The Hubbard model

IMPRS Focus Course, November 2018

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This lecture is based in large parts on the lecture notes by Richard Scalettar; see lab. sanef.org/teaching for details.

Tutorials and active learning: I highly encourage participants to take part in the hands-on part of this lecture. Basic knowledge of Mathematica, Matlab, Python, or higher-level programming required.
Hubbard model is minimal model to understand interacting electron systems: Mott insulators, magnetic phases, unconventional superconductors...

written down in early 1960's initially to model transition-metal monoxides (FeO, NiO, CoO), which are antiferromagnetic insulators even though electronic structure methods predicted them to be metals

exactly solvable only in two extreme limits of spatial dimension, \( D=1 \) (Lieb & Wu) and \( D=\infty \) (dynamical mean-field theory (DMFT) by Vollhardt & Mihrovic, Jorge & Kotliar).

2D Hubbard model particularly interesting because it contains a lot of physics relevant to high-temperature cuprate superconductors

many numerical techniques developed to tackle HTSC; here: basic introduction to get up to speed to learn more about advanced techniques and recent results
 Reminder: ladder operators $\hat{a}, \hat{a}^+$ of harmonic oscillator

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

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

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

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

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

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

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

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

4) Finite-temperature expectation value $\langle \hat{A} \rangle = Z^{-1} \text{Tr} [\hat{A} e^{-\beta \hat{H}}]$ and in particular $\langle \hat{n} \rangle = \frac{1}{e^{\beta \hbar \omega} - 1}$ Bose-Einstein distribution.

$\Rightarrow \hat{a}, \hat{a}^+$ are boson annihilation and creation operators

[From here on: $\hbar = 1$, $\hbar \omega \equiv 1$].

$\hat{H}$ is also written with creation and annihilation operators. These are 'fermionic' and differ from the bosonic ones in several ways.
Conceptual differences: Fermionic creation and annihilation operators are not defined based on $\psi, \rho$!
They rather stand on their own.

Technical differences:

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

(ii) Come with flavors.

(iii) Occupation numbers states come with collection of occupation numbers $|n_{1\uparrow}, n_{2\downarrow}, n_{3\uparrow}, n_{4\uparrow}, n_{5\downarrow}, n_{6\uparrow}, n_{7\downarrow}, n_{8\downarrow}, n_{9\uparrow}, n_{10\downarrow}, n_{11\uparrow}, n_{12\downarrow} >$.

(iii) Anti-commutation relations:

\[ \{ \hat{a}_{1\uparrow}, \hat{a}_{2\downarrow}^+ \} = \hat{A}_1 \hat{A}_2 + \hat{A}_2 \hat{A}_1 \]
\[ \{ \hat{c}_{j\sigma}^+, \hat{c}_{j\sigma}' \} = \delta_{jj'} \delta_{\sigma \sigma'} \]
\[ \{ \hat{c}_{j\sigma}, \hat{c}_{j\sigma}' \} = 0 = \{ \hat{c}_{j\sigma}^+, \hat{c}_{j\sigma}' \}. \]

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

A) Show how the Pauli principle follows from the anticommutator algebra.

B) Discuss what it means physically that a fermion is "created" or "annihilated"!

Hint: Do we talk about electron-positron annihilation in a solid?

Bookkeeping:

$$|\text{vac}\rangle = |0\ 0\ 0\ 0\ 0\ 0...\rangle$$

diff by

$$|1\ 0\ 1\ 0\ 0\ 0...\rangle = \epsilon_1^+ \epsilon_3^+ |\text{vac}\rangle$$

a sign

$$|1\ 0\ 1\ 0\ 0\ 0...\rangle = \epsilon_3^+ \epsilon_1^+ |\text{vac}\rangle$$

$$= -|1\ 0\ 1\ 0\ 0\ 0...\rangle$$

Thus we have to define a convention for the order of application of creation operators when building the occupation number states.

Once defined, stick to your convention!
**Hubbard Hamiltonian (HH)**

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

**Recent additional motivation:** optical lattice emulation via fermionic atoms with two hyperfine states corresponding to spin "up" and "down".

