① Hubbard model

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 <u>noninteracting electrons</u>, this led to <u>band theory</u> with good quasimomentum $\vec{k}$ and wavefunctions $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$ with periodic $u_{\vec{k}}(\vec{r}+\vec{R}) = u_{\vec{k}}(\vec{r})$ $\forall\ \vec{R} \in \{\vec{R}\}$ on the Bravais lattice.

However, electrons (quasielectrons) in a solid do interact in reality: with lattice vibrations (<u>electron-phonon interaction</u>) and one another (<u>electron-electron interaction</u>). This leads to interesting <u>phases of matter</u> 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 <u>Mott insulators</u>: 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 (e-e) Coulomb repulsion. The basic model that contains the competition between kinetic and potential (e-e) energy is the <u>Hubbard model</u>.

(Chopping)

Hubbard model:

- minimal model to understand interacting 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 $D = \infty$ (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

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

$$\hat{a}^+ = \text{—"—} \quad -i \quad \text{—"—}$$

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

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

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

Ground state $|0\rangle$: $\hat{a}|0\rangle = 0$, $\hat{H}|0\rangle = \frac{\hbar\omega}{2}|0\rangle$

Excited states: $\hat{a}^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$

$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$

$\Rightarrow \hat{H}\,|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle$

Finite-temperature expectation value $\langle \hat{A} \rangle = Z^{-1} \mathrm{Tr}\left[\hat{A} e^{-\beta \hat{H}}\right]$

and in particular $\langle \hat{n} \rangle = \frac{1}{e^{\beta\hbar\omega} - 1}$ Bose-Einstein distribution

$\rightarrow$ $\hat{a}, \hat{a}^\dagger$ are bosonic annihilation and creation op's

[from here on: $\hbar \equiv 1$, $k_B \equiv 1$]

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

<u>Conceptual difference</u>: fermionic creation and annihilation operators are <u>not</u> 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 <u>never</u> created or annihilated in solid state physics.

<u>Technical differences:</u>

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

$\Rightarrow$ come with flavors

↑ usually in a Wannier orbital localized around $\vec{r}_j$

(ii) occupation number states come with a collection of occupation numbers $|n_{1\uparrow}\, n_{2\uparrow}\, n_{3\uparrow}\, n_{1\downarrow} \ldots\rangle$

(iii) anti commutation relations

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

$$\{\hat{c}_{j\sigma}, \hat{c}^{+}_{l\sigma'}\} = \delta_{jl}\,\delta_{\sigma\sigma'}$$

$$\{\hat{c}^{+}_{j\sigma}, \hat{c}^{+}_{l\sigma'}\} = 0 = \{\hat{c}_{j\sigma}, \hat{c}_{l\sigma'}\}$$

→ e.g., $\hat{c}_{1\uparrow}\,\hat{c}^{+}_{1\uparrow} = 1 - \hat{c}^{+}_{1\uparrow}\,\hat{c}_{1\uparrow}$

$$\hat{c}_{1\uparrow}\,\hat{c}_{1\downarrow} = -\,\hat{c}_{1\downarrow}\,\hat{c}_{1\uparrow}$$

For a single flavor $\hat{c}^{+}_{j\sigma}|0\rangle = |1\rangle$ creates a fermion when acting on the vacuum $|0\rangle$ of that flavor. Here $|0\rangle$ means $|0\rangle_{j\sigma}$.

> Quiz: Show how the Pauli principle follows from the anticommutation algebra.

Hint: Compute $\hat{c}^{+}_{j\sigma}\,\hat{c}^{+}_{j\sigma}|0\rangle_{j\sigma}$.

Bookkeeping: $|\text{vac}\rangle \equiv |0\,0\,0\,0\,0\,0\ldots\rangle$ ← all possible fermion flavors for given system

$$|1\,0\,1\,0\,0\,0\ldots\rangle \equiv \hat{c}^{+}_{1}\,\hat{c}^{+}_{3}\,|\text{vac}\rangle$$

$$|1\,0\,1\,0\,0\,0\ldots\rangle \equiv \hat{c}^{+}_{3}\,\hat{c}^{+}_{1}\,|\text{vac}\rangle = -\,|1\,0\,1\,0\,0\,0\ldots\rangle$$

differ by a sign

⇒ 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 mimick 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. (Multiband generalizations are straightforward but deserve separate treatment — not here.)

