

Understanding correlated electron systems by a classification of Mott insulators

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Annals of Physics **303**, 226 (2003)



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



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”.

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. Fractionalized Fermi liquids (classes A and B)

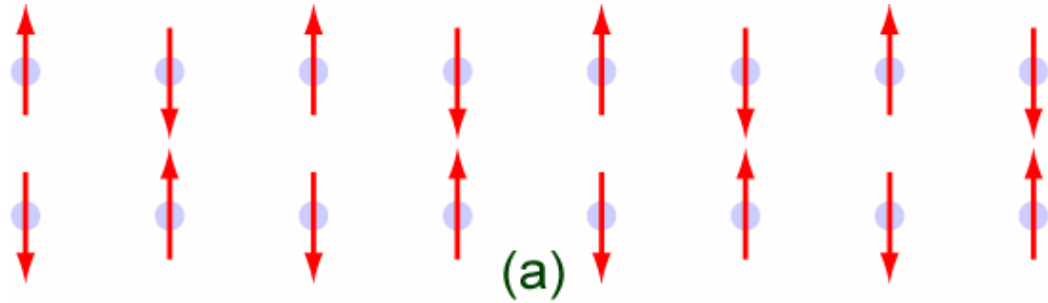
Applications to quantum criticality in heavy fermions

IV. Conclusions

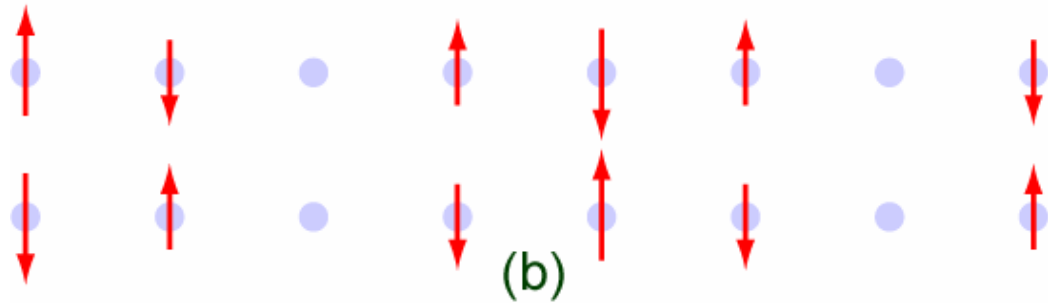
I. Order in Mott insulators

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

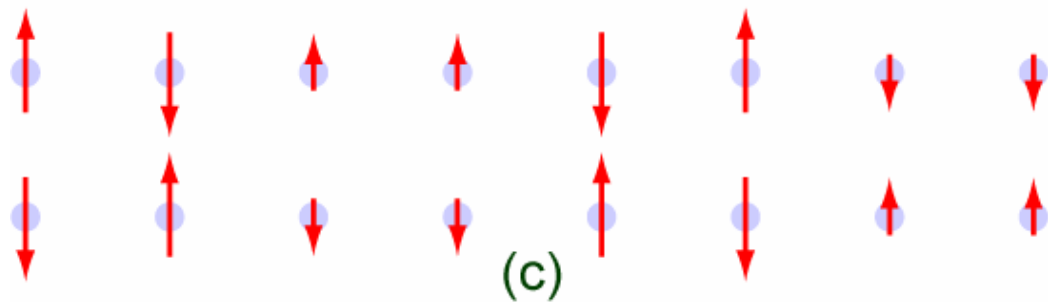
Class A. Collinear spins



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



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



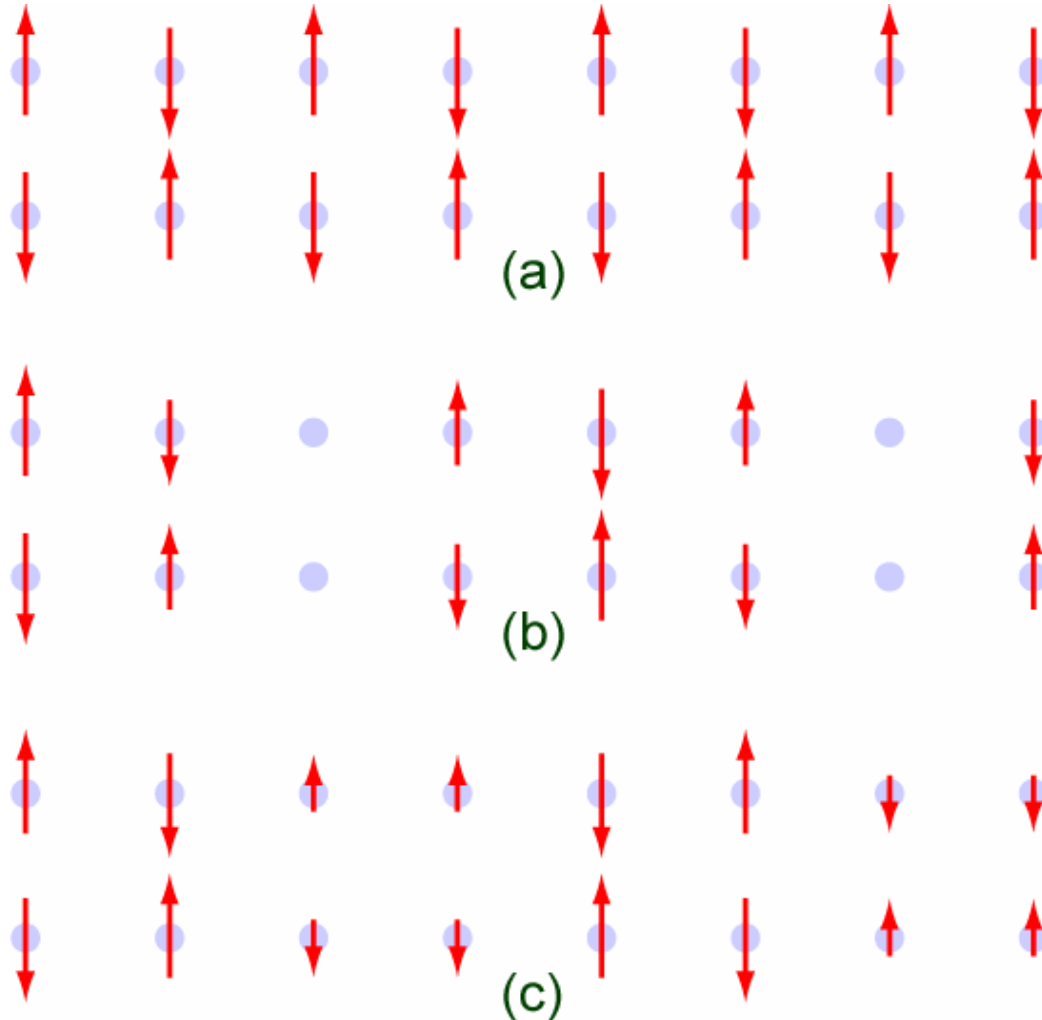
$$\vec{K} = (3\pi/4, \pi) ;$$

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

I. Order in Mott insulators

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Class A. Collinear spins



Key property

Order specified by a single vector N .