**Solids:** Consider cases with a single energy band near the Fermi energy.

$\Rightarrow$ Hubbard model provides effective low-energy description.

**Hubbard Hamiltonian** for the single-band Hubbard model:

\[
\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma = \uparrow, \downarrow} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_j n_{j\uparrow} n_{j\downarrow} - \mu \sum_j (n_{j\uparrow} + n_{j\downarrow}).
\]

- $t$ nearest-neighbor $\langle j,k \rangle$ hopping
- $U$ Hubbard on-site repulsion
- $\mu$ chemical potential
Symmetries help simplify the solution of a problem. For example, we can block-diagonalize the Hamiltonian by choosing an appropriate basis with good quantum numbers.

Important symmetry in the HH: particle-hole symmetry (PHS).

PHS is secured by allowing for any nearest-neighbor hopping, as we will see below.

PHS is important for Quantum Monte Carlo (QMC) simulations and useful for a mapping between the repulsive and attractive HH.

Bipartite lattice: partitioned into A + B sublattices

Define new operators $d^+_e e^{-} = (-1)^e c_{e\sigma}$

Where $(-1)^e = \begin{cases} +1 & e \in A \\ -1 & e \in B \end{cases}$
is a particle-hole transformation because $d^+_e d^+_r = 1 - c^+_e c^+_r$
which means that if $\langle c^+_e c^+_r \rangle = 1 \Rightarrow \langle d^+_e d^+_r \rangle = 0$
and vice versa.

**Question 2:** What happens to $\hat{H}$ under this particle-hole transformation?

**Kinetic Energy:** $c^+_e c^+_r = (-1)^{d_{e}d_{r}} d^+_e d^+_r = d^+_e d^+_r = -1$ for nearest-neighbor hopping

**Interaction Energy:** $U(\hat{n}_j - \frac{1}{2})(\hat{n}_j - \frac{1}{2})$ is unchanged as well

$$= U \hat{n}_j \hat{n}_j - \frac{U}{2} (\hat{n}_j \hat{n}_j + \hat{n}_j \hat{n}_j) + \frac{U}{4}$$

- shift of $\mu$
- trivial offset

$\Rightarrow$ PHS form of Hubbard model with $A-B$ hopping on biparticle $A-B$ lattice:

$$\hat{H} = -t \sum_{\langle \sigma \delta \rangle} (c^+_e c^+_r + c^+_r c^+_e) + U \sum_{\langle j \rangle} (\hat{n}_j - \frac{1}{2})(\hat{n}_j - \frac{1}{2})$$

$$- \mu \sum_{\langle j \rangle} \hat{n}_j$$
How do observables transform under the PHF?

Density \( \rho = \frac{N}{L} = \frac{\langle \sum_{\ell \sigma} c_{\ell \sigma}^+ c_{\ell \sigma} \rangle}{L} \)

\( L = \# \) sites

\[ \sum_{\ell \sigma} c_{\ell \sigma}^+ c_{\ell \sigma} \xrightarrow{\text{PHF}} \sum_{\ell \sigma} \left( 1 - d_{\ell \sigma}^+ d_{\ell \sigma} \right) \]

\( S \xrightarrow{\text{PHF}} 2 - S \quad (2 \text{ for spin } \eta_\text{d}) \)

Chemical potential term:

\[ -\mu \sum_{\ell \sigma} c_{\ell \sigma}^+ c_{\ell \sigma} \xrightarrow{\text{PHF}} -2 \mu + \mu \sum_{\ell \sigma} d_{\ell \sigma}^+ d_{\ell \sigma} \]

(trivial shift for fixed \( \mu \), sign of \( \mu \) reversed)

\[ \Rightarrow \rho(\mu) = 2 - \rho(-\mu) \]

\( \mu = 0 : \rho(0) = 2 - \rho(0) \Rightarrow \rho(0) = 1 \)

"half-filling"

The PHF Hubbard model (bipartite lattice) has a symmetric phase diagram about half-filling!