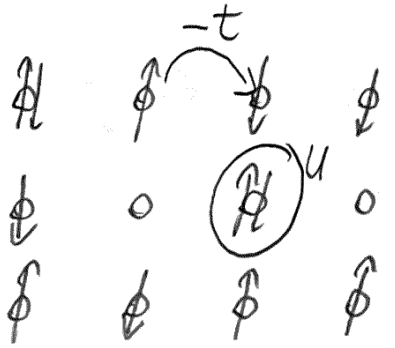
⇒ effective low-energy description

(write operators without hats)

Hubbard Hamiltonian

$$\hat{H} = -t \sum_{\langle j,\ell\rangle} \sum_{\sigma=\uparrow,\downarrow} \left(c_{j\sigma}^{+} c_{\ell\sigma} + c_{\ell\sigma}^{+} c_{j\sigma} \right) + U \sum_{j} n_{j\uparrow} n_{j\downarrow} - \mu \sum_{j} \left(n_{j\uparrow} + n_{j\downarrow} \right)$$

more precisely: $\hat{H} - \mu \hat{N} = \dots$



t nearest-neighbour $\langle j,\ell \rangle$ hopping amplitude (sites on lattice)

U on-site Coulomb repulsion, "Hubbard U"

$n_{j\sigma} \equiv c_{j\sigma}^{+} c_{j\sigma}$ = number operator

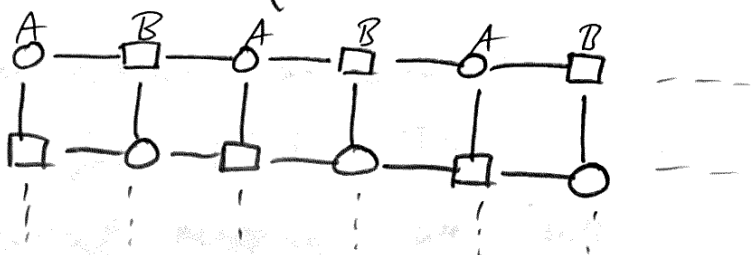
μ chemical potential (grand-canonical ensemble)

1.4 Symmetries

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

Important symmetry for HH: <u>particle-hole symmetry</u> (PHS).

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



e.g. 1D chain, 2D square lattice, 2D honeycomb lattice, 3D cubic lattices, ...

<u>not</u> true for triangular lattice

Define new operators: $d^+_{\ell\sigma} \equiv (-1)^\ell c_{\ell\sigma}$ where $(-1)^\ell = \begin{cases} +1 & \ell \in A \\ -1 & \ell \in B. \end{cases}$ This defines a particle-hole transformation (PHT) because $d^+_{\ell\sigma} d_{\ell\sigma} = 1 - c^+_{\ell\sigma} c_{\ell\sigma}$, which implies

$\langle c^+_{\ell\sigma} c_{\ell\sigma} \rangle = 1 \iff \langle d^+_{\ell\sigma} d_{\ell\sigma} \rangle = 0$,

$u \quad = 0 \qquad\qquad u \quad = 0$.

Quiz: Apply the PHT to the HH.

Kinetic energy: $c^+_{i\sigma} c_{j\sigma} = \underbrace{(-1)^{j+\ell}}_{\equiv -1} d_{i\sigma} d^+_{j\sigma} \overset{\text{anticomm.}}{=} d^+_{j\sigma} d_{i\sigma}$

U term: $U n_{j\uparrow} n_{j\downarrow} = U (1-\tilde{n}_{j\uparrow})(1-\tilde{n}_{j\downarrow})$ with $\tilde{n}_{j\sigma} = d^+_{j\sigma} d_{j\sigma}$

$= U \tilde{n}_{j\uparrow} \tilde{n}_{j\downarrow} - U (\tilde{n}_{j\uparrow} + \tilde{n}_{j\downarrow}) + U$ ← just an offset

chem. pot. term: $-\mu (n_{j\uparrow} + n_{j\downarrow}) = +\mu (\tilde{n}_{j\uparrow} + \tilde{n}_{j\downarrow}) - \mu$ ← just an offset

⇒ aside from trivial number terms that we can ignore (Why?), we map HH onto itself (for nn hopping on bipartite lattice) with

$$t \to t$$
$$U \to U$$
$$\mu \to U - \mu.$$

The last replacement suggests the choice $\mu = \frac{U}{2}$ as a condition for PHS. Then $\mu = \frac{U}{2} \to U - \mu = U - \frac{U}{2} = \frac{U}{2}$ is the identical mapping. We will see that $\mu = \frac{U}{2}$ is precisely the condition for <u>half-filling</u> for the PHS HH, i.e., one electron per site on average.

