_0.
(need not be an integer)

Then, in a metallic Fermi liquid state with a sharp electron-like Fermi surface:

$$2 \times \frac{v_0}{(2\pi)^d} \left(\text{Volume enclosed by Fermi surface} \right)$$

$$= n_T \left(\text{mod } 2 \right)$$

A "large" Fermi surface

Our claim

There exist "topologically ordered" ground states in dimensions $d > 1$ with a Fermi surface of **sharp** electron-like quasiparticles for which

$$2 \times \frac{v_0}{(2\pi)^d} \left(\text{Volume enclosed by Fermi surface} \right)$$

$$= (n_T - 1) (\text{mod } 2)$$

A "small" Fermi surface

Kondo lattice models

Model Hamiltonian for intermetallic compound with conduction electrons, $c_{i\sigma}$, and localized orbitals, $f_{i\sigma}$

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i \left(V c_{i\sigma}^\dagger f_{i\sigma} + V f_{i\sigma}^\dagger c_{i\sigma} + \varepsilon_f \left(n_{fi\uparrow} + n_{fi\downarrow} \right) + U n_{fi\uparrow} n_{fi\downarrow} \right) + \cdots$$

$$n_{fi\sigma} = f_{i\sigma}^\dagger f_{i\sigma} \quad ; \quad n_{ci\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$$

$$n_T = n_f + n_c$$

For small U, we obtain a Fermi liquid ground state, with a "large" Fermi surface volume determined by n_T (mod 2)

This is adiabatically connected to a Fermi liquid ground state at large U, where n_f=1, and whose Fermi surface volume must also be determined by

$$n_T \text{ (mod 2)} = (1 + n_c) \text{ (mod 2)}$$

The large U limit is also described (after a Schrieffer-Wolf transformation) by a Kondo lattice model of conduction electrons $c_{i\sigma}$ and S=1/2 spins on f orbitals

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} \left(J_K c_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{i\sigma} \cdot \vec{S}_{fi} \right) + \sum_{i<j} J_H \left(i, j \right) \vec{S}_{fi} \cdot \vec{S}_{fj}$$

This can have a Fermi liquid ground state whose "large" Fermi surface volume is $(1+n_c)(\text{mod } 2)$

We show that for small J_K, a ground state with a "small" electron-like Fermi surface enclosing a volume determined by $n_c(\text{mod } 2)$ is also possible.

III.A "Small" Fermi surfaces in Kondo lattices

Kondo lattice model:

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i \left(J_K c_{i\sigma}^\dagger \vec{\tau}_{\sigma\sigma'} c_{i\sigma} \cdot \vec{S}_{fi} \right) + \sum_{i<j} J_H (i,j) \vec{S}_{fi} \cdot \vec{S}_{fj}$$

Consider, first the case J_K=0 and J_H chosen so that the spins form a *bond ordered* paramagnet

This system has a Fermi surface of conduction electrons with volume n_c (mod 2)

However, because n_f=2 (per unit cell of ground state)
$\boldsymbol{n_T = n_f + n_c = n_c}$ **(mod 2)**, and
"small" Fermi volume="large" Fermi volume
(mod Brillouin zone volume)

These statements apply also for a finite range of J_K

Conventional Luttinger Theorem holds

III.A "Small" Fermi surfaces in Kondo lattices

Kondo lattice model:

$$H = \sum_{i<j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} \left(J_K c_{i\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{i\sigma} \cdot \vec{S}_{fi} \right) + \sum_{i<j} J_H (i,j) \vec{S}_{fi} \cdot \vec{S}_{fj}$$

Consider, first the case J_K=0 and J_H chosen so that the spins form a *topologically ordered* paramagnet

This system has a Fermi surface of conduction electrons with volume n_c (mod 2)

Now n_f=1 (per unit cell of ground state)

