Quantum Choreography: Exotica inside Crystals

U. Toronto - Colloquia 3/9/2006

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- Electrons inside crystals: Quantum Mechanics at room temperature

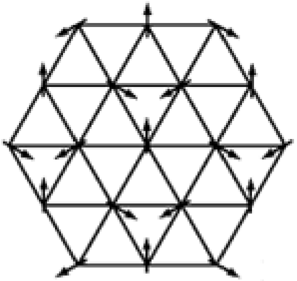
- Quantum Theory of Solids: Band Theory

  Metals/Insulators/Semiconductors …

Electrons do their own thing…

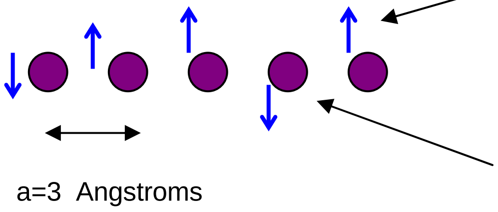
- Need revisiting…

Electrons are cooperative “dancers” -
exotic quantum dancers



Electrons in Solids:

Quantum mechanics at room temperature -



outer shell of electrons -
often are mobile

Ions - nuclei with closed
shell of electrons

Energy Scales:

Kinetic energy: Quantum zero point motion

$$E_{ke} \sim \frac{\hbar^2}{ma^2} \sim eV \sim 10^4 K >> T_{room}$$

Coulomb Interaction: between electrons and ions

$$E_{coul} \sim \frac{e^2}{a} \sim eV > T_{room}$$

Interest: Quantum Dynamics of 10^{23} electrons

Quantum Ground State Phases

Quantum Theory of Solids: Standard Paradigm

Landau Fermi Liquid Theory

Accounts for electronic behavior of simple metals, insulators and semiconductors

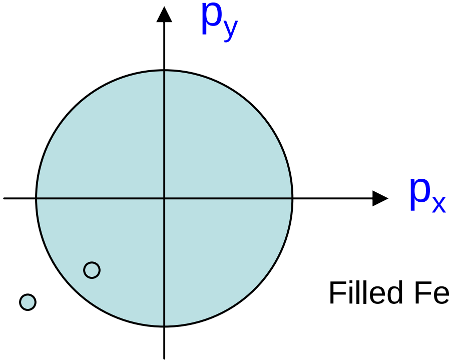
QuickTime?and a
TIFF (Uncompressed) decompressor
are needed to see this picture.

Landau Theory of Phase Transitions

Provides a framework to understand broken symmetry phases of metals, including -

- superconductors,
- ferromagnets,
- antiferromagnets,
- charge density waves,
- spin density waves,…

Fermi Liquid Theory



Free Fermions

$$H_0 = \sum_j \frac{\mathbf{p}_j^2}{2m}$$

particle/hole excitations

Filled Fermi sea

Interacting Fermions

$$H = \sum_j \frac{\mathbf{p}_j^2}{2m} + \sum_{ij} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Retain a Fermi surface

Luttingers Thm: Volume of Fermi sea
same as for free fermions

Particle/hole excitations are
long lived near FS

$$\frac{1}{\tau} \sim (E - E_F)^2$$

Vanishing decay rate

Add periodic potential from ions in crystal

$$H = \sum_j \frac{\mathbf{p}_j^2}{2m} + \sum_{ij} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_i V(\mathbf{r}_i)$$

- Plane waves become Bloch states
- Energy Bands and forbidden energies (gaps)
- Band insulators: Filled bands
- Metals: Partially filled highest energy band

Even number of electrons/cell - (usually) a band insulator

Odd number per cell - always a metal

Landau Theory of Phase Transitions

Order Parameter: A local observable, non-zero in one phase and zero in all others

Example: Electron Hamiltonian in metal

$$\mathcal{H} = \int d\mathbf{r} c_\alpha^\dagger(\mathbf{r})[-\nabla^2/2m]c_\alpha(\mathbf{r}) + \mathcal{H}_{int}$$

- Superconductor $\psi(\mathbf{r}) = \mathbf{c}_\uparrow(\mathbf{r})\mathbf{c}_\downarrow(\mathbf{r})$
- Ferromagnet $\mathbf{S}(\mathbf{r}) = \mathbf{c}_\alpha^\dagger(\mathbf{r})\sigma_{\alpha\beta}\mathbf{c}_\beta(\mathbf{r})$

Landau-Ginzburg-Wilson “Free energy” functional:

$$\mathcal{H}_{LGW} = \int d\mathbf{r}[|\nabla\psi|^2 + r|\psi|^2 + u\psi|^4 + ...]$$

Band Theory

- s or p shell orbitals : Broad bands

Simple (eg noble) metals: Cu, Ag, Au - 4s1, 5s1, 6s1: 1 electron/unit cell

Semiconductors - Si, Ge - 4sp3, 5sp3: 4 electrons/unit cell

Band Insulators - Diamond: 4 electrons/unit cell

Band Theory Works

Breakdown

- d or f shell electrons: Very narrow “bands”

Transition Metal Oxides (Cuprates, Manganites, Chlorides, Bromides,…): Partially filled 3d and 4d bands

Rare Earth and Heavy Fermion Materials: Partially filled 4f and 5f bands

Electrons can ``self-localize”

Electron "Fractionalization"

What is it?

