Plan for today

1. Comments on Mott insulators and quantum magnetism
2. Microscopic validity of "Hubbard-like" models.

Hubbard model at filling $1 \text{e}^{-/\text{site}}$:

Large-$U$ limit: "charge gap" $\sim O(U)$

and in perturbation theory in $t/U$, at $O(t^2/U)$, spin degeneracy is lifted by

$H_{\text{eff}} = \sum_{i<j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$

$J_{ij} > 0$, $\sim O(t^2/U)$

Higher orders of $t/U$: Different
- "Tij" will involve higher order terms in \( \frac{1}{N} \).

- New \( Tij \)'s will be generated with longer range than the \( Tij \)'s.

- Generate "multiple spin ring exchange" terms which involve cyclic permutations of spins along loops.

Postpone discussion of \( q \)-\( \mu \) magnetoism to later.

For now return to the basic question of the origin & validity of
Hubbard-type models in real solids.

Empirically, Mott insulators are typically found in materials where the active $e^-$s occupy narrow bands where Coulomb interaction can overwhelm the $e^-$ K.E.

(And of course integer # of $e^-$ per atom)

Such narrow bands are typically formed out of atomic d or f orbitals.

Classic examples of Mott insulators:

Transition metal oxides (NiO, MnO, FeO, V$_2$O$_3$,
Sulfides (NiS, NiS₂)
halides (MnF₂, K₂NiF₄, TlOCl)

La₂CuO₄

All of these involve 3d orbitals.

As the first d-shell, 3d orbital is close to the atomic nucleus - this enhances "on-site U" & decreases inter-site hopping thus enabling the Mott insulator.

Interesting example: 5d-based Mott insulator, e.g., Sr₂IrO₄,
where the active cs derive from Ir 5d orbitals.
Compared to 3d, these 5d orbitals are much more extended—how can they form a Mott insulator?

Answer: It has strong spin-orbit coupling which splits the wide bands derived from the 5d orbitals into narrower bands.

Microscopic validity of a "Hubbard-like" model.

Consider a system described by the "full" many-body Hamiltonian

\[ H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \sum_i V(\mathbf{r}_i) \]

\[ + \sum_{i \neq j} \frac{e^2}{4\pi \varepsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} + \text{electron-ion} \]
$V$ is the periodic ion-ion Coulomb potential of the ions. Diagonalizing $H_0$ alone will give energy bands $E(k)$. We are interested in a situation where bands are partially filled, i.e., chemical potential lies in the middle of a band.

Consider a particularly simple case where

0) there is one "active" band
interacts by chem. potl, and that is separated from remote bands by a band gap $E_0$.

2) Typical Coulomb e-e interaction strength $U \ll E_0$.

Let band width of active band be $W$. We make no a priori assumption about $U/W$.

If $U/W \ll 1$, material is weakly interacting.

Interesting regime is when $U/W \geq 1$. 
In the $\frac{1}{\epsilon_0}$ limit, it is appropriate to build an effective model by projecting $H_{\text{ee}}$ to just the active band.

To do this cleanly, first let us go to a 2nd quantized description:

$$H = \int d^d x \sum_\alpha \bar{\psi}_\alpha^+(x) \left(-\frac{\alpha^2}{2m} + V(x)\right) \psi_\alpha(x)$$

$$+ \gamma_3 \int d^d x \int d^d x' \bar{\psi}_\alpha^+(x) \psi_\alpha^+(x') \psi_\alpha(x')$$

$$\frac{e^2}{|x-x'|} \psi_\alpha(x') \psi_\alpha(x)$$

Go to the Wannier basis:
\[ |n\hat{R}\rangle = \frac{1}{\sqrt{N}} \sum_k e^{-i\mathbf{k} \cdot \hat{\mathbf{R}}} |n\hat{\mathbf{k}}\rangle \]

\( \hat{c} \) destruction operator

\[ \psi_x (\mathbf{r}) = \sum_{n\hat{R}} \psi_{n\hat{R}} (\mathbf{r}) e^{i\mathbf{k} \cdot \hat{\mathbf{R}}} c_{n\hat{R}a} \]