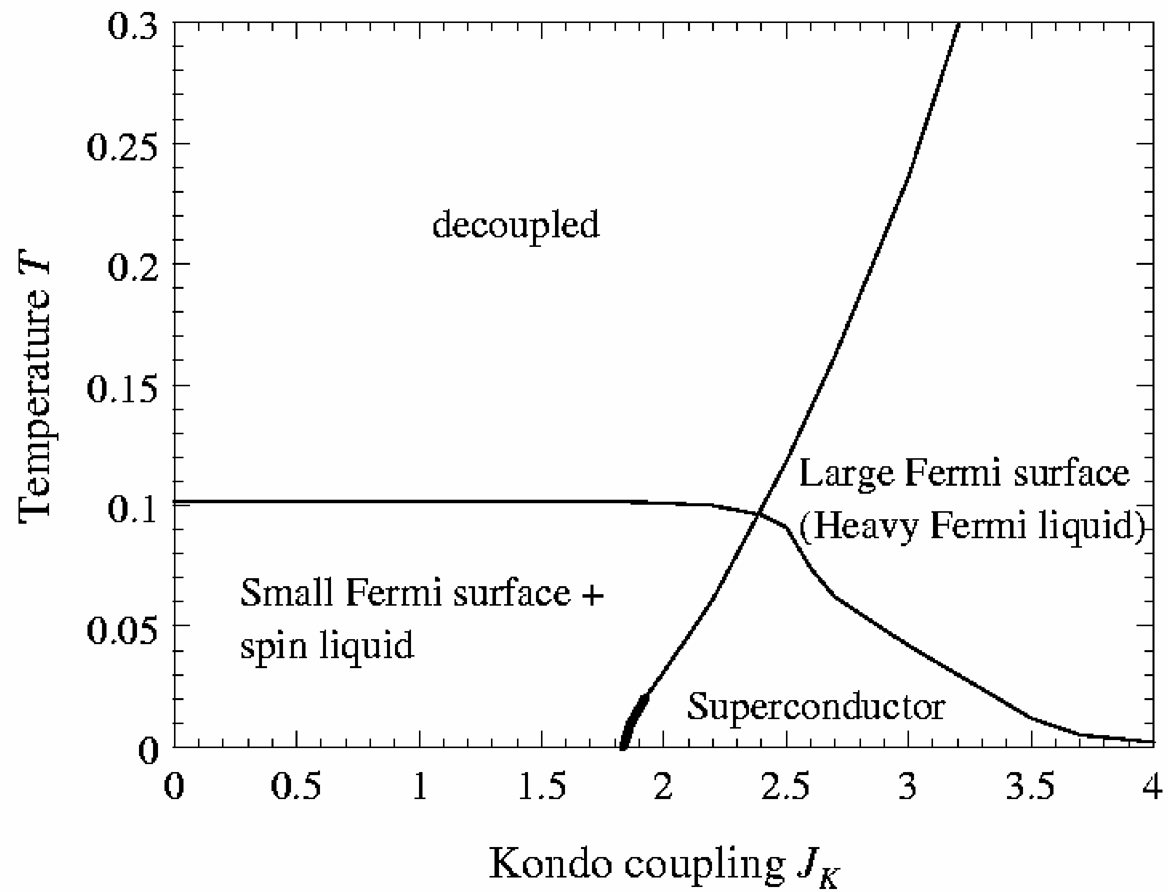
$$n_T = n_f + n_c \neq n_c \left(\text{mod } 2\right)$$

This state, and its Fermi volume, survive for a finite range of J_K

Perturbation theory is J_K is free of infrared divergences, and the topological ground state degeneracy is protected.

A "small" Fermi surface which violates conventional Luttinger theorem

Mean-field phase diagram (Sp(N), large N theory)



Pairing of spinons in small Fermi surface state induces superconductivity at the confinement transition

Small Fermi surface state can also exhibit a second-order metamagnetic transition in an applied magnetic field, associated with vanishing of a spinon gap.