Quantum Ground state of strongly correlated electron system which supports "particle-like" excitations which carry fractional quantum numbers

Not "built" from electrons: Q=e, s=1/2

Where does it occur?

- 1d systems of electrons: quantum wires, Carbon nanotubes
- 2d electrons in very strong magnetic fields: Fractional QHE
- Other 2d or 3d systems in ordinary crystals????

Holy Grail

Mott Insulators:

Insulating materials with an odd number of electrons/unit cell

Correlation effects are critical!

Hubbard model with one electron per site on average:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} [c^{\dagger}_{i\alpha} c_{j\alpha} + h.c.] + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

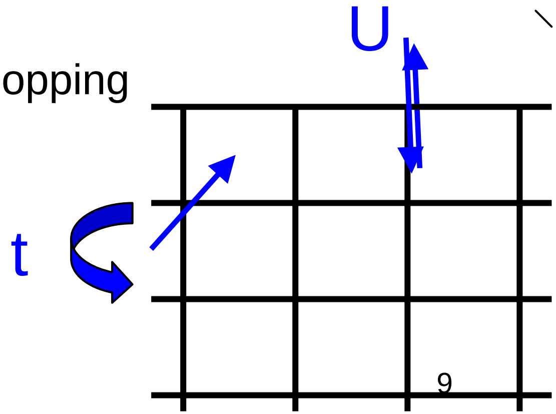
on-site repulsion

electron creation/annihilation
operators on sites of lattice

inter-site hopping

$$c^{\dagger}_{i\alpha}, c_{i\alpha}; \quad \alpha = \uparrow, \downarrow$$

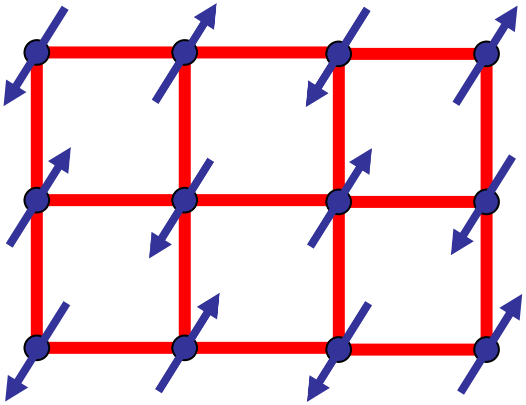
$$[c_{i\alpha}, c^{\dagger}_{j\beta}]_{-} = \delta_{ij} \delta_{\alpha\beta}$$



Spin Physics

For U>>t expect each electron gets self-localized on a site

(this is a Mott insulator)



Residual spin physics:

$$\vec{S}_i; \qquad [S_i^\mu, S_j^\nu] = i\delta_{ij}\epsilon_{\mu\nu\lambda}S_i^\lambda$$

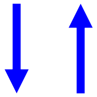
s=1/2 operators on each site

Heisenberg Hamiltonian:

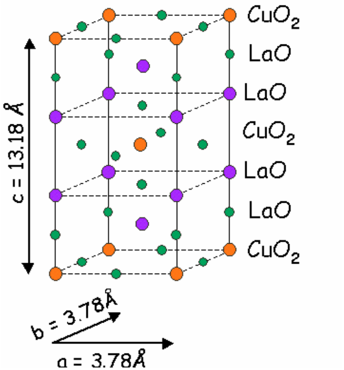
$$H_{spin} = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$$

Antiferromagnetic Exchange

$$J \sim t^2/U$$

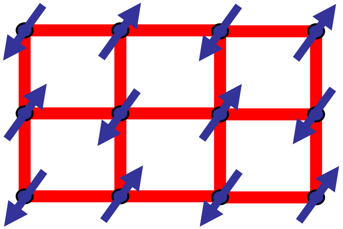


High Temperature Superconductors



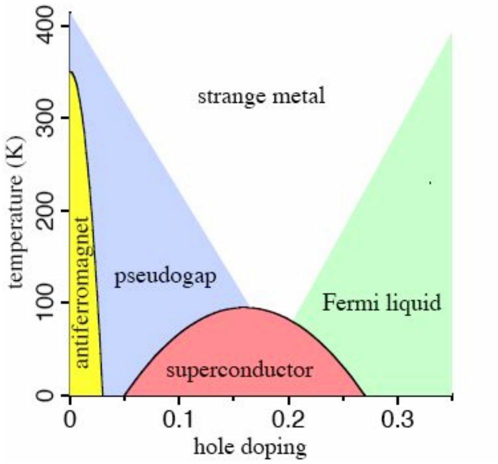
$La_{2-x}Sr_xCuO_4$

2d square lattice: Mott insulator with one electron/Cu atom

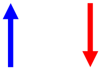


Remove electrons: dope in holes

Doped Mott insulator becomes a high temperature superconductor

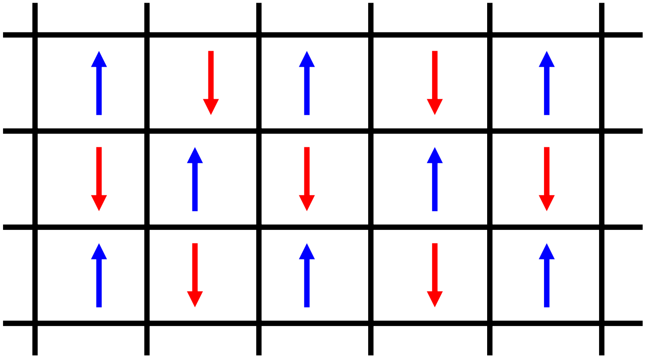


“Quantum Choreography”



