1.1 Correlations versus hopping — introduction

In Theoretical Solid State Physics I, you have learned about the Bloch theorem and tight-binding models. In the limit of noninteracting electrons, this led to band theory with good quasimomentum $\mathbf{k}$ and wave functions $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \psi_{\mathbf{k}}(\mathbf{r})$ with periodic $\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{\mathbf{k}}(\mathbf{r}) \quad \forall \mathbf{R} \in \mathbb{R}^3$ on the Bravais lattice.

However, electrons (quasi-electrons) in a solid do interact in reality, with lattice vibrations (electron-phonon interaction) and one another (electron-electron interaction). This leads to interesting phases of matter beyond simple metals and band insulators, namely for instance charge-density waves (CDW), spin-density waves (SDW), more exotic forms of magnetism or charge order, or superconductivity.

An important class of materials are Mott insulators; they do not conduct electricity although their Fermi level lies within a partially filled band, and band theory predicts them to be metallic. The reason is strong electron-electron Coulomb repulsion.

The basic model that contains the competition between kinetic and potential $(e-e)$ energy is the Hubbard model.
Hubbard model:

- minimal model to understand intrachain electron systems
- introduced in early 1960s to model transition-metal monoxides (FeO, NiO, CoO), which are antiferromagnetic insulators despite being predicted to be metals by band structure theory
- exactly solvable only in $D=1$ (Lieb & Wu 1968 via "Bethe ansatz") and $D=2$ (Metzner & Vollhardt 1989) + Georges and Kotliar 1992 via "dynamical mean-field theory"
- 2D Hubbard model is relevant to high-temperature cuprate superconductors
- many numerical techniques developed to tackle Hubbard model and its derivatives.

This lecture: basic notions and conceptual understanding

1.2 Recap: Creation and annihilation operators ("2nd quantization")

Reminder: ladder operators $\hat{a}$, $\hat{a}^+$ of harmonic oscillator

\[
\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i \sqrt{\frac{1}{2m\omega\hbar}} \hat{p}
\]

\[
\hat{a}^+ = -i \hat{x} - i \hat{p}
\]

\[
[\hat{p}, \hat{x}] = -i\hbar \quad \Rightarrow \quad [\hat{a}, \hat{a}^+] = 1
\]

\[
\hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} m\omega^2 \hat{x}^2 = \hbar \omega (\hat{a}^+ \hat{a} + \frac{1}{2})
\]

Number operator $\hat{n} = \hat{a}^+ \hat{a} \quad \Rightarrow \quad \hat{H} = \hbar \omega (\hat{n} + \frac{1}{2})$

Ground state $|0\rangle$: $\hat{a} |0\rangle = 0$, $\hat{H} |0\rangle = \frac{\hbar \omega}{2} |0\rangle$
Excited states:  
\[ \hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \]
\[ \hat{a} |n\rangle = \sqrt{n} |n-1\rangle \]

\[ \Rightarrow \hat{H} |n\rangle = \hbar w (n+\frac{1}{2}) |n\rangle \]

Finite-temperature expectation value
\[ \langle \hat{A} \rangle = \frac{1}{Z} \text{Tr} [A e^{-\beta \hat{H}}] \]

and in particular
\[ \langle n \rangle = \frac{1}{e^{\beta \hbar w} - 1} \]

Bose-Einstein distribution

\[ \Rightarrow \hat{a}, \hat{a}^\dagger \text{ are bosonic annihilation and creation operator's} \]

[from here on; \( \hbar = 1 \), \( k_B = 1 \)]

The Hubbard Hamiltonian is also written using creation and annihilation operators. These are fermionic and differ from the bosonic ones in several ways.

**Conceptual difference:** fermionic creation and annihilation operators are not defined based on \( \hat{x} \) and \( \hat{p} \). They "stand on their own".

Moreover, it makes sense to define them even though (quasi-) electrons are never created or annihilated in solid state physics.