Outline

I. Order in Mott insulators

Magnetic order

A. Collinear spins

B. Non-collinear spins

Paramagnetic states

A. Bond order and confined spinons

B. Topological order and deconfined spinons

II. Doping Mott insulators with collinear spins and bond order

A global phase diagram and applications to the cuprates

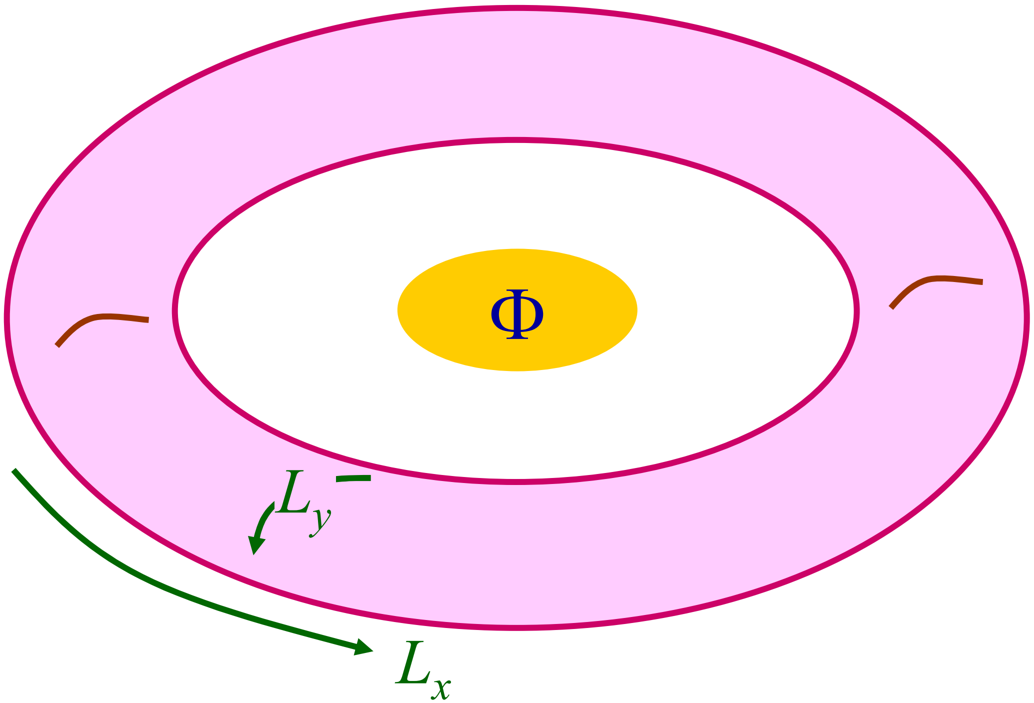
III. Doping Mott insulators with non-collinear spins and topological order

(A) A small Fermi surface state.

(B) Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-piercing arguments.

IV. Conclusions

III.B Lieb-Schultz-Mattis-Laughlin-Bonesteel-Affleck-Yamanaka-Oshikawa flux-piercing arguments



Unit cell a_x, a_y.
L_x/a_x, L_y/a_y
coprime integers

Adiabatically insert flux $\Phi=2\pi$ (units $\hbar$=c=e=1) acting on $\uparrow$ electrons.

State changes from $|\Psi\rangle$ to $|\Psi'\rangle$, and $UH(0)U^{-1} = H(\Phi)$, where

$$U = \exp\left[\frac{2\pi i}{L_x}\sum_{\boldsymbol{r}} x\,\hat{n}_{\boldsymbol{r}\uparrow}\right].$$

M. Oshikawa, *Phys. Rev. Lett.* **84**, 3370 (2000).

Adiabatic process commutes with the translation operator T_x, so momentum P_x is conserved.

$$\text{However } U^{-1} T_x U = T_x \exp\left[\frac{2\pi i}{L_x}\sum_{\boldsymbol{r}} \hat{n}_{T\boldsymbol{r}\uparrow}\right];$$

so shift in momentum ΔP_x between states $U|\Psi'\rangle$ and $|\Psi\rangle$ is

$$\Delta P_x = \frac{\pi L_y}{v_0} n_T \left(\text{mod}\,\frac{2\pi}{a_x}\right) \qquad (1).$$

Alternatively, we can compute ΔP_x by assuming it is absorbed by quasiparticles of a Fermi liquid. Each quasiparticle has its momentum shifted by $2\pi/L_x$, and so

$$\Delta P_x = \frac{2\pi}{L_x}\frac{(\text{Volume enclosed by Fermi surface})}{(2\pi)^2/(L_x L_y)}\left(\text{mod}\,\frac{2\pi}{a_x}\right) \qquad (2).$$