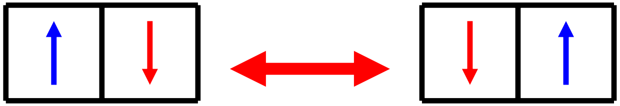
“males and females”

Rules: Electrons are -
- homophobes
- basically shy

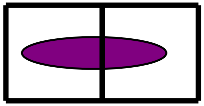


Antiferromagent
(boring)

Electrons like to dance

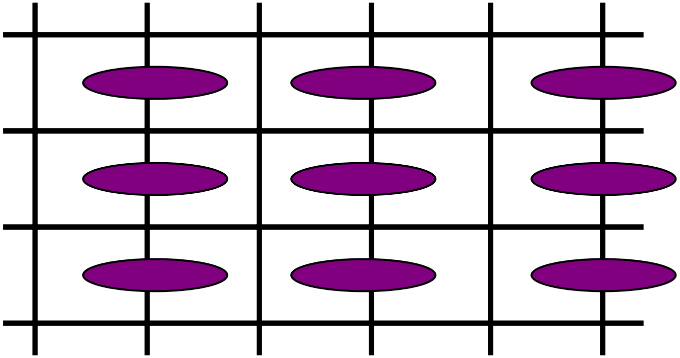


“Quantum Docey Doe”



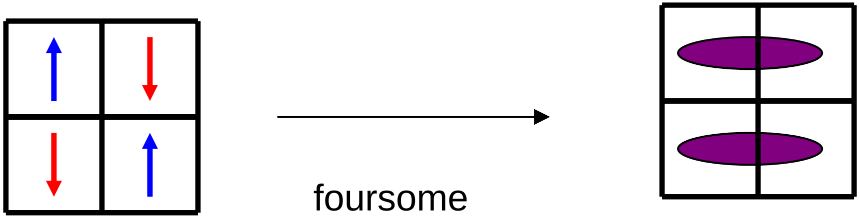
$$= \frac{1}{\sqrt{2}}[| \uparrow\downarrow\rangle - | \downarrow\uparrow\rangle]$$

singlet -valence/chemical bond



Valence Bond Crystal

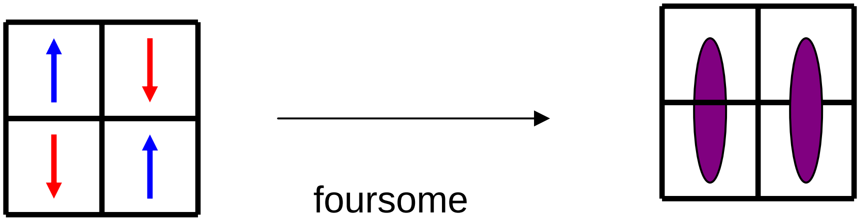
Electrons like to “swing”



foursome

“resonate”

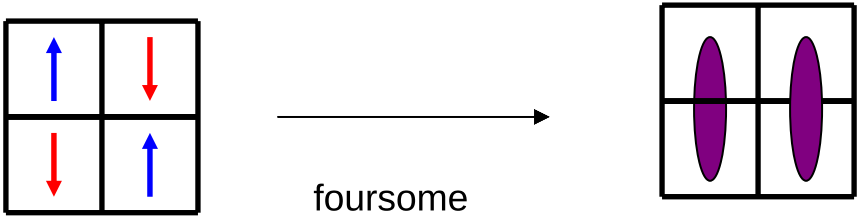
Electrons like to “swing”



foursome

“resonate”

Electrons like to "swing"



foursome

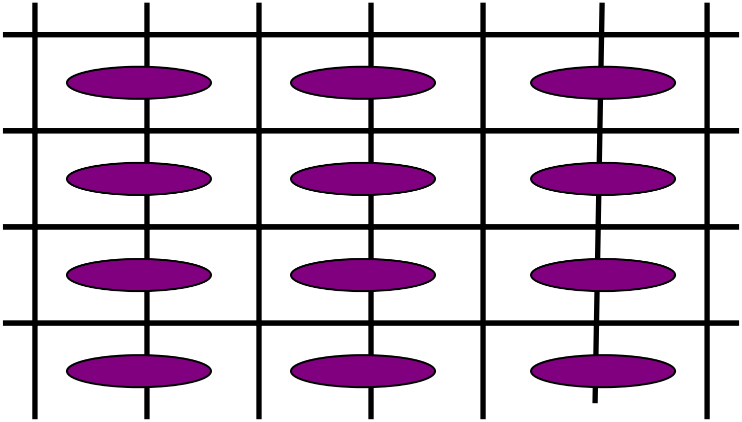
"resonate"

"Quantum Grand Right and Left"

“Quantum Grand Right and Left”

Resonating Valence Bond state (RVB)