**Technical differences:**

(i) fermionic operators \( \hat{c}_j^\dagger \) (\( \hat{c}_j \)) create (annihilate) an electron with spin \( \sigma \) on site \( j \) of a lattice.

\[ \Rightarrow \text{come with flavors} \]

\[ \text{Usually in a Wannier orbital localized around } \hat{r}_j \]

(ii) occupation number states come with a collection of occupation numbers \( \{ n_{1\uparrow}, n_{2\downarrow}, n_{3\uparrow} \ldots \} \)
(iii) and commutation relations
\[ \{ \hat{A},\hat{B}\bar{B} \} = \hat{A}\bar{B} + \bar{B}\hat{A} \]
\[ \{ \hat{C}_{\sigma_0},\hat{C}_{\sigma_1}^+ \} = \delta_{\sigma_0}\sigma_1 \]
\[ \{ \hat{C}_{\sigma_0},\hat{C}_{\sigma_1}^+ \} = 0 = \{ \hat{C}_{\sigma_1},\hat{C}_{\sigma_0}^+ \} \]

- e.g., \( \hat{C}_{\tau\tau}^+ \hat{C}_{\tau\tau} = 1 - \hat{C}_{\tau\tau}^+ \hat{C}_{\tau\tau} \)
\( \hat{C}_{\tau\tau} \hat{C}_{\tau\tau} = - \hat{C}_{\tau\tau} \hat{C}_{\tau\tau} \)

For a single flavor \( \hat{C}_{\sigma_0}^+ |0\> = |1\> \) creates a fermion when acting on the vacuum \( |0\> \) of that flavor. Here \( |0\> \) means \( |0\>_{\sigma_0} \).

**Quiz:** Show how the Pauli principle follows from the anti-commutation algebra.

**Hint:** Compute \( \hat{C}_{\sigma_0}^+ \hat{C}_{\sigma_0}^+ |0\>_{\sigma_0} \).

**Bookkeeping:** \( |\text{vac}\> \equiv 1000000... \Rightarrow (\text{all possible fermion flavors for given system for each possible \( \sigma_0 \).}) \)
\( |101000... \equiv \hat{C}_1^+ \hat{C}_3^+ |\text{vac}\> \)
\( |101000... \equiv \hat{C}_2^+ \hat{C}_4^+ |\text{vac}\> = - |101000... \) differ by a sign

\( \Rightarrow \) need to define a convention for the construction of basis states in occupation number basis.

Once defined: stick to convention!
1.3 Hubbard Hamiltonian (HH)

Goal: A minimal model to study competition between delocalization in energy bands and localization due to Coulomb repulsion.

Scope: Materials with (strongly correlated electrons), cold atoms in optical lattices (hyperfine states mimic spin up/down).

Remark: 1) "Condensed matter physics" has by now replaced the term "solid state physics" as an umbrella term for all things related to "condensed matter" (beyond solids).

2) In recent years, we speak of "quantum materials" as materials in which quantum effects manifest themselves at meso- and macroscopic scales. The term usually encompasses materials with strong correlations ("where band theory fails") and/or topology/quantum geometry (another topic not part of this lecture).

Hubbard model: Consider a single isolated energy band near the Fermi level. (Multi-band generalizations are straightforward but deserve separate treatment — not here.)

\[ \hat{H} = -t \sum_{\langle j, \ell \rangle} \sum_{\sigma} (\hat{c}^+_j \hat{c}_{\ell \sigma} + \hat{c}_{\ell \sigma} \hat{c}^+_j) + U \sum_j n_{j \uparrow} n_{j \downarrow} - \mu \sum_j (n_{j \uparrow} + n_{j \downarrow}) \]

More precisely:

\[ \hat{H} = -t \sum_{\langle j, \ell \rangle} \sum_{\sigma} (\hat{c}^+_j \hat{c}_{\ell \sigma}) \]

\[ \text{nearest-neighbor} \langle j, \ell \rangle \]

\[ t \text{ hopping amplitude} \]

\[ U \text{ on-site Coulomb repulsion, "Hubbard U"} \]

\[ n_{j \sigma} = \hat{c}^+_j \hat{c}_{j \sigma} = \text{number operator} \]

\[ \mu \text{ chemical potential} \]

(Grand-canonical ensemble)
1.4 Symmetries

As usual, symmetries help simplify the solution to a problem. E.g., block-diagonalize a matrix by exploiting eigenbasis of operators that commute with Hamiltonian.