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

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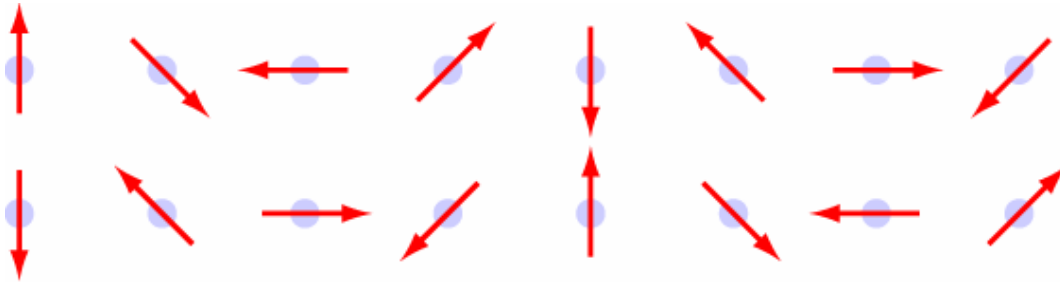
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I. Order in Mott insulators

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

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



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

$$N_2^2 = N_1^2, N_1 \cdot N_2 = 0$$

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

$$N_1 + iN_2 = \begin{pmatrix} z_\downarrow^2 - z_\uparrow^2 \\ i(z_\downarrow^2 + z_\uparrow^2) \\ 2z_\uparrow z_\downarrow \end{pmatrix}$$

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

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

I. Order in Mott insulators

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

Class B. Noncollinear spins

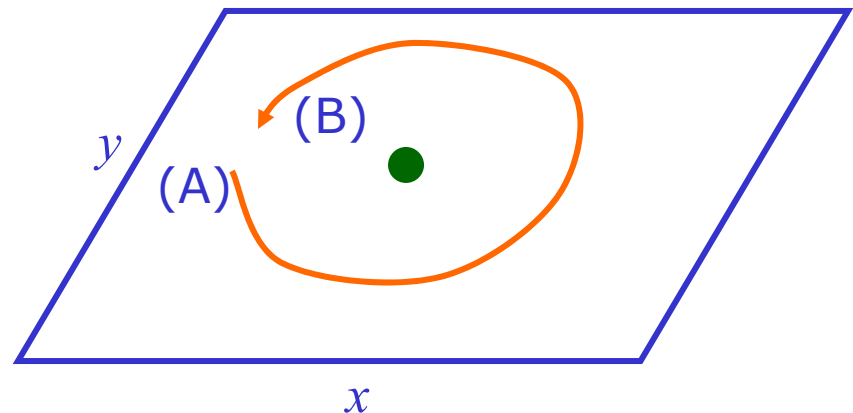
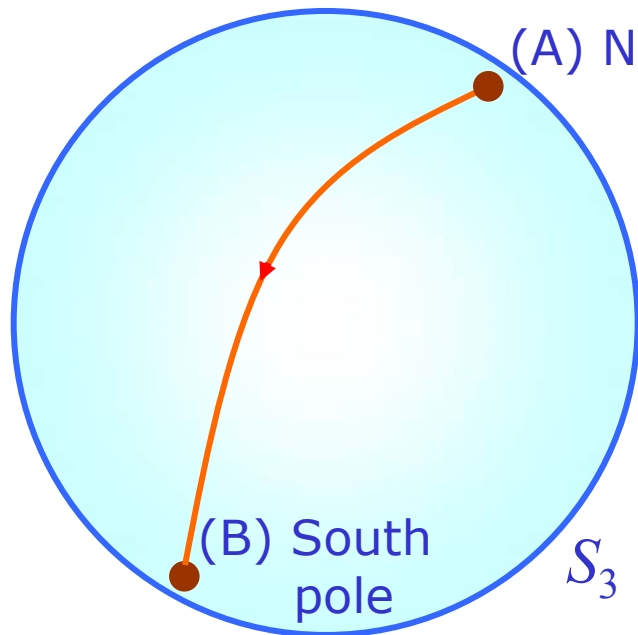
$$N_1 + iN_2 = \begin{pmatrix} z_{\downarrow}^2 - z_{\uparrow}^2 \\ i(z_{\downarrow}^2 + z_{\uparrow}^2) \\ 2z_{\uparrow}z_{\downarrow} \end{pmatrix}$$

Order parameter space: S_3/Z_2

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

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

Become “visons” in paramagnet



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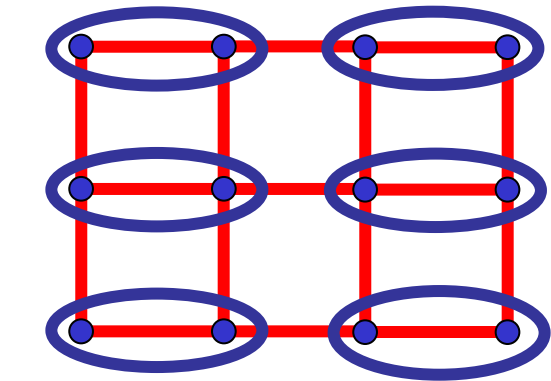
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IV. Conclusions

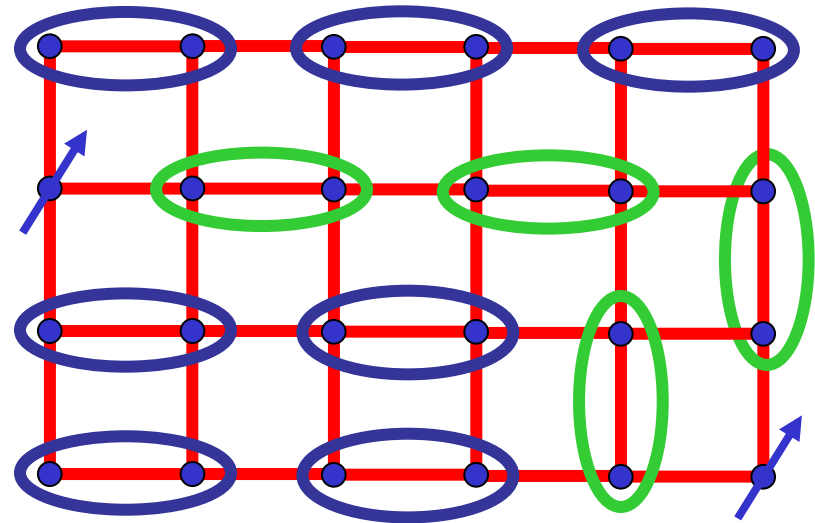
I. Order in Mott insulators

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

Class A. Bond order and spin excitons in $d=2$



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



$S=1/2$ 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 N becomes the $S=1$ spin exciton and Berry phases induce bond order

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

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

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

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

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

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

Small $g \rightarrow$ Spin-wave theory about Neel state receives minor modifications from Berry phases.