(relevant) to high-\( T_c \) cuprate superconductors (2D square lattice), where a diagonal next-nearest-neighbor hopping \( t' \) breaks PHF, making the phase diagram asymmetric!
We can set $t=0$ in the HH and have $L$ independent sites.

In this case: $[\hat{H}, \hat{n}_{i0}] = 0$

for each site

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

$\Rightarrow$ drop site index

States: $\{\ket{10}, \ket{11}, \ket{01}, \ket{00}\}$

Quiz 3:

(A) What is the partition function, $Z = \text{Tr} [e^{-\beta \hat{H}}]^2$?

(B) What is the occupation $s = \langle n_1 + n_2 \rangle$?

(C) Plot $s(\mu)$ for $t=0$, $U=4$, $T=\frac{4}{\beta} \in \{2.00, 0.50, 0.25\}$ and an interval $\mu \in [6,6]$

(D) Plot the compressibility $\Delta = \frac{\partial s}{\partial \mu}$ for the same parameters as in (C)

[end of document]
Answer: \[ \hat{H} = U (n+\frac{1}{2}) (n+\frac{1}{2}) - \mu (n_\uparrow + n_\downarrow) \]

\( \hat{A} |0\rangle = \frac{U}{4} |0\rangle \)

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

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

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

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

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

\( \mu = 0; \quad S = 1 \quad \text{(true even for } t \neq 0) \)

\[ t = 0, \quad u = 4 \]

\[ t = 0.25, \quad t = 2 \]

Graph showing the change in the system over time with different values of \( t \) and \( u \).
Compressibility: $\kappa$

\[
\text{Eo.25}
\]

\[
\begin{align*}
-\frac{\mu}{2} & \quad \frac{\mu}{2} \\
\text{inside "Hubbard"} & : \kappa = 0
\end{align*}
\]

- High temperature: Thermal fluctuations lead to sharp jumps in $f(\mu)$

- At $T=0$, $\mu=0$: Quantum fluctuations due to hopping can play a "similar role" destroying the Hubbard plateau — much more complicated than in the simple single-site limit through.

Local spin moment:

\[
\langle m^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n_\uparrow + n_\downarrow \rangle - 2 \langle n_\uparrow n_\downarrow \rangle
\]

\[
= g - 2D
\]

- Local moment is zero for $|1\uparrow\rangle$ and $|1\downarrow\rangle$
- But takes maximal value for either $|1\uparrow\rangle$ or $|1\downarrow\rangle$ ($=1$)

Quiz 4: A) Plot $\langle m^2 \rangle$ as a function of $U$. For $T=2$, $\mu=0$.
Answer: \( \langle m^2 \rangle \)

### Local moments
- Form at large \( U \)
- Destroyed by thermal fluctuations

6. **Noninteracting limit → band picture**

**Starting point:** \( U=0 \) \( H \) \( H \)

\[
\hat{H} = -t \sum_{\langle ij \rangle} \left( \hat{c}_i \hat{c}_j + h.c. \right) - \mu \sum_{j \sigma} \hat{n}_{j\sigma}
\]

**Two points of view:**
- (i) real space
- (ii) momentum space

(i) real space:

\[
[\hat{H}, \hat{N}_\sigma] = 0, \quad [\hat{H}, \hat{N}_\sigma] = 0 \quad \text{(show!)}
\]

\[
\hat{N}_\sigma = \sum_j \hat{n}_{j\sigma}
\]
How to see this? Use a link i-j

\[ \left[ \hat{c}_i^\dagger, \hat{c}_j + \hat{c}_j^\dagger, \hat{c}_i \right] \mid \nu_i + \nu_j \rangle = 0 \]

Which can be shown using \[ [AB, C] = A \{B, C\} - \{A, C\} B \]

\[ \text{anticommutator } BC + CB \]

Another way to understand it: \( \hat{c}_i \hat{c}_j \) does have as many annihilation as creation operators \( \hat{c}_i \hat{c}_j \) does not change the particle number for either spin, and does not flip a spin.

