MOTT TRANSITIONS

Oxide Interface Group Meeting
Outline

- What is a Mott insulator?
- Mott transitions as quantum phase transitions
- Physics near the Mott transition
Imagine varying the lattice spacing of a solid

- When the spacing is large compared to the Bohr radius, it should be an insulator

\[ 2\Delta = E_{\text{ion}} - E_{\text{aff}} \]

- When spacing is reduced, orbitals overlap, and bands form, leading to a metallic state
Usually, we require a Mott Insulator to have an odd number of electrons per unit cell.

Then the “atomic” states are degenerate.

Usually there is magnetic (or occasionally more complex) order at low temperature.

A complication: the low-T state usually has an enlarged unit cell, with an even number of electrons in it, that could be interpreted as a band insulator.
Physically, a Mott Insulator is one which is insulating due to interaction-induced localization, not due to band physics.

This is a question of energy scales.

Deep in the Mott state:

- Magnetic insulator
- Paramagnetic insulator

\[ 0 \quad T_{\text{mag}} \quad \Delta \sim U \quad T \]
Hubbard Model

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

- Two dimensionless parameters
  - \( U/(z t) \): Coulomb energy/Bandwidth
  - Filling \( n = \langle n_{i\uparrow} + n_{i\downarrow} \rangle \) (\( = 1 \) for MI)
- More generally have
  - multiple hopping parameters
  - more orbitals
  - more interactions
When doped away from half-filling, the Mott insulator becomes a (bad) conductor

- particles/holes can hop without additional energy cost
- many complex things can occur: phase separation, stripes, localization...
Mott Transition

- Mott state
  - Single particle gap
  - insulating
  - local moments

- Metal
  - Fermi surface
  - conducting
  - Pauli paramagnetism

U/W

Mott Insulator

filling control

n

Metal

bandwidth control
Quantum Phase Transitions

- Any phase transition at $T=0$ is a quantum phase transition (QPT).
  - “Quantum” because at $T=0$ there is perfect phase coherence.
  - At $T>0$, there is always some finite dephasing length, beyond which the physics is effectively classical.
- The Mott transition (at $T=0$) is a QPT.
**Types of QPTs**

- **First order transition**
  - “Level crossing”
  - Two phases are unrelated
  - Observables jump at QPT

- **Second order transition**
  - Phases smoothly transform into one another
  - Diverging correlation length
  - “Quantum criticality”
Mott originally argued for a first order transition. But he changed his mind later! If it is, a line of first order transitions must exist at $T>0$. This is often seen in experiment.
First order Mott transitions

- Vanadates (from Mott’s RMP!)
- \( \text{V}_2\text{O}_3 \) phase diagram
  - McWhan, 1971
- Nickelates (perovskites)
  - first order
**First order Mott Transitions**

- Seen in several organic quasi-2d conductors

\[ \kappa-(ET)_2\text{Cu}[\text{N(CN)}_2]\text{Cl} \]

\[ \kappa-(ET)_2\text{Cu}_2(\text{CN})_3 \]
Second order Mott transitions?

- Second order (continuous) QPTs are rare, but they do exist
  - e.g. magnon BEC transitions (edges of magnetization plateaus)

But I do not know of any experimentally clear examples of continuous Mott transitions
Continuous Mott Transitions?

- Theoretically, this is an active suggestion
- Might occur in frustrated situations
- Even if it doesn’t, the most interesting situation is when the transition is only “weakly” first order
- In this case, the material combines features of metals and insulators, and exhibits strong fluctuations, near the transition
Some physical features
Features of the Mott Transition

- On the metallic side
  - formation of band at the Fermi energy
  - mass enhancement
  - anomalous scattering
- On the insulating side
  - magnetic order
  - quasiparticle gap
**Band evolution**

- High energy scale picture (deep in the Mott state)
  - Zaanen-Sawatzky-Allen scheme
In perovskites

![Graph showing the electronic and magnetic phase diagrams for perovskite-type compounds. The graph illustrates the variation of the quasiparticle residue energy with respect to the correlation strength (U/W) and the charge disproportionation (Δ/W).]

- **Insulator**: Demonstrates the phase where the material is electrically insulating.
- **Mott insulator**: Indicating the regime with strong electron-electron repulsion.
- **Charge Transfer insulator**: Signifying the transition from metallic to insulating behavior.

**Graphical Illustration**

- **Metals** and **Insulators** are marked on the diagram, showing the phase boundaries.
- **TiO** and **O 2p** states are highlighted, with **CT** (charge transfer) band marked.
- **YTiO** is depicted, showcasing the optical conductivity.

**Example**

- **Optical conductivity (Ω^{-1}cm^{-1})**: Demonstrates the range from 1000 to 3000, indicating strong optical properties.
- **Energy (eV)**: From 0 to 6, reflecting the electronic transitions.

The diagram is a visual representation of the electronic and magnetic phase diagrams for perovskite-type compounds, highlighting the correlation effects and the role of the ionic radius on the electronic properties.
Band Evolution

- Low energy picture
- Different scenarios
Band Evolution

- Low energy picture
- Different scenarios

DOS

E

DMFT
Filling Control

• Spectral weight transfer

Sawatzky

FIG. 12(a) Density of states of La$_{2-x}$Sr$_x$CuO$_4$

FIG. 12(b) Chemical potential shift as a function of hole concentration in La$_{2-x}$Sr$_x$CuO$_4$

Shifts expected from band-structure calculation and the $T$ term in specific heat (which is proportional to the quasiparticle DOS at $E_F$) are also plotted in (b).
Mass Enhancement

- LaNiO$_3$: $\gamma/\gamma_{\text{band}} = 10$
- V$_{2-y}$O$_3$
There is a lot left for the next meeting!