Plan for today

1. Comments on the Hubbard model & its limitations.

2. Slides on some illustrative correlated materials

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Active band near chem. potl.

Derive effective interacting model by projecting Coulomb interaction to active band.

Use Wannier basis to get an effective lattice model of the form

\[ H = \sum \epsilon_{n\sigma} (c_n^\dagger \sigma c_n^\sigma + h.c.) \]
\[ U_{RR'}^{kk} (k_x k_y) \]
\[ + \sum_{R_1 R_2 R_3 R_4} \sum_{\alpha \beta \gamma \delta} c_{\alpha R_1}^T c_{\beta R_2}^T c_{\gamma R_3} c_{\delta R_4} \]
\[ U(CR_i R_j) = \frac{1}{2} \int d^d x \int d^d x' w_{R_i}^* (x) w_{R_j} (x) \]
\[ \frac{e^2}{|x - x'|} \left( \frac{w_{R_2}^* (x') w_{R_4} (x)}{R_2 R_4} \right) \]

If \( w_{R_i} (x) \) is strongly localized near \( x \approx R_i \), then biggest \( U \) is the on-site "Hubbard" interaction

\[ U = \frac{1}{2} \int_{x \neq x'} |w_{R_i} (x)|^2 \frac{e^2}{|x - x'|} \]
In principle we could keep terms when $R_1 = R_3$, $R_2 = R_4$ to write

$$U(R_1, R_2) = \frac{1}{2} \int \int \left| w_{R_1}(x) \right|^2 \frac{e^{2}}{|x - x'|} \left| w_{R_2}(x') \right|^2$$

This is a Coulomb repulsion between $e$'s at $R_1$ and $R_2$.

Qualitatively: $U(R_1, R_2)$ is long ranged and decays as

$$\frac{1}{|R_1 - R_2|}$$

for large $|R_1 - R_2|$. This is how we can boot a fire
Coulomb interaction is important for some phenomena (e.g., plasma oscillations in a metal etc.) - but the essential difficulty in treating the strong correlation problem comes from the short range part. This motivates studying the simplified Hubbard model.

Other complications in real materials.

1. Phonons

2. There may be more than one active band near the chem. pott.
   - then the tight-binding model must involve multiple orbitals
3. Depending on the system, spin-orbit may need to be included as an essential feature of the low energy model.
(Certainly true for eg Ir oxides and all f-electron Mott insulators)

4. A fundamental limitation: If the active band is topological, then we know we cannot write down localized Wannier functions. If such a band is partially filled, & has strong e-e interactions, then the Hubbard-like
Lattice formulation fails.

Eg: (a) A partially filled Chern band (no Wannier rep. possible)

(b) A partially filled symmetry protected topological band.

Here a localized Wannier rep. is possible but at the cost of losing a local realization ("on-site") of some physical symmetry.

Keeping track of such a non-trivial symmetry is hard (a dangerous strategy).

Despite these limitations, the Hubbard
model is a useful toy model to study competition between local physics of interactions and "itinerant" physics of the band kinetic energy.

Conde phase diagram:

Dimensions parameters $U/E$ and $\nu$.

$\nu = \# \text{ of } e^s / \text{unit cell}$.

Diagram:

- Band insulator
- Metal
- Fully filled band

x-axis: $y=0$, $y=1$, $y=2$

y-axis: Metal, Band insulator

$U/E$ parameter variation