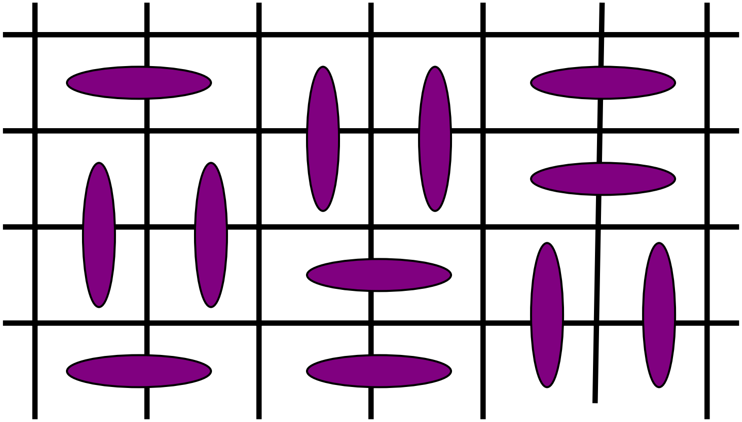
PW Anderson



"Quantum Grand Right and Left"

Resonating Valence Bond state (RVB)

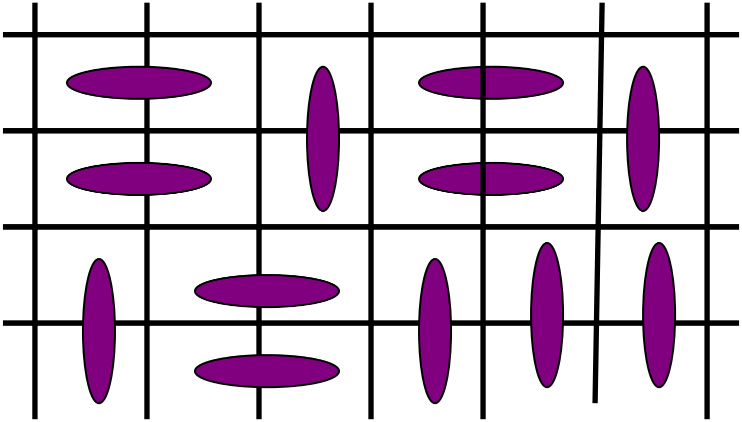
PW Anderson



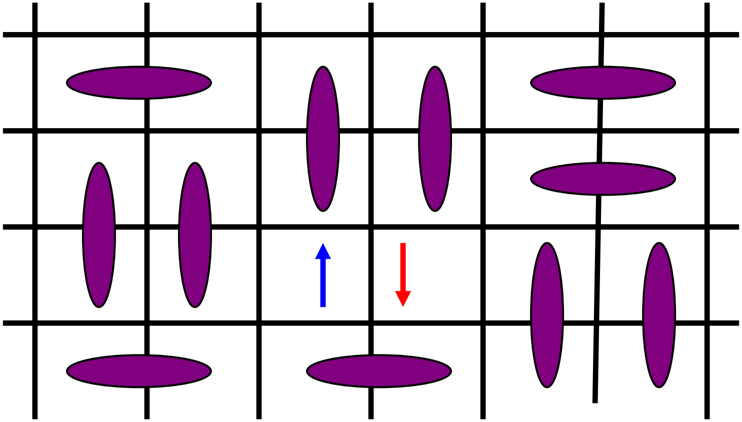
“Quantum Grand Right and Left”

Resonating Valence Bond state (RVB)

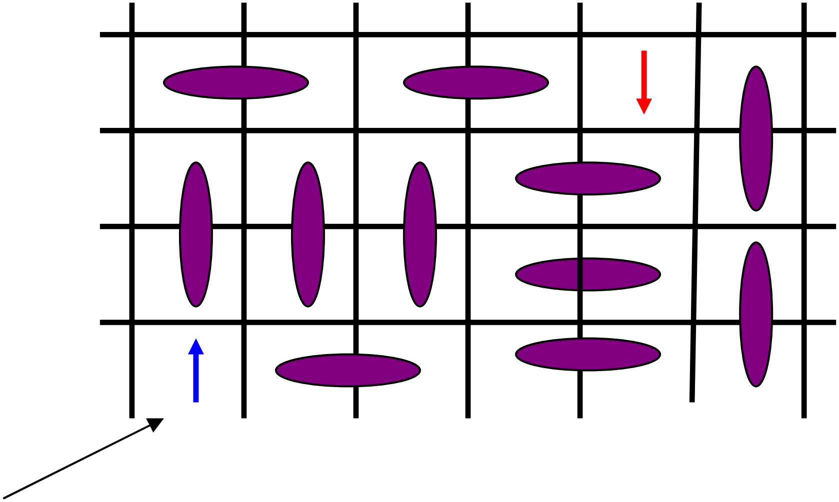
PW Anderson



Breakups - break valence bonds



Separation



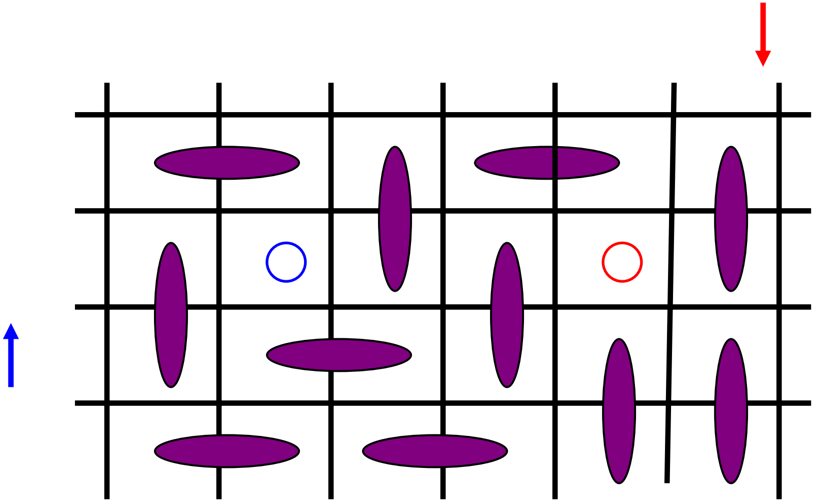
Loners - “Spinons”