Upshot: sectors of total \( N_p, N_d \) can be considered separately (even for \( U(1) \)).

Example: \( N_p = 1, N_d = 0 \)

Basis:
\[ \{ 1 0 0 0 0 \ldots \}, \{ 0 1 0 0 0 \ldots \}, \ldots \]  
\[ \{ 0 0 1 0 0 \ldots \}, \ldots \]  
\[ \text{dim} = L \text{ for } L\text{-site chain} \]

\[ \hat{H} \mid 0 1 0 0 0 \ldots \rangle = -\mu \mid 0 1 0 0 0 \ldots \rangle \]
\[ -t \mid 1 0 0 0 0 \ldots \rangle \]
\[ -t \mid 0 0 1 0 0 \ldots \rangle \]
In this basis we have:

$$H = \begin{pmatrix} -\mu - t & \cdot & \cdot & \cdot & -t \\ -t & -\mu - t & \cdot & \cdot & \cdot \\ \cdot & -t & -\mu - t & \cdot & \cdot \\ \cdot & \cdot & -t & -\mu - t & \cdot \\ \cdot & \cdot & \cdot & -t & -\mu \end{pmatrix}$$

(periodic boundary conditions)

= hopping between sites 1 and L

= L×L tridiagonal matrix with 'a' as diagonal and 'b' as upper/lower diagonal

Element has eigenvalues:

$$\lambda_n = a + 2b \cos(k_n)$$

$$k_n = \frac{2\pi n}{L}, \quad n = 1, \ldots, L$$

How to see this?

Ansatz: \( u_e = e^{ik_eL} \) into eigenvalue eq.

\( au_e + bu_{e-1} + bu_{e+1} = \lambda u_e \)

together with periodicity \( u_0 = u_L \)

= see forces discrete values of \( k \)
\[ \varepsilon(k) = -2t \cos(k) - \mu \]

and eigenvectors:
\[ (\hat{V}_k)^e = e^{i k e} \]

*ith spatial component of eigenvector with label \( k \).

For \( U=0 \) one can simply build eigenstates for arbitrary particle number as product states (obeying the Pauli principle) of single-particle eigenstates!

(Does not work as soon as \( U \neq 0 \))

(ii) momentum space

Simpler way to solve \( U=0 \) H.H.: canonical transformation of operators:
\[ C_{k0}^+ = \frac{1}{\sqrt{L}} \sum_{e} e^{i k e} C_{e0}^+ \]

Orthogonality:
\[ \frac{1}{L} \sum_{k} e^{i (k_n-k_m)e} = \delta_{n,m} \]
\[ \frac{1}{L} \sum_{n} e^{i k_n (e-j)} = \delta_{e,j} \]
**Quiz 5:**

A) Prove that \( c_{k\sigma}^+ = \frac{1}{N^*} \sum_{k} e^{-i k \cdot \vec{a}_e} c_{k\sigma}^+ \)

("inverse Fourier transform")

B) Prove that
\[
\{ c_{k\sigma}, c_{p\sigma'}^+ \} = \delta_{kp} \delta_{\sigma\sigma'}
\]
\[
\{ c_{k\sigma}, c_{p\sigma'} \} = 0
\]
\[
\{ c_{k\sigma}^+, c_{p\sigma'}^+ \} = 0
\]

(fermionic anticommutation)

Total number operator: \( \hat{N} = \sum_{\sigma} \hat{n}_{k\sigma} = \sum_{k\sigma} \hat{c}_{k\sigma}^+ \hat{c}_{k\sigma} \)

\( \hat{n}_{k\sigma} = c_{k\sigma}^+ c_{k\sigma} \)

**Quiz 6:**

Derive the \( U=0 \) HH in momentum space.

