Mott Insulators:
Exotica inside Crystals

- Interest: Novel Electronic properties of Mott insulators
- Particularly: “Spin liquids” -disordered due to “frustration”
- Theory: Explore various such “Spin liquids” - topological, critical
- Goal: Find experimental examples, and understand them!

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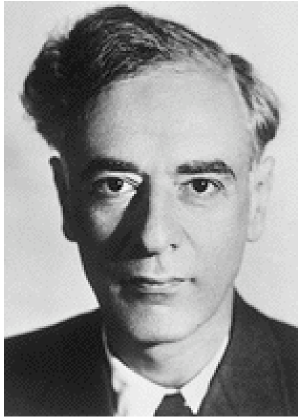
Quantum Theory of Solids: Standard Paradigm

Landau Fermi Liquid Theory



Accounts for electronic behavior of simple metals, insulators and semiconductors

Landau Theory of Phase Transitions

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

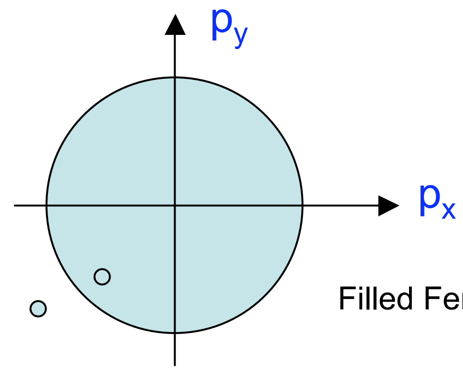
- superconductors,
- ferromagnets,
- antiferromagnets,
- charge density waves,
- spin density waves,…

Fermi Liquid Theory

Free Fermions

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

particle/hole excitations



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

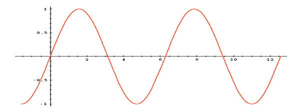
Particle/hole excitations are long lived near FS

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

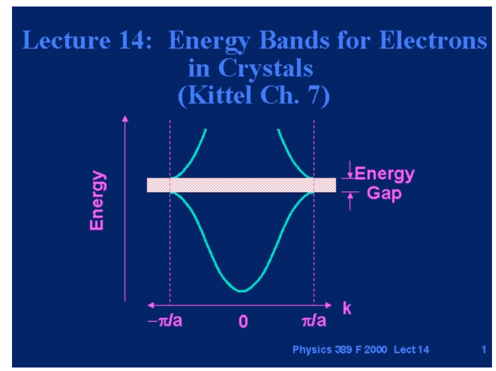
Vanishing decay rate

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

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

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

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”

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:

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

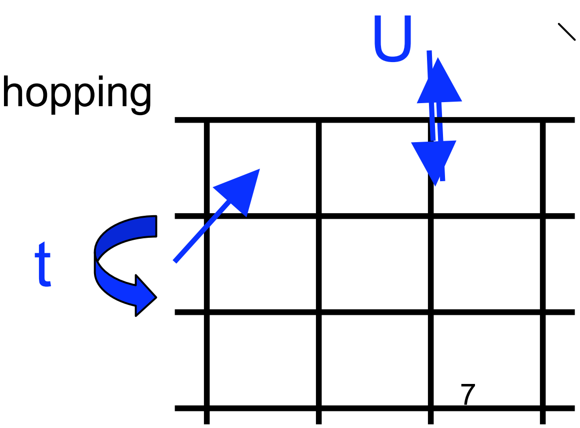
inter-site hopping

on-site repulsion

electron creation/annihilation operators on sites of lattice

$$c_{i\alpha}^{\dagger}, c_{i\alpha}; \qquad \alpha = \uparrow, \downarrow$$

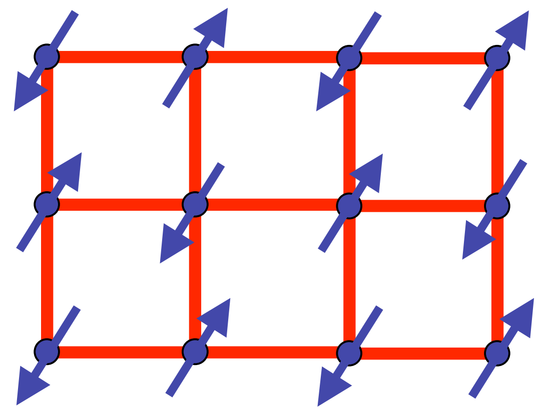
$$[c_{i\alpha}, c_{j\beta}^{\dagger}]_{-} = \delta_{ij} \delta_{\alpha\beta}$$



Spin Physics

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

(this is a Mott insulator)



Residual spin physics:

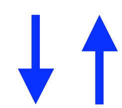
$$\vec{S}_i; \quad [S_i^\mu, S_j^\nu] = i\delta_{ij}\epsilon_{\mu\nu\lambda}S_i^\lambda$$