s=1/2 , Q=0 , fermions

spin of electron
but no charge

Electron Fractionalization: Spin-Charge separation

Dejected and ejected: Dope in holes



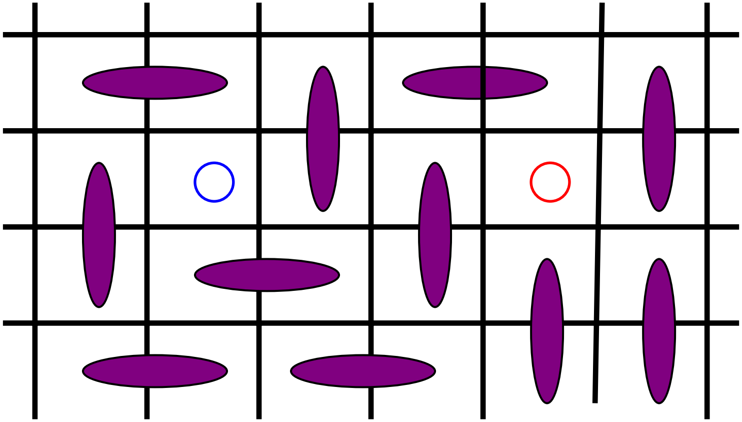
“Holons” s=0 , Q=e, bosons

electron charge
but no spin

Kivelson et. al.

Electron Fractionalization: Spin-Charge separation

Condensation of holons - Superconductivity



Liberating the electron of its spin/statistics, allows the bosonic charge e to condense

Doping an RVB “spin liquid” - route to high T_c superconductivity?

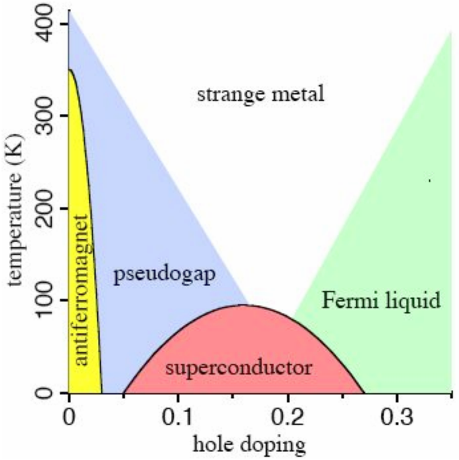
Doped high Tc Superconductor

- undoped Mott state is a boring AFM, NOT an RVB spin liquid

- AFM destroyed with low doping - “Pseudogap phase”

- Pseudogap an RVB spin liquid?

- How can one tell?

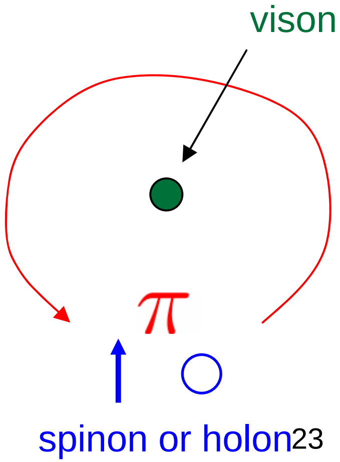


Topological Order

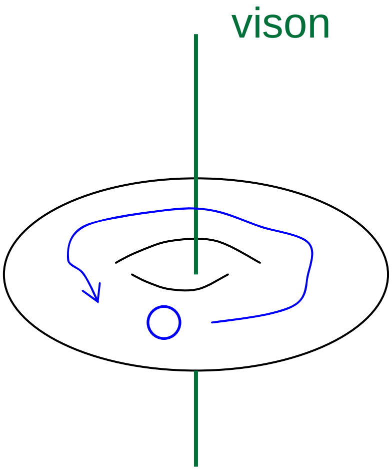
Simplest RVB spin liquid has “hidden” Z_2 symmetry,

In addition to the spinons and holons which carry a Z_2 “electric charge”, there are particles carrying Z_2 “magnetic charge” - “visons”

π phase change upon encircling vison



Topological Order:



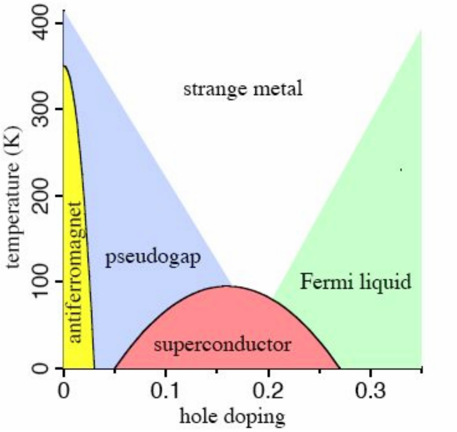
Four fold degeneracy on a torus - vison/no vison threading holes of torus

π phase change for holon upon encircling hole

Essence of:

- Superconductor - Expulsion of Magnetic field
- Z_2 RVB Spin liquid - Expulsion of visons (“Z_2 magnetic field”)