This can also be absorbed into the U term:

$$H_{PHS} = -t \sum_{\langle ij \rangle} \sum_{\sigma=\uparrow,\downarrow} \left(c^\dagger_{j\sigma} c_{i\sigma} + c^\dagger_{i\sigma} c_{j\sigma} \right) + U \sum_j \left(n_{j\uparrow} - \frac{1}{2} \right) \left(n_{j\downarrow} - \frac{1}{2} \right) - \mu \sum_{j\sigma} n_{j\sigma}$$

$\frac{1}{2}$: on average $\frac{1}{2}$ 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 PHT?

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

L = # sites

$$\sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} \xrightarrow{PHT} \sum_{i\sigma} \left(1 - d^\dagger_{i\sigma} d_{i\sigma} \right)$$

$$\Rightarrow \quad \rho \xrightarrow{PHT} 2 - \rho \qquad \left(2 \text{ is from } \sum_{\sigma=\uparrow,\downarrow} \right)$$

$$-\mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} \xrightarrow{\text{PHT}} \underbrace{-2L\mu}_{\text{trivial shift for fixed } \mu} + \underbrace{\mu \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma}}_{\text{sign of } \mu \text{ reversed}}$$

$$\Rightarrow \quad \rho(\mu) = 2 - \rho(-\mu)$$

$$\mu = 0: \quad \rho(0) = 2 - \rho(0) \Rightarrow \boxed{\rho(0) = 1}$$

"half-filling"

The PHS Hubbard model (bipartite lattice, nn hopping only) has a symmetric phase diagram about half-filling.

1.5 Single-site limit

Set $t = 0$ in HH $\Rightarrow$ L independent sites.

In this case: $[\hat{H}, n_{j\sigma}] = 0$ (prove this!)

$\Rightarrow$ can use number eigenstates for each site as basis that simultaneously diagonalizes $\hat{H}$.

$\Rightarrow$ drop site index.

states: $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$

$$|0\rangle \equiv |n_\uparrow = 0, n_\downarrow = 0\rangle$$
$$|\uparrow\rangle = |n_\uparrow = 1, n_\downarrow = 0\rangle$$
$$|\downarrow\rangle = |n_\uparrow = 0, n_\downarrow = 1\rangle$$
$$|\uparrow,\downarrow\rangle = |n_\uparrow = 1, n_\downarrow = 1\rangle$$

Quiz:

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

(B) Compute the occupation $\rho = \langle n_\uparrow + n_\downarrow \rangle$.

(C) Plot $\rho(\mu)$ for $t = 0$, $U = 4$, $\beta \in \{4, 2, \frac{1}{2}\}$ and $\mu \in [-6, 6]$.

(D) Plot the compressibility $\kappa = \frac{\partial \rho}{\partial \mu}$ 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) $\hat{H}|0\rangle = \frac{U}{4}|0\rangle$

$\hat{H}|\uparrow\rangle = (-\frac{U}{4} - \mu)|\uparrow\rangle$

$\hat{H}|\downarrow\rangle = (-\frac{U}{4} - \mu)|\downarrow\rangle$

$\hat{H}|\uparrow\downarrow\rangle = (\frac{U}{4} - 2\mu)|\uparrow\downarrow\rangle$