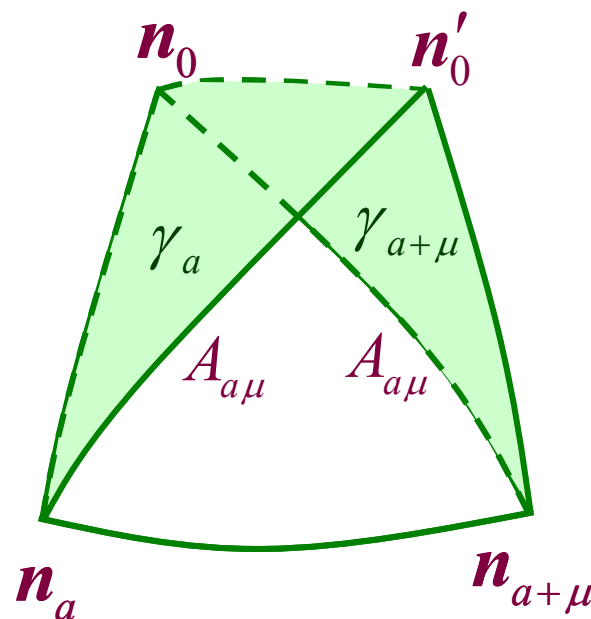
Large $g \rightarrow$ Berry phases are crucial in determining structure of "quantum-disordered" phase with $\langle \mathbf{n}_a \rangle = 0$

Integrate out \mathbf{n}_a to obtain effective action for $A_{a\mu}$

Change in choice of \mathbf{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 \mathbf{n}_a and the two choices for \mathbf{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 $A_{a\mu}$

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.

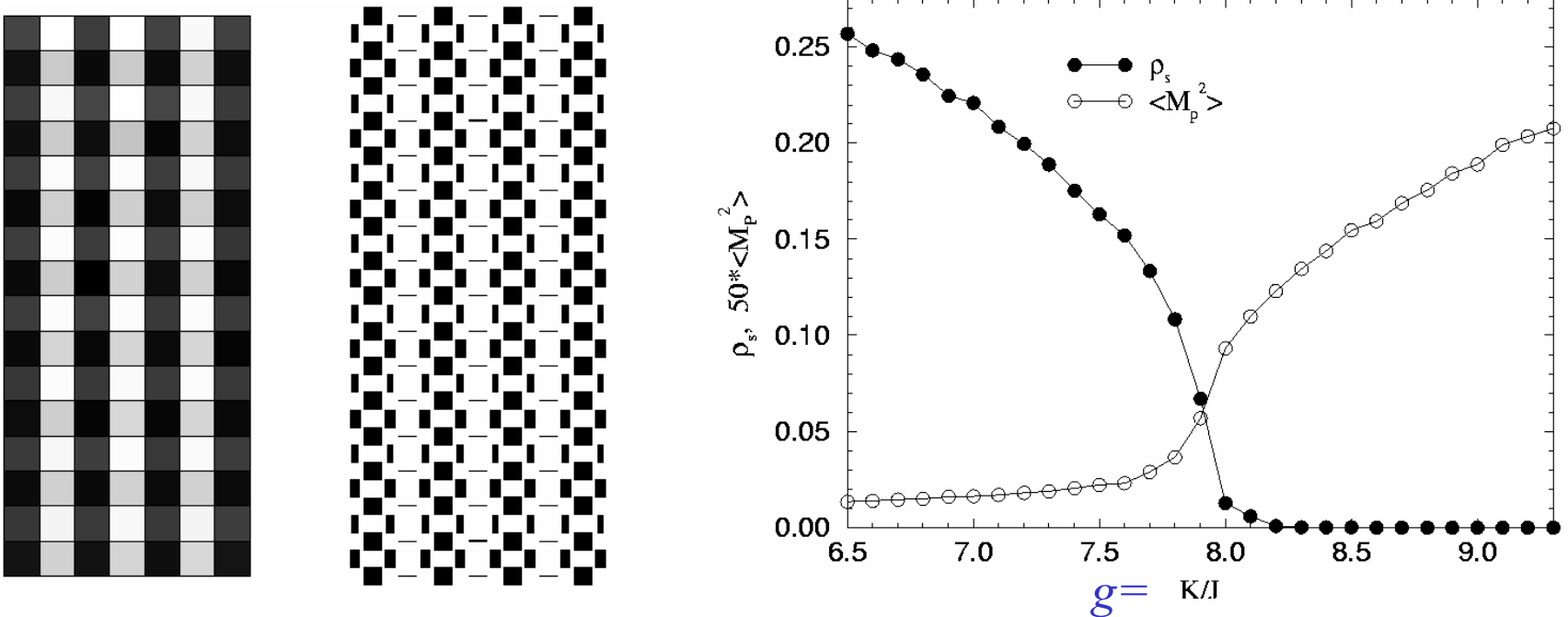
$d=2$: The gauge theory is *always* in a *confining* phase and there is bond order in the ground state.

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

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



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

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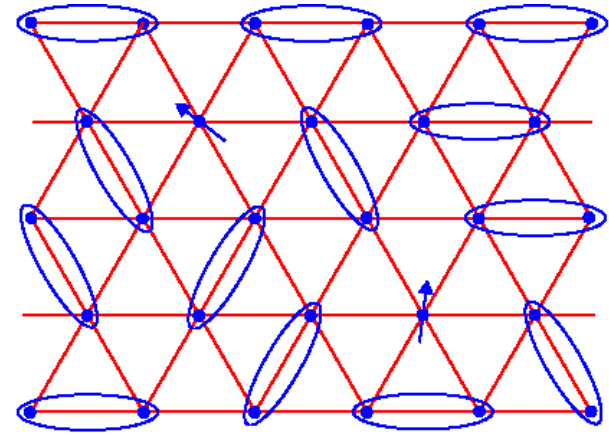
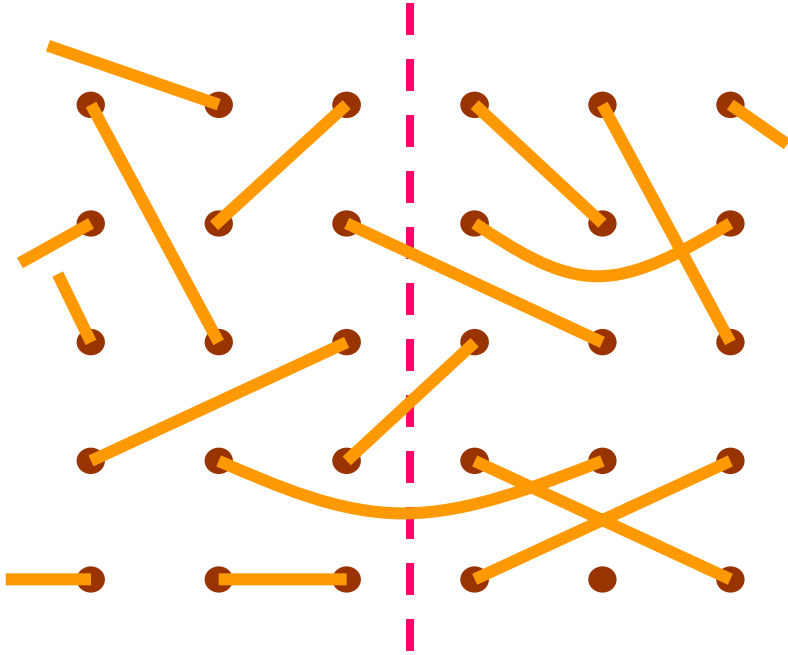
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I. Order in Mott insulators

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

Class 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).