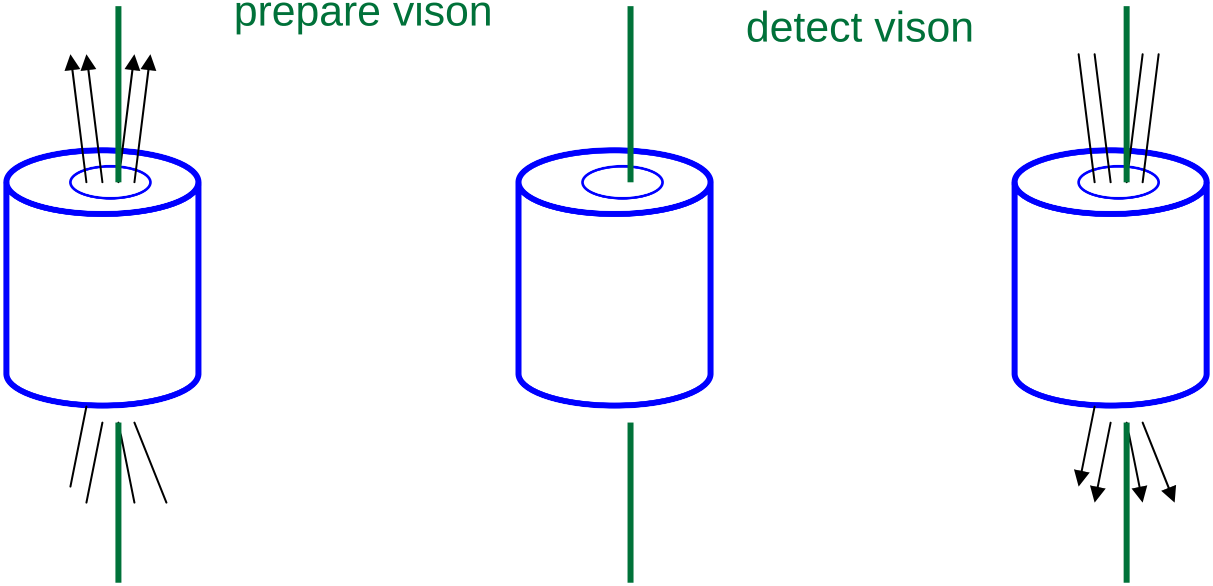
Vison detection: (Senthil, MPAF)



Tune from pseudogap into superconductor

RVB Liquid →	superconductor
holons →	condense
spinons →	BCS quasiparticle
visons →	hc/2e vortex

Set-up: Superconductor with Hole



prepare vison

detect vison

cool sc in non-zero B-field, trapping hc/2e flux

heat into pseudogap and turn off B-field

cool back into sc - nucleate hc/2e vortex if vison is trapped

Vison detection experiment

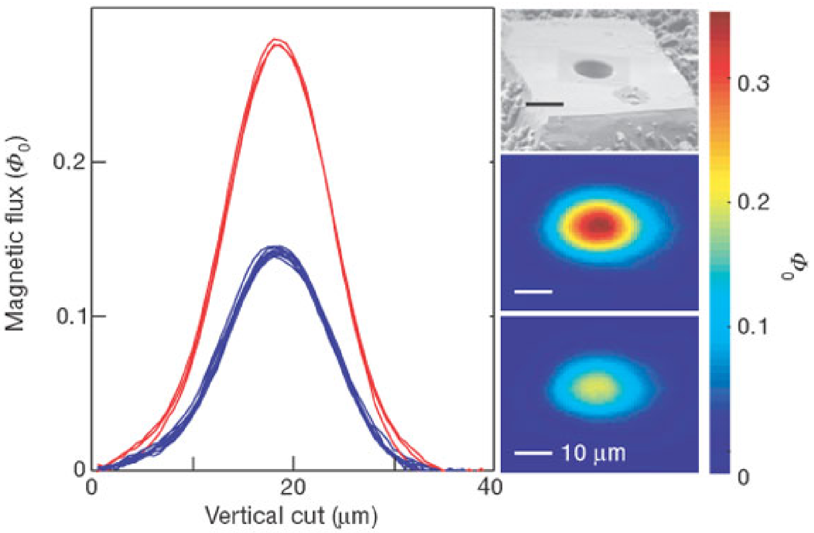
K. Moler et. al. *Nature* **414**, 887-889 (2001)

Single crystal of very underdoped $YBa_2Cu_3O_{6.35}$ with $T_c = 10$ K

Drill 10 micron diameter hole in 40 x40 (micron)^2 sample

Measure trapped flux with scanning SQUID magnetometer

Cycle T into/out of sc



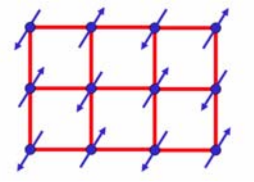
No trapped flux - ie. vison escaped from hole

Conclusion: Pseudogap apparently not Z_2 spin liquid

Avoid symmetry breaking without hole doping?