Answers: \( \hat{A} = \sum_{k\sigma} (\varepsilon_k - \mu) c_{k\sigma}^+ c_{k\sigma} = \sum_{k\sigma} (\varepsilon_k - \mu) \hat{n}_{k\sigma} \)

\( \varepsilon_k = -t \sum_{\ell} e^{i k \cdot \vec{a}_e} \)

\( \vec{a}_e = \) real space vectors connecting a site with each nearest neighbor \( \ell \)

1D chain: \( \vec{a}_e = \pm \hat{x} \)

\( \varepsilon_k = -2t \cos k \)

(Lattice Constant = 1)
the noninteracting HH (and multiband/multiorbital generalizations) is determined by the single-particle energy dispersion ("band structure") \( E_k \)

Useful quantity: density of states (DOS)

\[
N(E) = \frac{4}{L} \sum_k \delta(E - E_k)
\]

Continuum limit \( L \to \infty \):

\[
\frac{4}{L} \sum_k \longrightarrow \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d}
\]

\( d \) = spatial dimension

**Quiz 7:** Compute \( N(E) \) for 1D chain, \( E_k = -2t \cos k \).

**Answer:**

\[
N(E) = \frac{4}{\pi} \int_{-\pi}^{\pi} \frac{dx}{4k^2 - x^2} \delta(E - x)
\]

\( x = -2t \cos k, \ dx = 2t \sin k \ \ d k = 2t \sqrt{1 - \cos^2 k} \ \ d k \)

\( k \in [0, \pi] \Rightarrow x \in [-2t, 2t] \)

\[
\int_{-2t}^{2t} \frac{dx}{4k^2 - x^2} \delta(E - x)
\]

N(E) = \begin{cases} \frac{4}{\pi \sqrt{4k^2 - E^2}} & |E| \leq 2t \\ 0 & |E| > 2t \end{cases} \quad (t > 0)

("Van Hove Singularity")

\( N(E) \) divergence!
Knowledge of $\varepsilon_k \Rightarrow$ knowledge of all statistical properties.

Partition function $Z = \text{Tr} [e^{-\beta \hat{H}}] = \prod_k \prod_{\ell \in \{0,1\}} e^{-\beta (\varepsilon_k-k)} = \prod_k \left(1 + e^{-\beta (\varepsilon_k - \mu)}\right)$

Density $f = Z^{-1} \text{Tr} \left[\sum_k \hat{n}_k e^{-\beta \hat{H}}\right] = \sum_k \left(1 + e^{\beta (\varepsilon_k - \mu)}\right)^{-1} = \sum_k f(\varepsilon_k) = \sum_k \frac{1}{e^{\beta (\varepsilon_k - \mu)}} - 1$

Potential function $f(\varepsilon_k) = \left(1 + e^{\beta (\varepsilon_k - \mu)}\right)^{-1}$

Internal energy $E = Z^{-1} \text{Tr} \left[\hat{H} e^{-\beta \hat{H}}\right] = \sum_k \varepsilon_k \left(1 + e^{\beta (\varepsilon_k - \mu)}\right)^{-1} = \sum_k \varepsilon_k f_k$

Entropy $S = \beta (E - F) = \beta E - \ln Z$

\[ F = -\ln Z / \beta \]

\[ E = F - TS \]
Introduction to exact diagonalization: the two-site HH

So far: Single-site HH \rightarrow Mott plateau, local moment formation due to $U$

but: no interplay of $t$ and $U$

minimal extension where exact full diagonalization is still possible: two-site HH

Occupation number basis: $|n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}\rangle$

# basis states: $2^4 = 16$

Use particle number conservation $[\hat{H}, \sum_{i=1,2} \hat{n}_{i\sigma}] = 0$ for each $\pi_{in}$

to divide Hilbert space into sectors:

\[
(n_{1\uparrow} + n_{2\uparrow}, n_{1\downarrow} + n_{2\downarrow}) = (0,0), (1,0), (0,1), (1,1), (2,0), (2,1), (2,2)
\]

9 sectors

dimensions: $1, 2, 1, 2, 4, 2, 4, 1, 2, 1$

- the 1st sectors are trivially diagonal, $E = \pm \frac{U}{2}$
- the 2nd sectors are almost as simple, with one fermion being able to hop, $E = \pm t$; $N=1$ and $N=3$ particle sectors are related by PHS
- there is only one "nontrivial sector" $(1,1)$ with dimension 4