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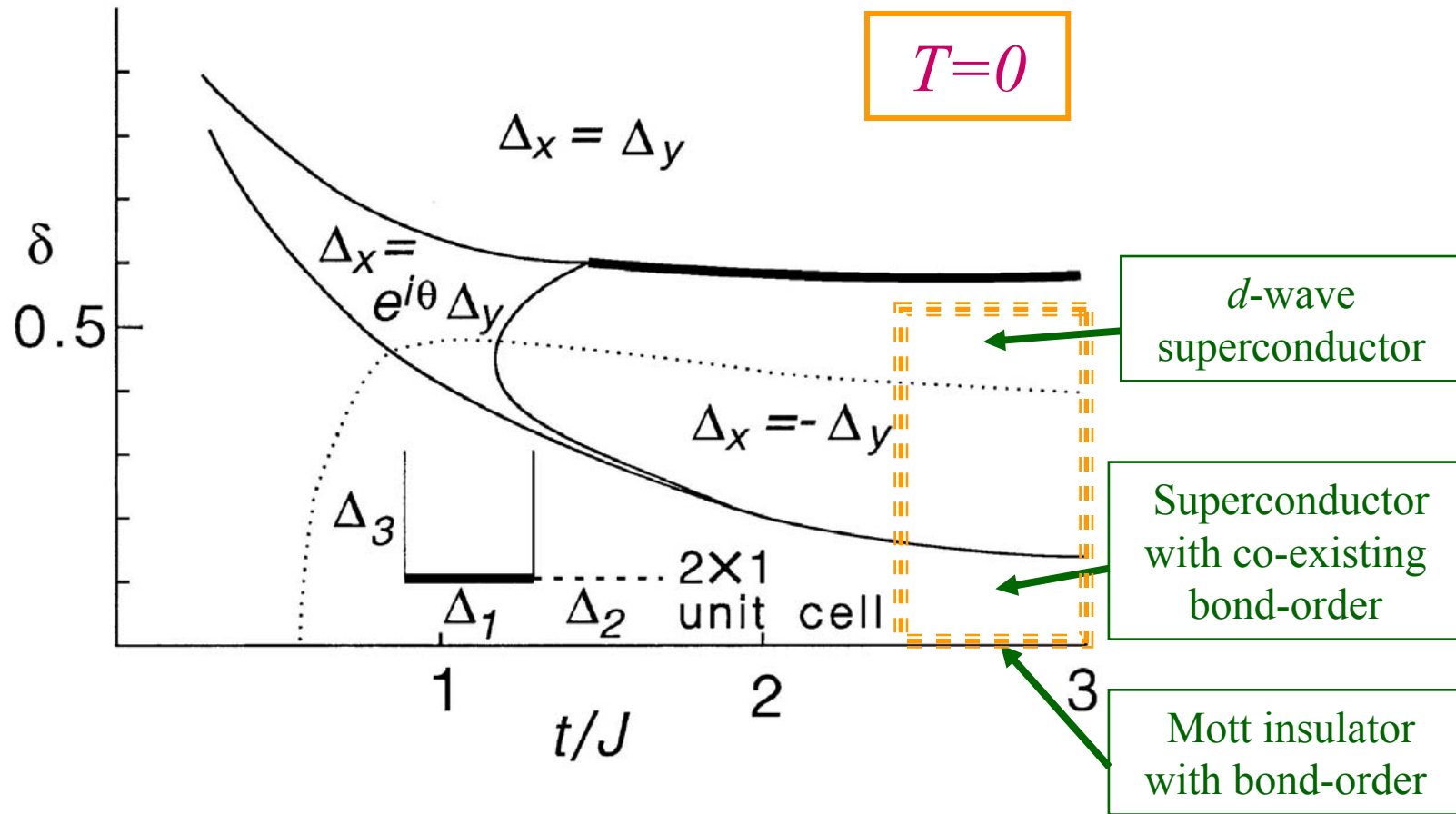
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II. Doping Class A

Doping a paramagnetic bond-ordered Mott insulator

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

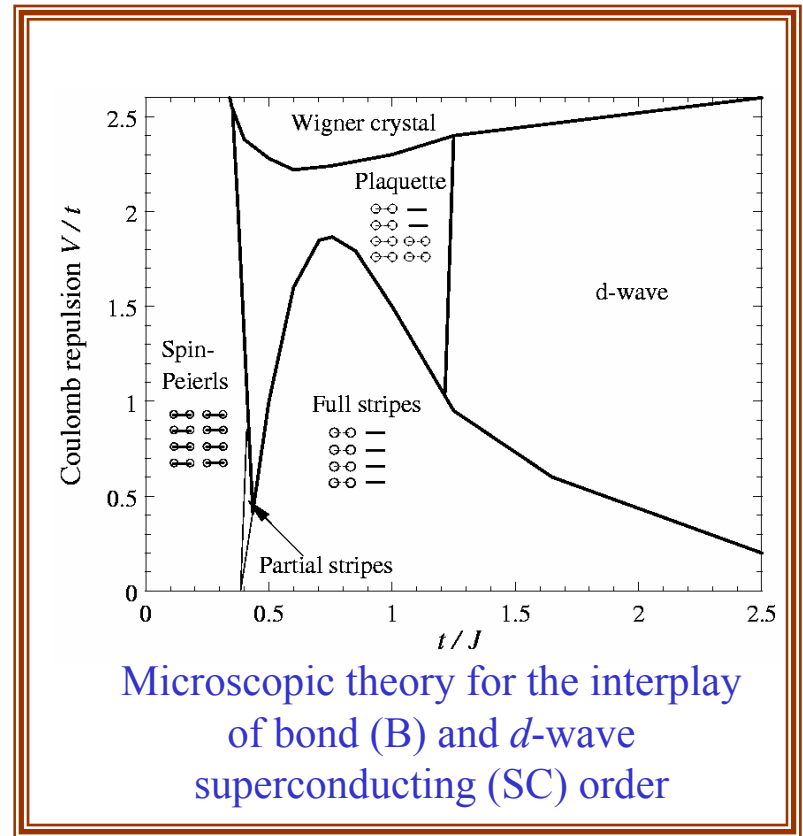
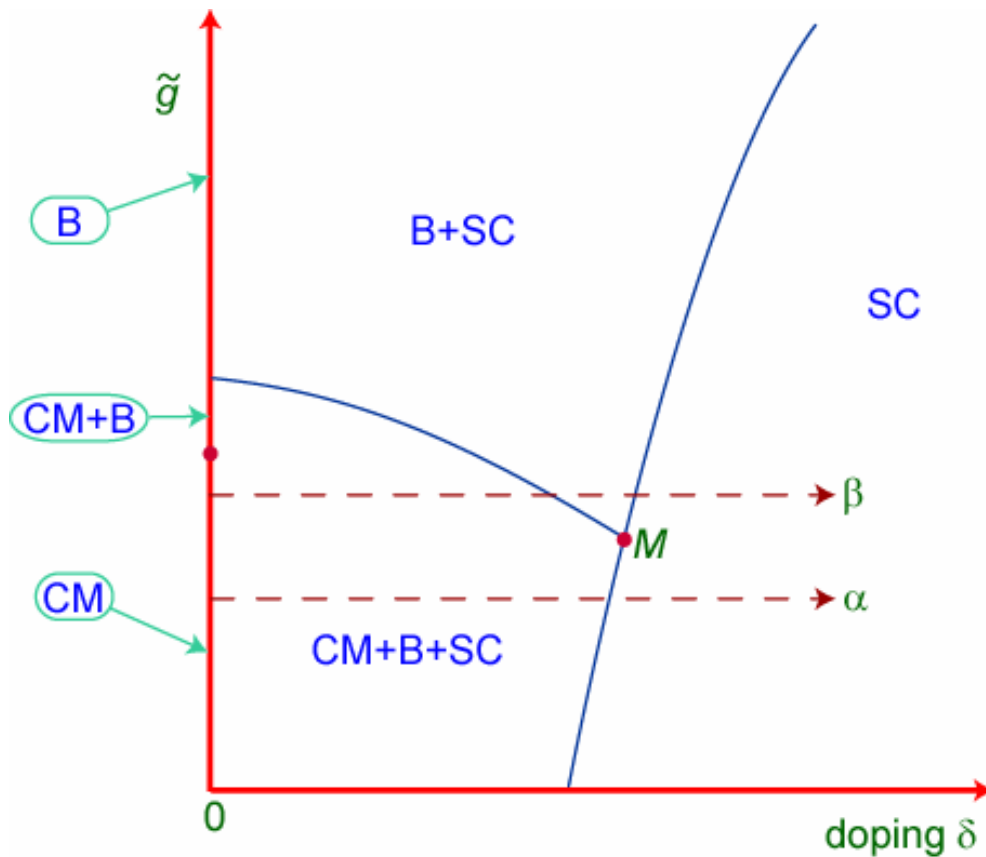