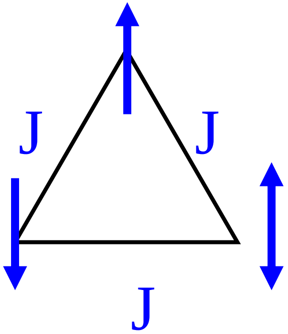
Mott insulator - symmetry breaking instability - unit cell doubling

eg. AFM order in undoped cuprates

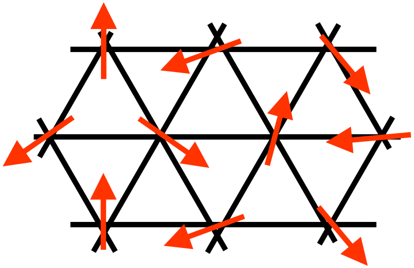


Geometrical Frustration

Triangular plaquette of antiferromagnetically coupled spins cannot all be “satisfied”



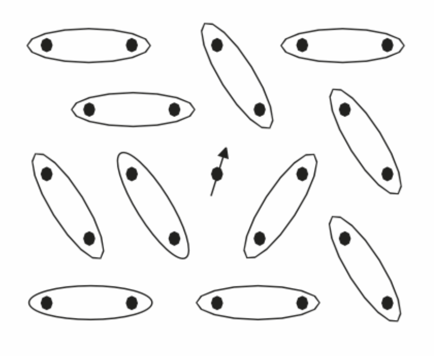
Oftentimes the system can still find a way to order, but not always. Example: Coplaner 3-sublattice arrangement on triangular lattice -



Spin liquids come in two varieties:

• "Topological Order"

- Gap to all excitations in the bulk
- Ground state degeneracy on a torus
- "Fractionalization" of Quantum numbers
- Decoherence free Quantum computing

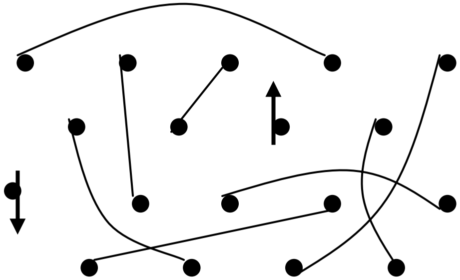


RVB State

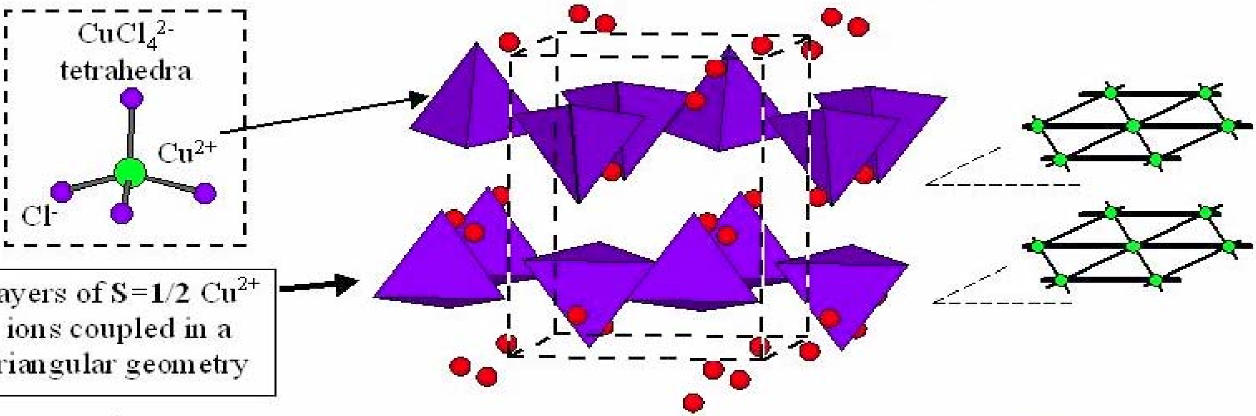
Free "spinon", with s=1/2

• "Algebraic or critical Spin Liquid"

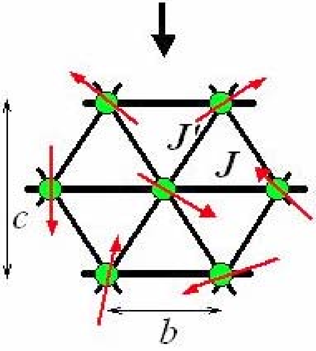
- Gapless Excitations
- "Critical" Power Laws
- No free particle description



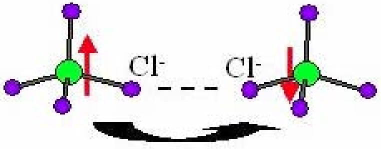
Crystal structure and magnetism of Cs_2CuCl_4



Layers of $S=1/2$ Cu^{2+} ions coupled in a triangular geometry

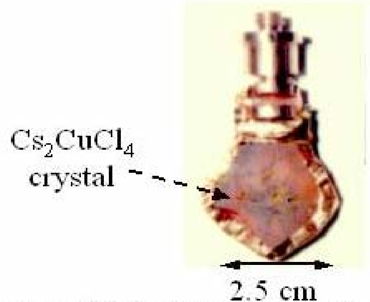


J, J' antiferromagnetic



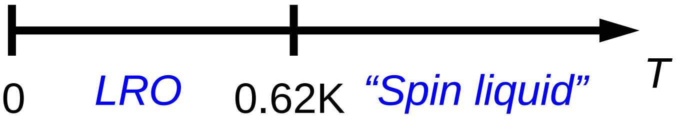
Low antiferromagnetic superexchange $J \sim 4$ K