\( k \)-space operators for band states

Define lattice \( \hat{c} \) operators

\[ c_{n\hat{R}a} = \frac{1}{\sqrt{N}} \sum_k e^{i\mathbf{k} \cdot \hat{\mathbf{R}}} c_{n\hat{\mathbf{k}}a} \]

so that

\[ \psi_x (\mathbf{r}) = \sum_{n\hat{R}} \psi_{n\hat{R}} (\mathbf{r}) c_{n\hat{R}a} \]

The one-electron Ham.
lattice tight binding model

\[ H_0 = \sum_n \sum_{R'} e^{i c_n} \psi^+_n \psi^+_R \eta_n \bar{\eta}_R + h.c. \]

Now re-express Coulomb interaction in this basis.

\[ H_{e-e} = \frac{1}{2} \int d^d x \int d^d x' \psi^+_\alpha(x) \psi^+_\alpha(x') \]

\[ \frac{e^2}{|x-x'|} \psi_\alpha(x') \psi_\alpha(x) \]

\[ = \frac{1}{2} \int d^d x \int d^d x' \sum_n \sum_{R_1, R_2} w^+_{\eta_R_1}(x) w^+_{\eta_R_2}(x') \]

\[ \left\{ c_{\eta_R_1}^+ c_{\eta_R_2}^+ \right\} \frac{e^2}{|x-x'|} w_{\eta_{R_3}}(x') \]

\[ w_{\eta_{R_4}}(x) \]

\[ c_{\eta_{R_1}}^+ c_{\eta_{R_2}}^+ \eta_{R_3} \eta_{R_4} \]
\[ U(L; R; \beta) = \frac{1}{2} \int x^{\kappa} \left( \frac{e^2}{1-x^2} \right) \left( w_{\eta_1}^*(\kappa) w_{\eta_2}^*(\kappa) \right) \left( w_{\eta_1}^*(\kappa) w_{\eta_2}^*(\kappa) \right) \]

So far everything is exact.

To project onto "active band", in \( H_0 \), we simply drop all terms except those corresponding
\[ \psi_{\alpha}(\vec{r}) = \psi_{\eta_0} \phi_{\alpha}(\vec{r}) \cdot \eta_0 \phi_{\alpha} \]

(Drop the subscript \( \eta_0 \) when there is no chance of confusion).

In the interaction, if \( \mathcal{U}(L, R; \eta) \)

for any \( \eta : \eta = \eta_0 \) is \( \ll E_0 \)

then we can ignore all terms

where all \( \eta \neq \eta_0 \), i.e., we only keep

\[ \mathcal{U}(\eta_0 R_1, \eta_0 R_2, \eta_0 R_3, \eta_0 R_4) \]

\[ \cong \mathcal{U}(R_1, R_2, R_3, R_4) \]

We get
$$H_{\text{eff}} = \sum_{RR'} t_{RR'} \left( c_{R}^{+} c_{R'} + h.c. \right)$$

$$+ \sum_{R_1 R_2 R_3 R_4} U(R_1 R_2 R_3 R_4)$$

$$c_{R_1}^{+} c_{R_2}^{+} c_{R_3} c_{R_4}$$

$$U(R; \vec{R}) = \frac{1}{2} \int_{\vec{x}' \vec{x}} \left( \begin{array}{c} w_{R_1}^{x}(x) \\ w_{R_2}^{x}(x) \end{array} \right) \left( \begin{array}{c} w_{R_1}^{x'}(x') \\ w_{R_2}^{x'}(x') \end{array} \right)$$

$$\frac{e^2}{1_{x-x'}} \left( \begin{array}{c} w_{R_2}^{x}(x) \\ w_{R_4}^{x}(x) \end{array} \right)$$

If Wannier functions are strongly localized at their centers, then in the integral above, the biggest term will be

$$U(R, R, R, R) \equiv U = \text{on-site}$$
\[
U = \frac{1}{2} \int d^d x \, d^d x' \left| \psi_R(x) \right|^2 \frac{e^2}{|x-x'|} \left| \psi_R(x') \right|^2
\]

In principle, we could keep other terms where \( R_1 = R_2 \), and \( R_3 = R_4 \) to write

\[
U(R_1, R_2) = \frac{1}{2} \int \int d^d x \, d^d x' \left| \psi_R(x) \right|^2 \frac{e^2}{|x-x'|} \left| \psi_R(x') \right|^2
\]

= Coulomb repulsion between \( e^- \)'s at sites \( R_1 \) and \( R_2 \).