Air 8: Write $H$ in the $(1,1)$ sector and compute its eigenvalues!
Choose a basis \( |\uparrow, \downarrow>, |0, \uparrow>, |N, 0>, |10, \uparrow> \):

\[
\hat{H} = -t \sum_c (C_{1c}^+ C_{2c} + C_{2c}^+ C_{1c}) + U \sum_{i=1}^{N} \langle \hat{n}_i \rangle (\hat{n}_i - \frac{1}{2}) (\hat{n}_i - \frac{1}{2})
\]

in the above basis:

\[
H = \begin{pmatrix}
-u/2 & 0 & -t & -t \\
0 & -u/2 & -t & -t \\
-t & -t & u/2 & 0 \\
-t & -t & 0 & u/2
\end{pmatrix}
\]

check:

- \( t \ C_{1\uparrow}^+ C_{2\uparrow} |0, \uparrow\rangle = \begin{pmatrix} \circ \end{pmatrix} |\uparrow, \downarrow\rangle \) 4-14
- \( t \ C_{1\downarrow}^+ C_{2\downarrow} |0, \uparrow\rangle = \begin{pmatrix} \circ \end{pmatrix} |\uparrow, \downarrow\rangle \) 24
- \( t \ C_{2\uparrow}^+ C_{1\uparrow} |N, 0\rangle = \begin{pmatrix} \circ \end{pmatrix} |\uparrow, \downarrow\rangle \) 13
- \( t \ C_{2\downarrow}^+ C_{1\downarrow} |N, 0\rangle = \begin{pmatrix} \circ \end{pmatrix} |\uparrow, \downarrow\rangle \) 23

Consistency:

\( C_{1\uparrow}^+ C_{2\downarrow} |0, \uparrow\rangle \equiv C_{2\uparrow}^+ C_{1\downarrow} |N, 0\rangle = |\uparrow, \downarrow\rangle \)

Eigenvalues of \( H (\Psi) \): \( -u/2, u/2, \pm \sqrt{4t^2 + u^2/4} \)

For \( u/t \gg 1 \) we can expand

\[
\pm \sqrt{4t^2 + u^2/4} = \pm \frac{u}{2} \sqrt{1 + 16t^2/u^2} \approx \pm \frac{u}{2} \left( 1 + \frac{8t^2}{u^2} \right)
\]

\[
= \begin{cases} 
\frac{u}{2} - \frac{4t^2}{u} = E_5, \text{see below} \\
\frac{u}{2} + \frac{4t^2}{u}
\end{cases}
\]

Together with the states \( |\uparrow, \downarrow\rangle \) and \( |\downarrow, \downarrow\rangle \), which both have energy \( -\frac{u}{2} \), we have in the half-filled
Sector: \((N = 2\) on \(L = 2\) sites):

\[
E \begin{cases} 
+ \frac{U}{2} + \frac{4t^2}{U} & \text{sector with one doubly occupied site} \\
+ \frac{U}{2} & \text{"Nephew gap"} \end{cases}
\]

\[
\rightarrow \begin{cases} 
\text{"Upper Hubbard band"} & \text{(UHB)} \\
\text{\(\frac{U}{2}\) (3-fold degenerate)} & \text{(LHB)} \\
\text{\(\frac{U}{2} - \frac{4t^2}{U}\) (1-fold)} & \text{sector without doubly occupied sites}
\end{cases}
\]

Eigenstates in the lower sector at limit \(U/t \gg 1\):

\[
\begin{aligned}
\text{Singlet} & \quad \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \quad 1 \text{-fold} \\
\text{Triplets} & \quad \frac{1}{\sqrt{2}} \left( |\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle \right) \\
& \quad \begin{cases} 
|\uparrow\uparrow\rangle \\
|\downarrow\downarrow\rangle 
\end{cases} \quad 3 \text{-fold}
\end{aligned}
\]