=> saturation fields ~ 9 T



Large high-purity single crystals grow from solution

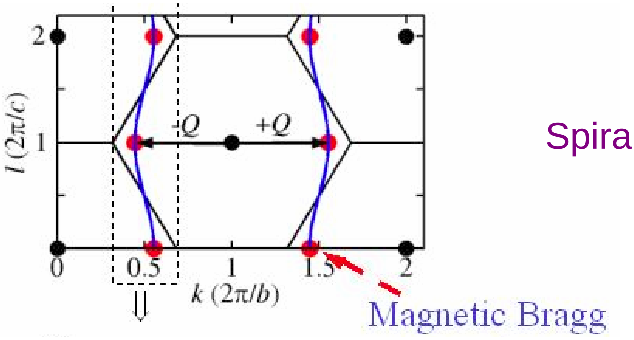
Phase Diagram:



Neutron Scattering from Cs_2CuCl_4

R. Coldea *et al*. PRL **86,** 1335 (2001)
Y. Shimizu *et al*. PRL **91**, 107001 (2003)

- Magnetic Bragg peaks at Q



Spiral Order at low T

- Continuum Inelastic Scattering near Q

$$\langle S^+(\mathbf{Q},\omega)S^-(-\mathbf{Q},-\omega)\rangle \sim \frac{A}{\omega^{2-\eta}} \qquad \eta \approx 0.75$$

Power law scaling: Suggestive of “critical” spin liquid ??

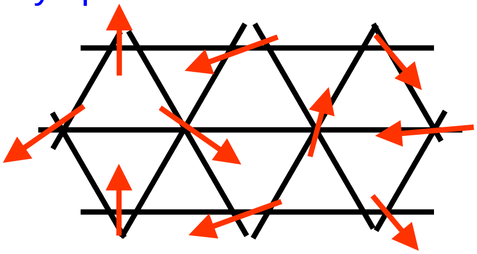
Theoretical approach to s=1/2 Triangular AFM

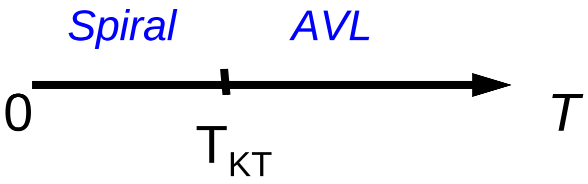
(Alicea, Motrunich, MPAF)

- Duality from spins to "vortices"
- Fermionize vortices via Chern-Simons flux attachment
- Flux smeared mean-field treatment
- Dirac equation with U(1) gauge field and SU(4) flavor symmetry (QED3)

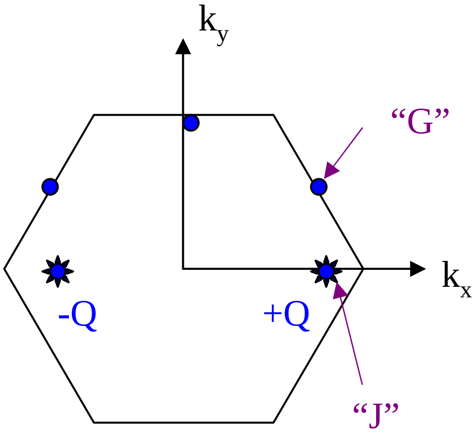
- ***"Algebraic vortex liquid" (AVL)***
  - "Critical Phase" with no free particle description
  - No broken symmetries - rather an emergent global SU(4) symmetry
  - Power-law correlations
  - Stable gapless spin-liquid (no fine tuning)

Weak instability to spiral coplaner driven by spin-orbit interactions





Comparison with Cs_2CuCl_4



1st B-zone of triangular lattice

Key prediction:

$$\langle S^+(\mathbf{Q}_j,\omega)S^-(-\mathbf{Q}_j,-\omega)\rangle \sim \frac{A_j}{\omega^{2-\eta}}$$

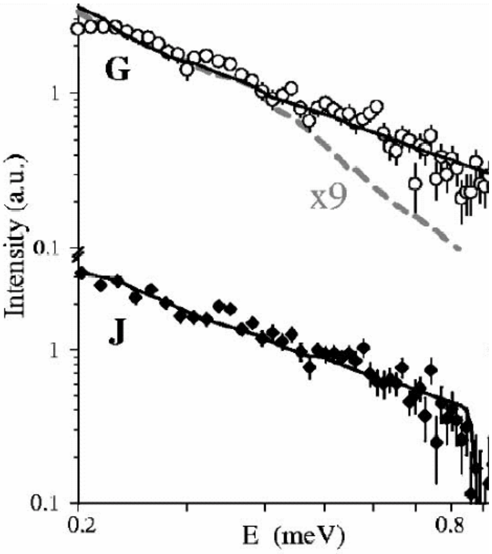
Same η for all $\mathbf{Q}_i; \quad i = 1, 2, ..., 5$

Inelastic Neutron Scattering

Experiments find same scaling exponent "near" G, J

- but energy scans are NOT at fixed k
- closer look between J and G would be good

R. Coldea, D. A. Tennant, and Z. Tylczynski
Phys. Rev. B **68**, 134424 (2003)



Summary

- Materials with one d or f shell electron per atom are often insulating - Mott insulators - in contrast to band theory predictions.
- If not symmetry broken, the ground state of such a Mott insulator is guaranteed to be an exotic “spin liquid”
- Spin liquids come in two varieties - “topological” and “critical”
- Cuprate pseudogap is not the (simplest) Z_2 topologically ordered spin liquid. So what is it??
- Frustrated AFM (eg triangular) show promise for observing “critical” spin liquids
- “Exotic” quantum world awaits discovery and exploration!