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



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

Symmetry Breaking

Mott Insulator ➡ Unit cell doubling ("Band Insulator")

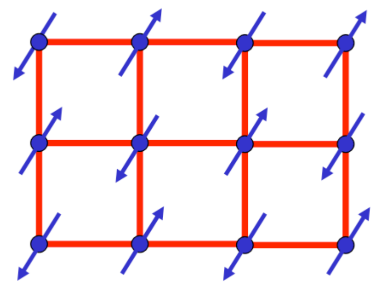
Symmetry breaking instability

- Magnetic Long Ranged Order (spin rotation sym breaking)

Ex: 2d square Lattice AFM

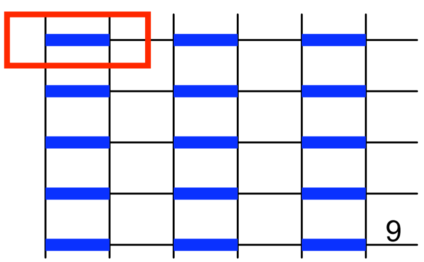
(eg undoped cuprates La_2CuO_4)

2 electrons/cell



- Spin Peierls (translation symmetry breaking)

2 electrons/cell



Valence Bond (singlet)

$$— = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

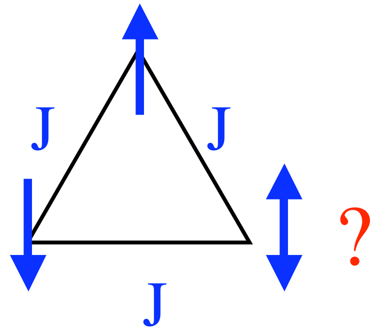

ORDERVILLE


Fisher's
GOLD &
JEWELRY
ROCKS & GEMS

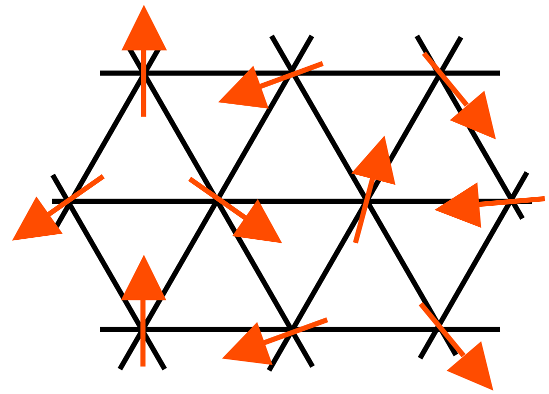
Suppress the Ordering

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 Liquid: Holy Grail

Theorem: Mott insulators with one electron/cell and NO symmetry breaking, have low energy excitations above the ground state with $(E_1 - E_0) < \ln(L)/L$ for system of size L by L.   (Matt Hastings, 2005)

> Remarkable implication - Exotic Quantum Ground States are guaranteed in a Mott insulator with no broken symmetries

Such quantum disordered ground states of a Mott insulator are generally referred to as “spin liquids”

Spin liquids come in two varieties:

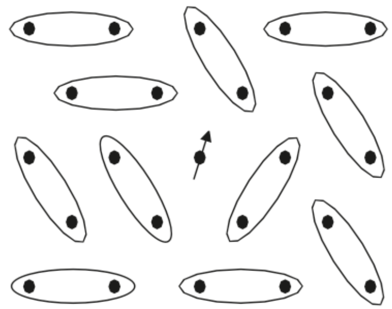
• "Topological Order" (Lecture 2)

• Gap to all excitations in the bulk

• Ground state degeneracy on a torus

• "Fractionalization" of Quantum numbers

• Decoherence free Quantum computing



RVB State

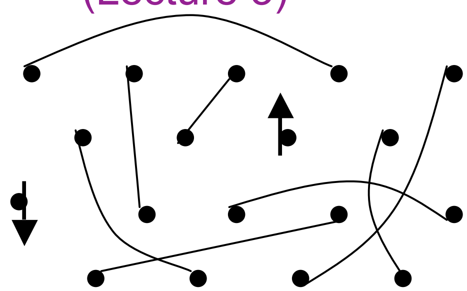
Free "spinon", with s=1/2

• "Algebraic or critical Spin Liquid" (Lecture 3)

• Gapless Excitations

• "Critical" Power Laws

• No free particle description



Lecture 4: Quantum phase transitions

- T=0 phase transitions in the ground state
- Standard Paradigm: Landau theory - order parameter
- "Deconfined" quantum criticality - violates Landau

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 guaranted to be an exotic “spin liquid”

- Spin liquids come in two varieties - “topological” and “critical”