S. Sachdev and N. Read, *Int. J. Mod. Phys. B* **5**, 219 (1991).

A 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).

Evidence cuprates are in class A

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- 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).

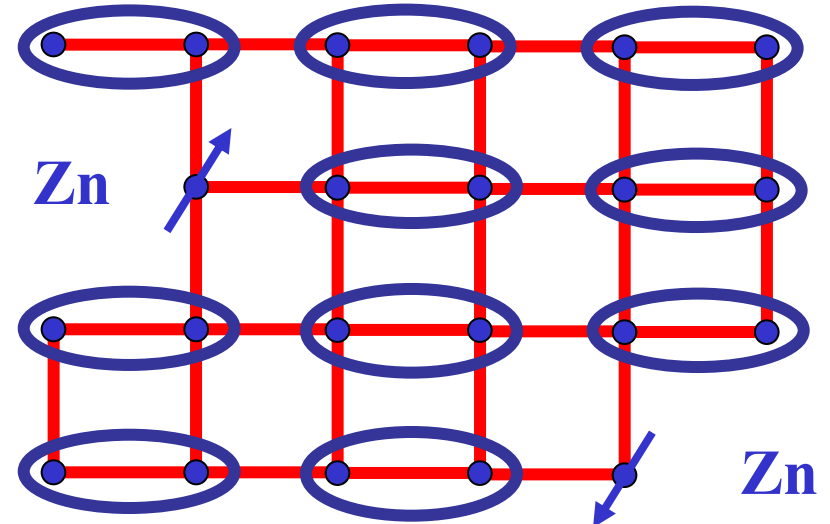
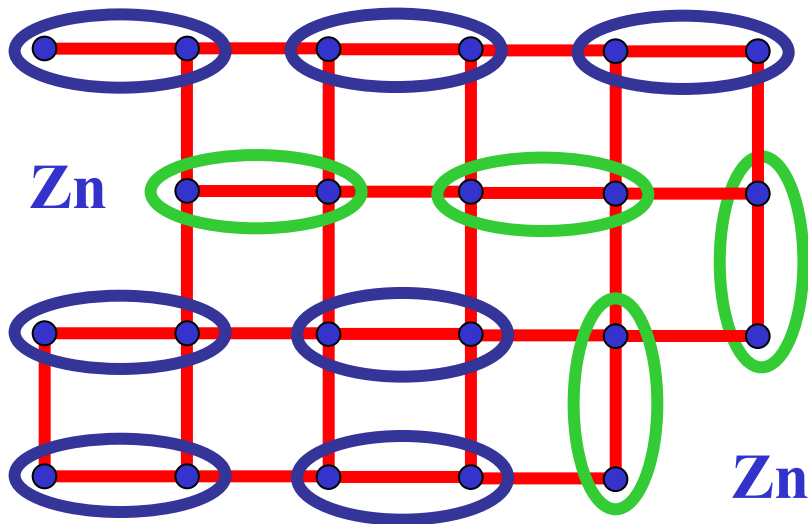
D. A. Bonn, J. C. Wynn, B. W. Gardner, Y.-J. Lin, R. Liang, W. N. Hardy, J. R. Kirtley, and K. A. Moler, *Nature* **414**, 887 (2001).

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).

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- Non-magnetic impurities in underdoped cuprates acquire a $S=1/2$ moment

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



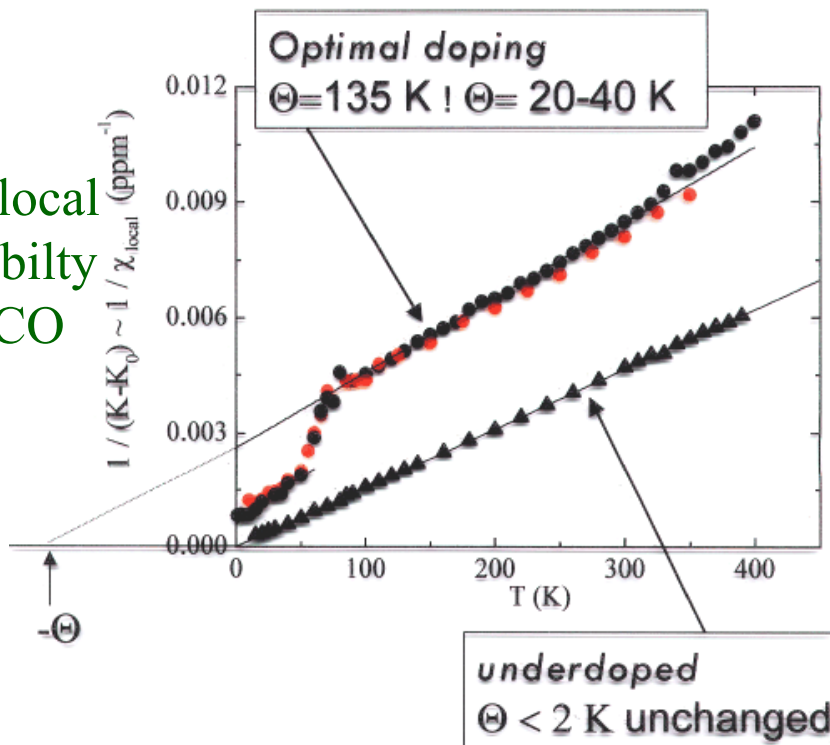
Spinon confinement implies that free $S=1/2$ moments form near each impurity

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

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

^7Li 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.