Important symmetry for HH: **particle-hole symmetry (PHS).**

PHS is secured by restricting hopping to only nearest-neighbors on a **bipartite lattice** (lattice that has A-B sublattice structure):

![Bipartite Lattice Diagram](image)

- e.g., 1D chain, 2D square lattice, 2D honeycomb lattice, 3D cubic lattices, ...
  - not true for triangular lattice

Define new operators:  
\[ d_{e\sigma}^+ = (-1)^k d_{e\sigma}, \quad \text{where } (-1)^k = \begin{cases} +1 & \text{if } k \in A \\ -1 & \text{if } k \in B \end{cases} \]

This defines a particle-hole transformation (PHT) because  
\[ d_{e\sigma}^+ d_{e\sigma} = 1 - C_{e\sigma} d_{e\sigma}^+ C_{e\sigma} \]

which implies  
\[ \langle C_{e\sigma} d_{e\sigma} \rangle = 1 \quad \Rightarrow \quad \langle d_{e\sigma}^+ d_{e\sigma} \rangle = 0, \]

\[ u = 0, \quad u' = 0. \]

**Quiz:** Apply the PHT to the HH.

Kinetic energy:  
\[ C_{e\sigma} C_{e\sigma}^+ = (-1)^k d_{e\sigma}^+ d_{e\sigma} = d_{e\sigma}^+ d_{e\sigma} \]

**U term:**  
\[ U \langle n_{j\uparrow} n_{j\uparrow} \rangle = U \left( 1 - \tilde{n}_{j\uparrow} \right) \left( 1 - \tilde{n}_{j\downarrow} \right) \]

with  
\[ \tilde{n}_{j\sigma} = d_{j\sigma}^+ d_{j\sigma} \]

\[ = U \tilde{n}_{j\uparrow} \tilde{n}_{j\downarrow} - U \left( \tilde{n}_{j\uparrow} + \tilde{n}_{j\downarrow} \right) + U \]

just an offset

**Chem. pot. term:**  
\[ -\mu \left( n_{j\uparrow} + n_{j\downarrow} \right) = -\mu \left( \tilde{n}_{j\uparrow} + \tilde{n}_{j\downarrow} \right) - \mu \]

just an offset
Aside from trivial number terms that we can ignore (why?), we map $HHH$ onto itself (for no hopping on bipartite lattice) with
\[ t \rightarrow t, \quad U \rightarrow U, \quad \mu \rightarrow U - \mu. \]

The last replacement suggests the choice $\mu = \frac{U}{2}$ as a condition for PHS. Then $\mu = \frac{U}{2} \rightarrow U - \mu = U - \frac{U}{2} = \frac{U}{2}$ is the identical mapping. We will see that $\mu = \frac{U}{2}$ is precisely the condition for half-filling for the PHS $HHH$, i.e., one electron per site on average. This can also be absorbed into the $U$ term:

\[
H_{\text{PHS}} = -t \sum_{\langle ij \rangle} \sum_{\sigma = \uparrow, \downarrow} (c_{i\sigma}^+ c_{j\sigma} + c_{i\sigma}^+ c_{j\sigma}) + U \sum_{j} \left( \Psi_{j\downarrow} - \frac{1}{2}\right) \left( \Psi_{j\uparrow} - \frac{1}{2}\right) - \mu \sum_{j\sigma} \Psi_{j\sigma}
\]

\[
\downarrow \quad \text{on average} \quad \frac{1}{2} \text{ electron of each spin per site}
\]

This is a redefined chemical potential, since the $\frac{U}{2}$ part was absorbed into the $U$ term.

How do observables transform under $HHH$?