Single-triplet splitting:

\[
\frac{4t^2}{U} = E_T - E_S
\]

\(\rightarrow\) Mapping of Hubbard model to Heisenberg model in large \(U\) limit! \((\text{spin-1/2})\)

\(\rightarrow\) no hopping of charge, spin physics only

"charge degree of freedom is frozen" for \(U/t \gg 1\)
Heisenberg model on two sites:

\[ A = J \mathbf{S}_1 \cdot \mathbf{S}_2 \]

Trick to obtain spectrum:

\[ J (\mathbf{S}_1 \cdot \mathbf{S}_2) = \frac{J}{2} \left( (\mathbf{S}_1^2 + \mathbf{S}_2^2) - \mathbf{S}_1^2 - \mathbf{S}_2^2 \right) \]

\[ \mathbf{S}_1^2 = \mathbf{S}_2^2 = \frac{3}{4} \]

[cf. \( \mathbf{S}_2^2 = \mathbf{S} (S+1) \)]

Addition of two \( S = \frac{1}{2} \) combines to \( S_{\text{tot}} = 0, 1 \)

\[ \Rightarrow \mathbf{S}_{\text{tot}}^2 = (\mathbf{S}_1^2 + \mathbf{S}_2^2)^2 = 0, 2 \]

\( \Rightarrow \) two options for \( J(\mathbf{S}_1 \cdot \mathbf{S}_2) \):

\[ \frac{J}{2} \left( 0 - \frac{3}{4} - \frac{3}{4} \right) = -\frac{3J}{4} = \tilde{E}_s \quad \text{singlet} \]

\[ \frac{J}{2} \left( 2 - \frac{3}{4} - \frac{3}{4} \right) = +\frac{J}{4} = \tilde{E}_t \quad \text{triplet} \]

\( \Rightarrow \tilde{E}_t - \tilde{E}_s = J \)

Comparison with Hubbard:

\[ J = \frac{4t^2}{U} \]

Pictorial:

- Initial: \[ \uparrow \rightarrow \downarrow \]
- Magnetic exchange coupling: \[ -t \rightarrow t \]
- Exchange of spins via virtual intermediate state:

\[ \frac{(-t) \cdot (-t)}{U} = \frac{t^2}{U} \]

"exchange of spins"
Mott gap and spectral function

Useful quantity for spectroscopy: Green's function

=> spectra of excitations

For example: Single-particle Green's function contains information about single-particle excitations (energies, lifetimes)

We will again focus on the two simple limits

$U=0$ and $t=0$.

8.1 Green's functions at $U=0$

Definition: $G_{j\nu}(T):= \langle C_{j}(T) C_{\nu}^d(0) \rangle$ $(T > 0)$

will $C_{j}(T) = e^{\hat{H}T}C_{j}(0) e^{-\hat{H}T}$ ($\dagger$)

$T$: "imaginary time" (but $T \in \mathbb{R}$)

because in real time we have $C_{j}(t) = e^{i\hat{H}t}C_{j}(0)e^{-i\hat{H}t}$

and $t \rightarrow -iT$ gives ($\dagger$)

\[
\begin{array}{c}
\mathbb{R} \\
\downarrow
\end{array}
\rightarrow \begin{array}{c}
\mathbb{C} \\
\downarrow
\end{array}
\]

Complex-time plane

What is $C_{k}(T)$? We know that $\frac{dC_{k}(T)}{dT} = [\hat{H}, C_{k}(T)]$

and $\hat{H} = \sum_{\nu} \varepsilon_{\nu} C_{\nu}^d C_{\nu}$, such that

\[
\frac{dC_{k}(T)}{dT} = \sum_{k'} \varepsilon_{k'} \left[ C_{k'}^d C_{k} + C_{k} C_{k'} \right] = -\varepsilon_{k} C_{k}
\]