From (1) and (2), same argument in y direction, using coprime $L_x/a_x, L_y/a_y$:

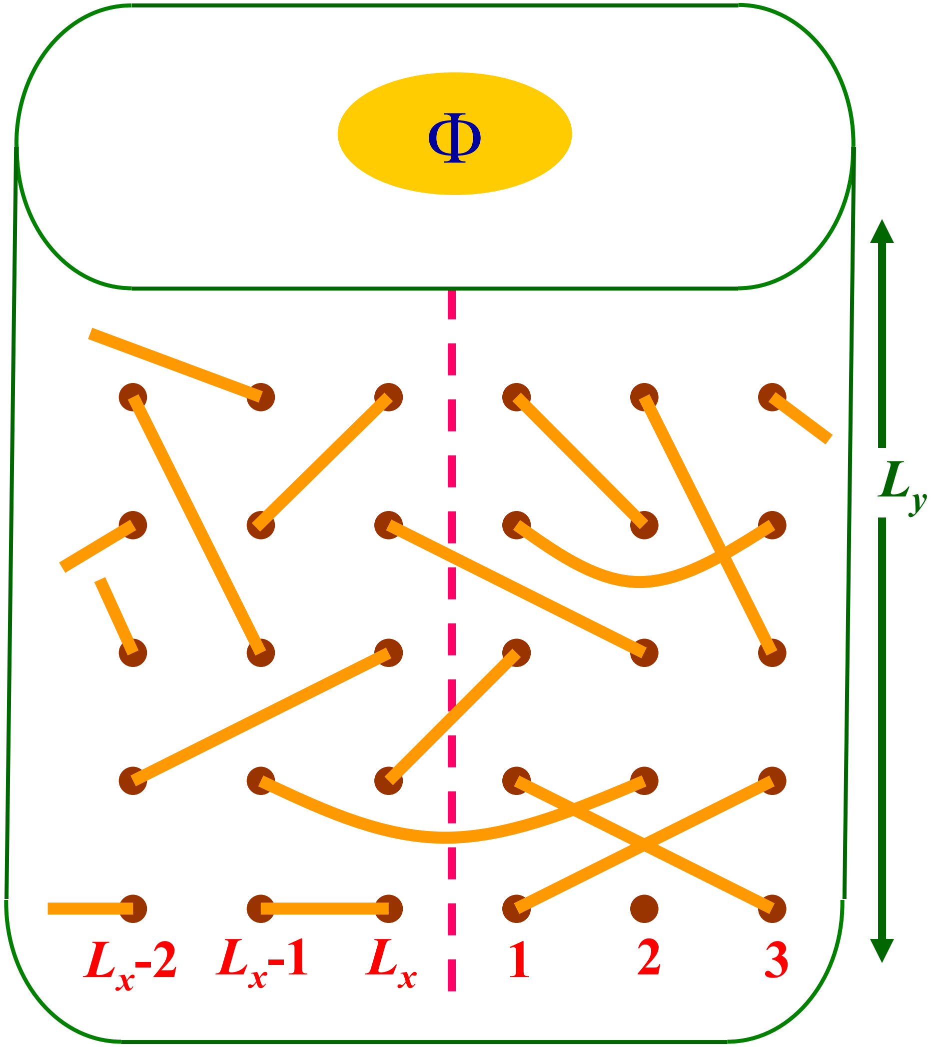
$$2\times\frac{v_0}{(2\pi)^2}(\text{Volume enclosed by Fermi surface}) = n_T\ (\text{mod } 2)$$