Density $\rho = \frac{N}{L} = \frac{\langle \sum_{\langle i \rangle} c_{i}^+ c_{i} \rangle}{L}$

\[
\sum_{\langle i \rangle} c_{i}^+ c_{i} \xrightarrow{HHH} \sum_{\langle i \rangle} (1 - d_{i\uparrow} d_{i\downarrow})
\]

\[ \Rightarrow \quad \rho = \frac{1}{4} \frac{1}{2} - \rho \quad (2 \text{ is from } \sum_{\sigma = \uparrow, \downarrow}) \]
\[-\mu \sum_{\ell \sigma} c_{\ell \sigma}^+ c_{\ell \sigma} + \mu \sum_{\ell \sigma} d_{\ell \sigma}^+ d_{\ell \sigma} \text{ VHS} \]

\[= \sum_{\ell \sigma} \rho_{\ell \sigma} \text{ trivial shift for fixed } \mu \]

\[
\mu = 0: \quad \mathcal{P}(0) = 2 - \mathcal{P}(-\mu) \Rightarrow \mathcal{P}(0) = 1
\]

The PM Hubbard model (bipartite lattice, no hopping only) has a symmetric phase diagram about half-filling.

1.5 Single-site limit

Set \(t = 0\) \(\mu \notin H \) \(\Rightarrow \) independent sites. 
In this case: \([\hat{H}, n_{i\sigma}] = 0\) (prove this!)

\(\Rightarrow\) can use number eigenstates for each site as basis that simultaneously diagonalize \( \hat{H} \).

\(\Rightarrow\) drop site index.

states: \(\{ |0\rangle, |1\rangle, |u\rangle, |T\rangle \}\)

| \( |0\rangle \) | \( |n_n = 0, n_u = 0\rangle \)
| \( |1\rangle \) | \( |n_n = 1, n_u = 0\rangle \)
| \( |u\rangle \) | \( |n_n = 0, n_u = 1\rangle \)
| \( |T\rangle \) | \( |n_n = 1, n_u = 1\rangle \)

Quiz:

A. Compute the partition function \( Z = \text{Tr} [e^{-\beta \hat{H}}] \) at inverse temperature \( \beta \equiv \frac{1}{k_B T} \).

B. Compute the occupation \( \mathcal{P} = \langle n_n + n_u \rangle \).

C. Plot \( \mathcal{P}(\mu) \) for \( t = 0, U = 4, \beta \in \{4, 2, 1\} \) and \( \mu \in [-5, 5] \).

D. Plot the compressibility \( \chi_e = \frac{\partial \mathcal{P}}{\partial \mu} \) for the same parameters as in (C).
Answer: \[ \hat{H} = U (n_{\uparrow} - \frac{1}{2}) (n_{\downarrow} - \frac{1}{2}) - \mu (n_{\uparrow} + n_{\downarrow}) \]

(A) \[ \hat{H} |\uparrow\rangle = \frac{\mu}{4} |\uparrow\rangle \]
\[ \hat{H} |\uparrow\rangle = (\frac{\mu}{4} - \mu) |\uparrow\rangle \]
\[ \hat{H} |\downarrow\rangle = (\frac{\mu}{4} - 2\mu) |\downarrow\rangle \]
\[ Z = \text{Tr} \left( e^{-\beta \hat{H}} \right) = e^{-\beta \frac{\mu}{4}} + 2 e^{-\beta (\frac{\mu}{4} - \mu)} + e^{-\beta (\frac{\mu}{4} - 2\mu)} \]

(B) \[ \langle n_{\uparrow} + n_{\downarrow} \rangle = Z^{-1} \text{Tr} \left[ (n_{\uparrow} + n_{\downarrow}) e^{-\beta \hat{H}} \right] \]
\[ = Z^{-1} \left( 2 e^{-\beta (\frac{\mu}{4} - \mu)} + 2 e^{-\beta (\frac{\mu}{4} - 2\mu)} \right) \]

\[ \mu = 0 \Rightarrow \langle n_{\uparrow} + n_{\downarrow} \rangle = 1 \quad \text{(true even for } t \neq 0, \text{ see above)} \]

\( \beta = 4 \) (low \( T \))
\( \beta = \frac{1}{2} \) (high \( T \))

\( t = 0 \quad U = 4 \)

\( \beta = 4 \) = incompressible inside Mott gap; \( \delta \epsilon = 0 \)
\( \beta = \frac{1}{2} \) = precursor of Mott insulating behavior in extended system for large \( U/t \) ratio.