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- Tests of phase diagram in a magnetic field

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

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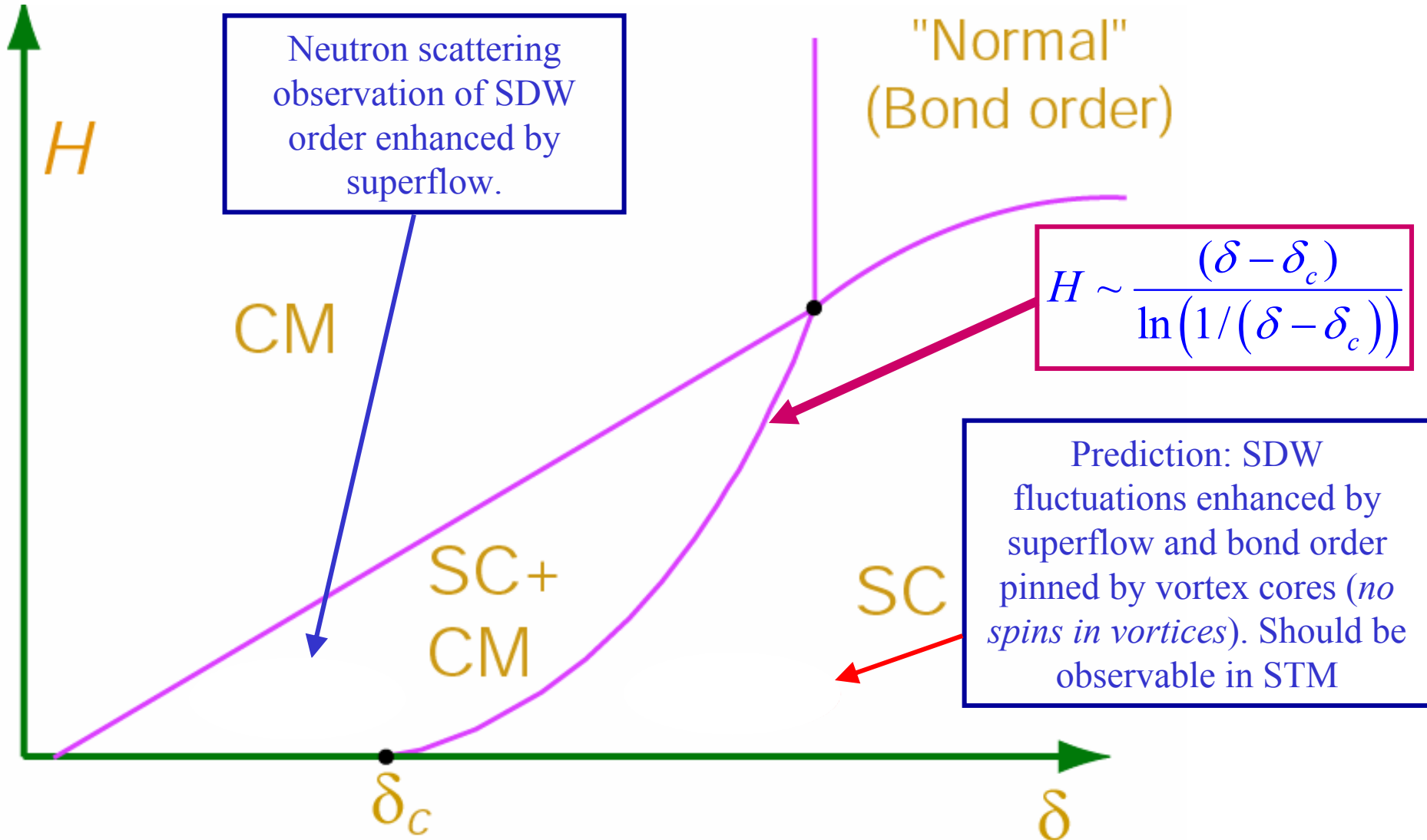
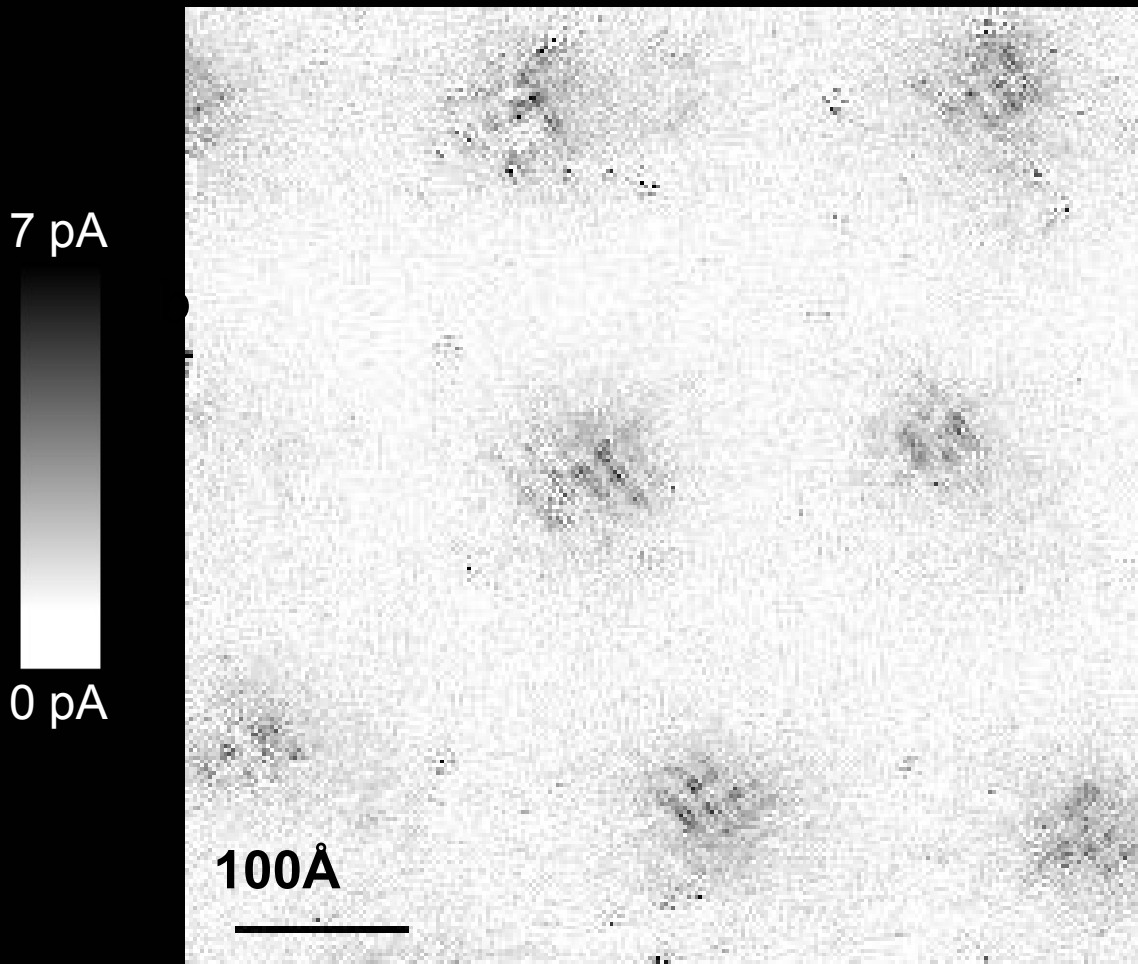