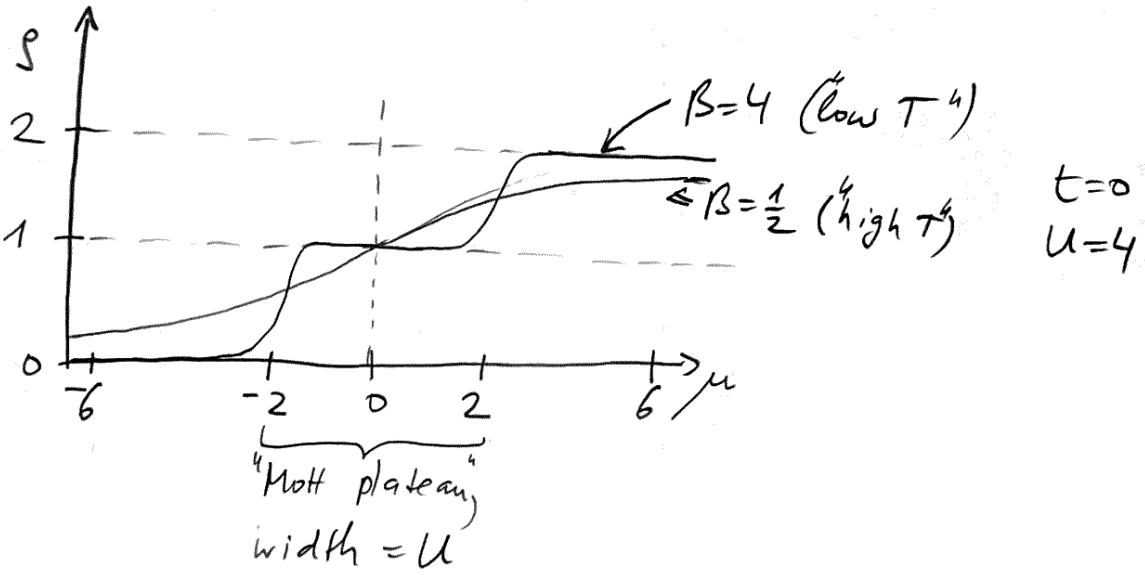
$Z = \mathrm{Tr}[e^{-\beta H}] = e^{-\beta\frac{U}{4}} + 2e^{-\beta(-\frac{U}{4}-\mu)} + e^{-\beta(\frac{U}{4}-2\mu)}$

(B) $\rho = \langle n_\uparrow + n_\downarrow \rangle = Z^{-1}\,\mathrm{Tr}[(n_\uparrow + n_\downarrow)e^{-\beta H}]$

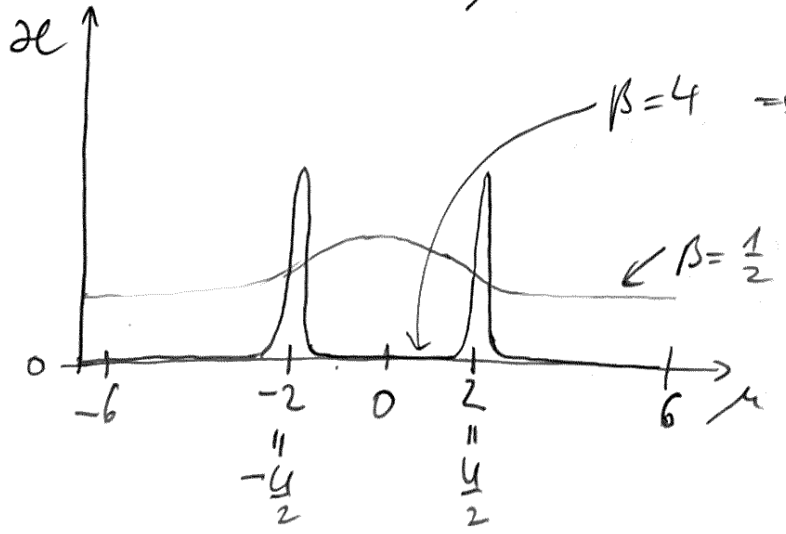
$= Z^{-1}\left(2e^{-\beta(-\frac{U}{4}-\mu)} + 2e^{-\beta(\frac{U}{4}-2\mu)}\right)$

$\mu = 0 \Rightarrow \rho = 1$ (true even for $t \neq 0$, see above)

(C)



(D) Compressibility $\varkappa = \frac{\partial \rho}{\partial \mu}$ is the derivative of the plot above



$\beta = 4$ ⇒ incompressible inside "Mott gap": $\varkappa = 0$

⇒ precursor of Mott-insulating behavior in extended system for large U/t ratio.