M. Oshikawa, *Phys. Rev. Lett.* **84**, 3370 (2000).

Effect of flux-piercing on a topologically ordered quantum paramagnet

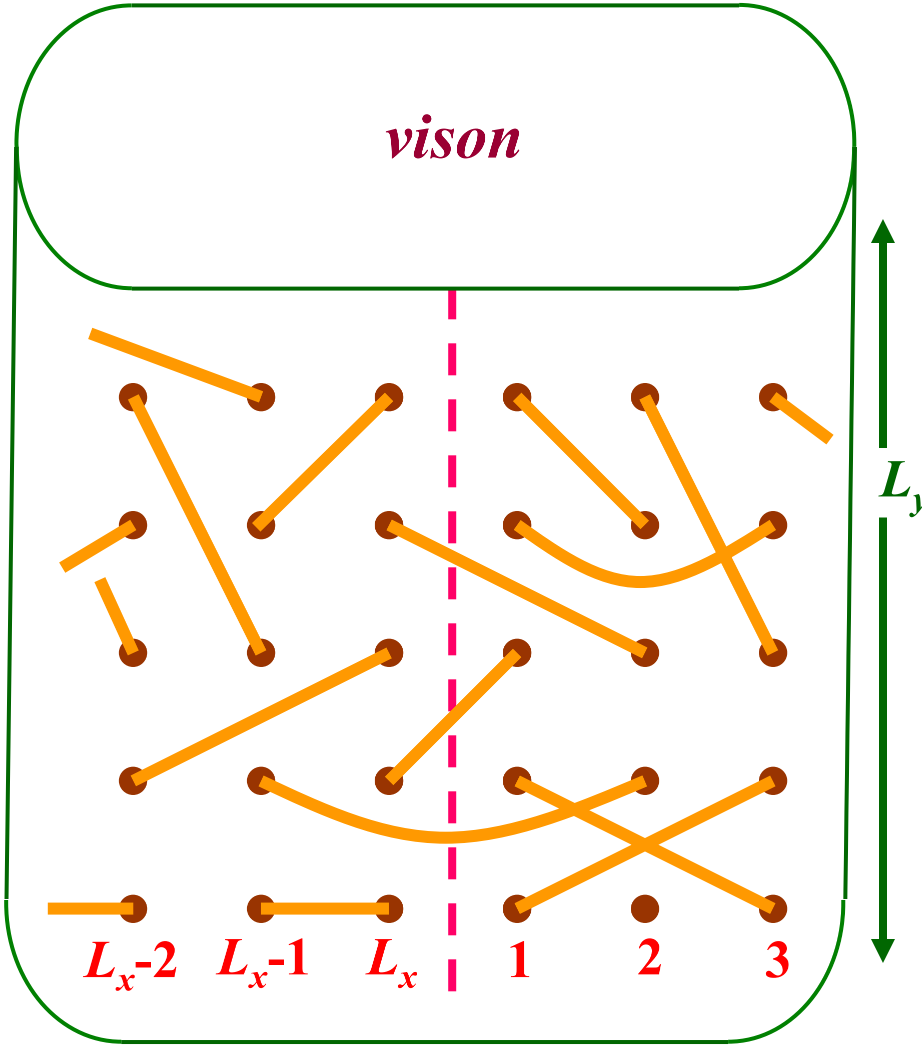
N. E. Bonesteel, *Phys. Rev.* B **40**, 8954 (1989).
G. Misguich, C. Lhuillier, M. Mambrini, and P. Sindzingre, *Eur. Phys. J.* B **26**, 167 (2002).

$$|D\rangle =$$



$$|\Psi\rangle = \sum_D a_D |D\rangle$$

Effect of flux-piercing on a topologically ordered quantum paramagnet



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$$|\Psi\rangle = \sum_D a_D |D\rangle$$

After flux insertion $|D\rangle \Rightarrow$

$$(-1)^{\text{Number of bonds cutting dashed line}} |D\rangle;$$

Equivalent to inserting a ***vison*** inside hole of the torus.

Vison carries momentum $\pi L_y / v_0$

Flux piercing argument in Kondo lattice

Shift in momentum is carried by n_T electrons, where

$$n_T = n_f + n_c$$

In topologically ordered, state, momentum associated with n_f=1 electron is absorbed by creation of vison. The remaining momentum is absorbed by Fermi surface quasiparticles, which enclose a volume associated with n_c electrons.

A small Fermi surface.

cond-mat/0209144

Conclusions

I. Two classes of Mott insulators:

(A) Collinear spins, bond order, confinements of spinons.

(B) Non-collinear spins, topological order, free spinons

II. Doping Class (A)

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.

III. Doping Class (B)

New "Fermi liquid" state with a small Fermi surface.