FIG. 1. Phase diagram in the H - δ plane. δ_c is the critical value of δ for the onset of superconductivity.

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

Y. Zhang, E. Demler and S. Sachdev, *Phys. Rev. B* **66**, 020501 (2002).

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



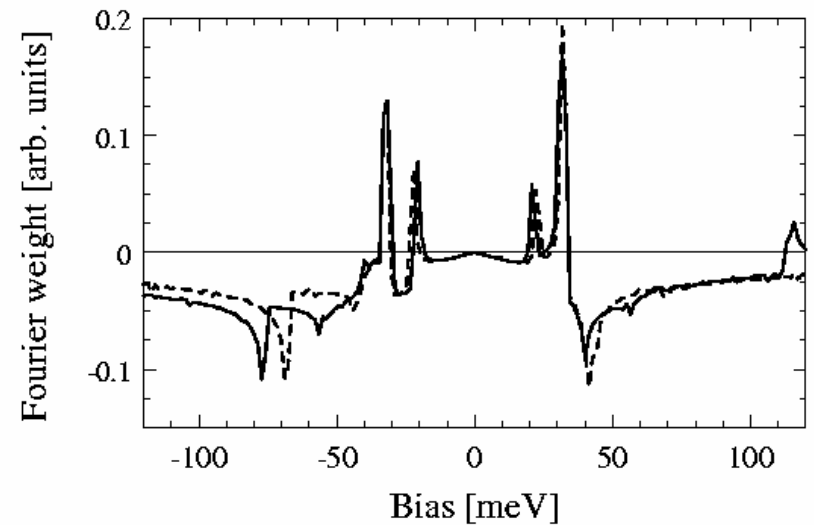
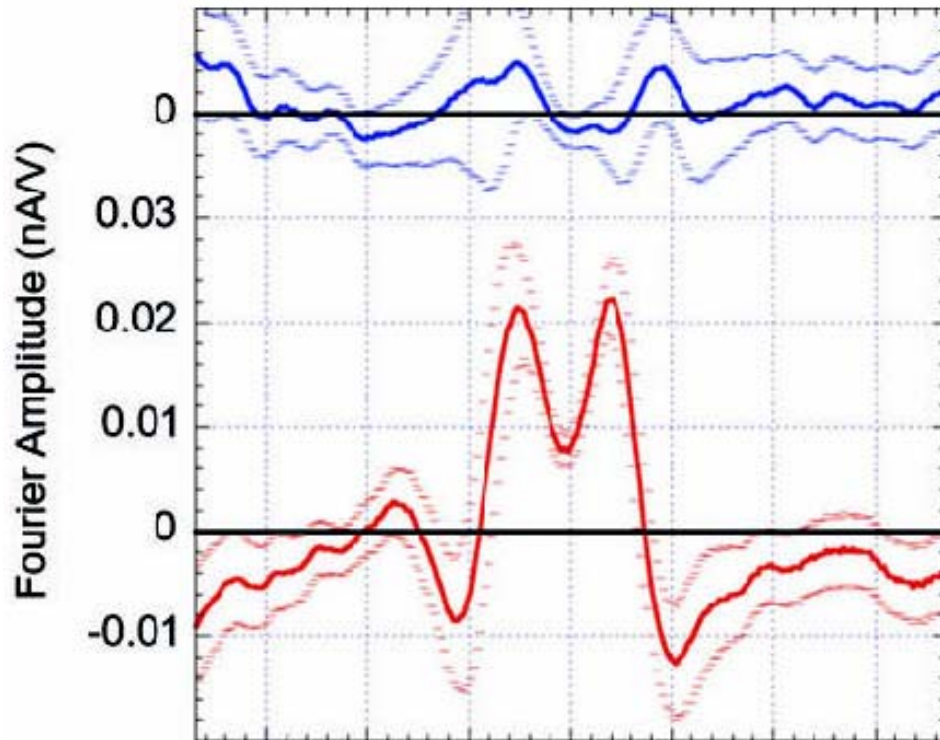
Our interpretation:
LDOS modulations are
signals of bond order of
period 4 revealed in
vortex halo

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).

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

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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:

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

A Fermi liquid (FL)

Our claim

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

$$2 \times \frac{v_0}{(2\pi)^d} (\text{Volume enclosed by Fermi surface}) \\ = (n_T - 1) \pmod{2}$$

A Fractionalized Fermi Liquid (FL*)

T. Senthil, S. Sachdev, and M. Vojta, *Phys. Rev. Lett.* in press, cond-mat/0209144

T. Senthil, M. Vojta, and S. Sachdev, cond-mat/0305193

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 f spins form a topologically ordered (U(1) or Z_2) paramagnet

This system has a Fermi surface of conduction electrons with volume $n_c \pmod{2}$

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

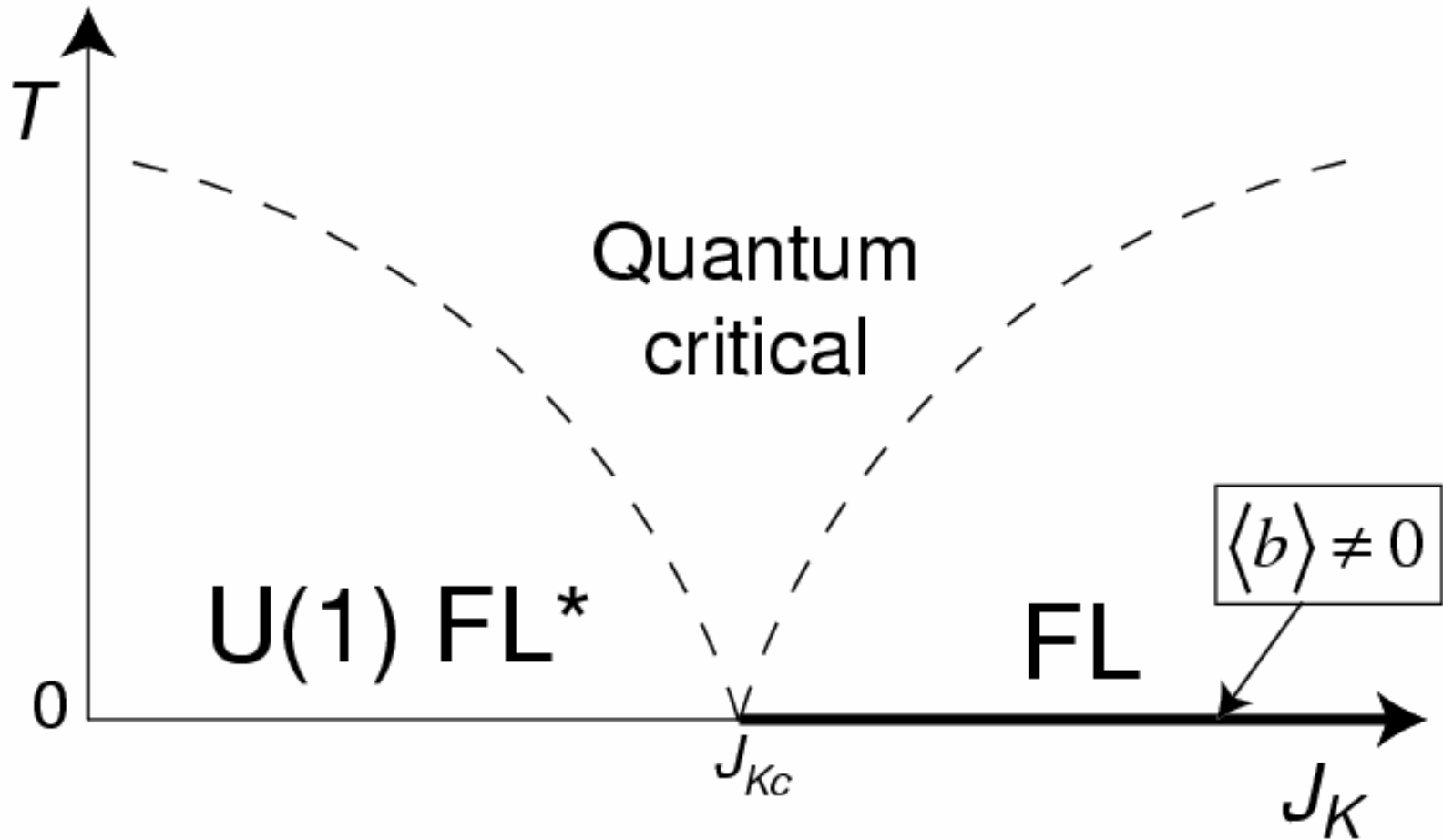
$$n_T = n_f + n_c \neq n_c \pmod{2}$$

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

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

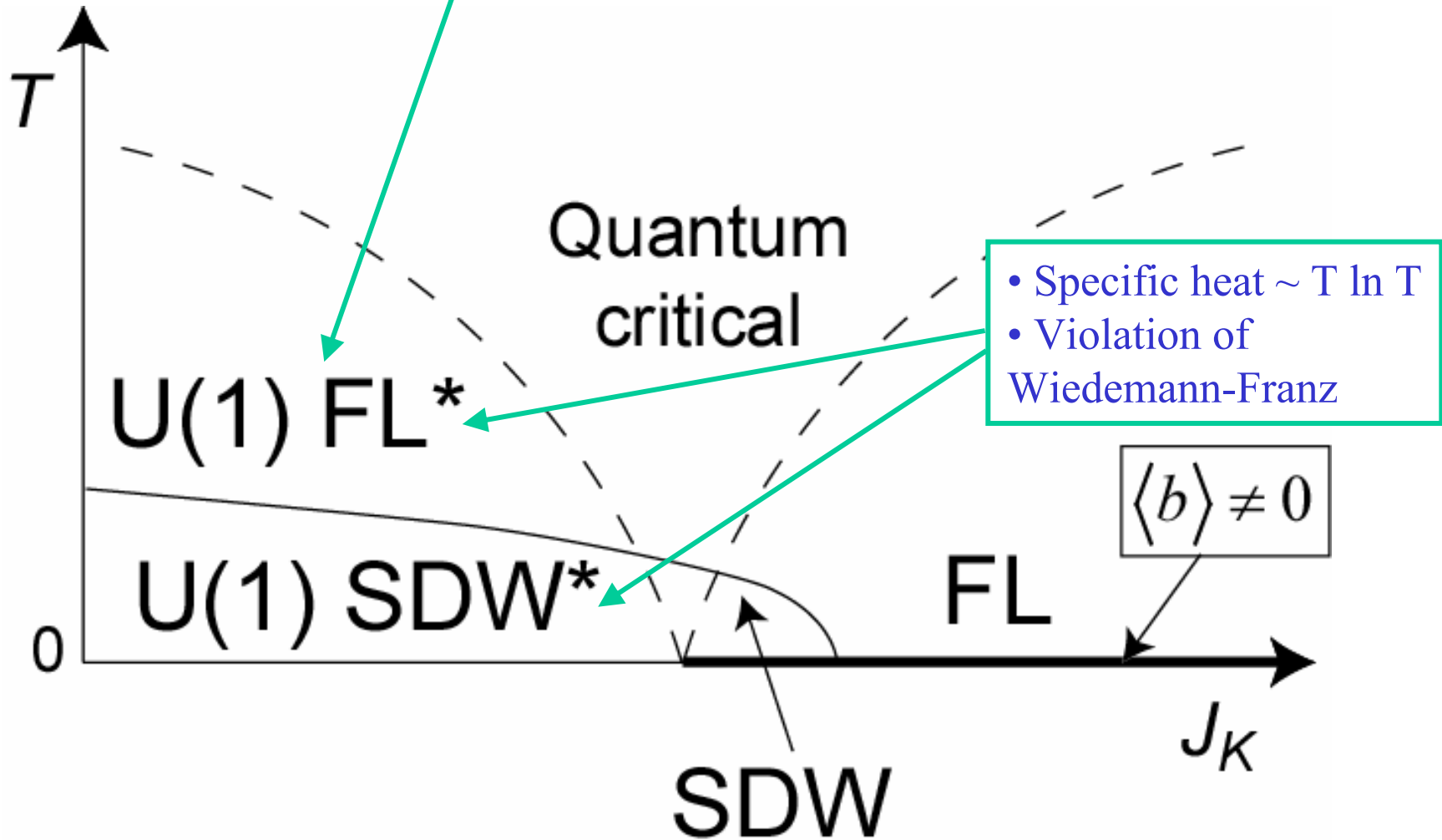
FL*

Phase diagram (U(1), $d=3$)



Phase diagram (U(1), $d=3$)

Fermi surface volume does not include local moments



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.
- III. New “Fractionalized Fermi liquid” state, with possible applications to the heavy fermion compounds