$C_{k}^d C_{k} - C_{k} C_{k} = \delta_{k,0} \delta_{k,0} (-\varepsilon_{k})$
\[ \Rightarrow \ \frac{\partial C_k}{\partial T} = - E_k C_k \Rightarrow \]

\[ C_k(t) = e^{-E_k T} C_k(0) \]

\[ \Rightarrow \ G_{j,n}(T) = \frac{1}{N} \sum_k e^{i k (n-j)} (1 - f_k) e^{-E_k T} \]

\[ \text{using } \langle C_k C_k^+ \rangle = 1 - f_k \]

\[ \Rightarrow \ G_{j,n} = G(j-n) \text{ for translationally invariant } \hat{H} \]

More precisely, \[ G_k(T) := - \langle T_T C_k(T) C_k^+(0) \rangle \]

with time ordering \( T_T \)

\[ T_T \ C_k(T) C_k^+(0) = \begin{cases} 
C_k(T) C_k^+(0) & \text{for } T > 0 \\
-C_k^+(0) C_k(T) & \text{for } T < 0 
\end{cases} \]

\[ \Rightarrow \ G_k(T + \beta) = - G_k(T) \text{ for } -\beta < T < 0 \]

\[ \Rightarrow \text{ define Fourier transform for discrete frequencies} \]

\[ G_k(T) = \frac{1}{\beta} \sum_{\omega_n} G_k(i \omega_n) e^{-i \omega_n T} \]

\[ G_k(i \omega_n) = \int_0^\beta dT \ G_k(T) e^{i \omega_n T} \]

\[ \omega_n = \frac{\pi}{\beta} (2n+1) \text{ Fermionic Matsubara frequencies} \]

We have \[ G_k(T) = \begin{cases} 
- e^{-E_k T (1 - f_k)} & \text{for } 0 < T < \beta \\
e^{-E_k T} f_k & \text{for } -\beta < T < 0 
\end{cases} \]
\[ G_k (i\omega_n) = \frac{1}{i\omega_n - E_k} \]

This noninteracting Green's function forms the basis of many-body perturbation theory and is also a central quantity for DMFT (cf. Chapter 1).

8.2) Greens functions at \( t=0 \)

Consider again a single site with two spins. Let us compute
\[ \hat{H} = U (\hat{n}_s - \frac{1}{2}) (\hat{n}_s - \frac{1}{2}) \]
\[ G^t_{\uparrow} (T) = \langle C^\uparrow (T) C^\downarrow (0) \rangle. \tag{*} \]

We need to consider only two states, namely \( |00\rangle \) and \( |10\rangle \). (Why?)

\[ C^\uparrow (T) C^\downarrow (0) |00\rangle = e^{HT} C^\uparrow e^{-HT} C^\downarrow |10\rangle \]
\[ = e^{HT} C^\uparrow e^{-HT} |10\rangle \]
\[ = e^{HT} C^\uparrow e^{UT/4} |10\rangle \]
\[ = e^{HT} e^{UT/4} |10\rangle \]
\[ = e^{UT/2} |00\rangle \]

**Question:** Repeat the same for \( |10\rangle \)!

What is \( G^t_{\downarrow} (T) \) in (\( * \)?)
Answer: \[ G_\tau (\tau) = Z^{-1} \text{Tr} \left[ e^{-\beta \hat{H}} C_\tau (\tau) C_\tau^+ (0) \right] \]
\[ = Z^{-1} \sum_n e^{-\beta E_n} \langle n | c_\tau (\tau) c_\tau^+ (0) | n \rangle \]

Where \( n \in \{ | 100 \rangle, | 010 \rangle, | 110 \rangle, | 111 \rangle \} \)

for the occupation number state \( | n \rangle = | n_0, n_1, n_2 \rangle \).

We had (c.f. Chapter 5)
\[ Z = \frac{1}{2} e^{-\beta \frac{u}{4}} + 2 e^{\beta \frac{u}{4}} \] \hspace{1cm} (***)

and \[ \langle 00 | \hat{H} | 00 \rangle = \frac{u}{4}, \]
\[ \langle 01 | \hat{H} | 10 \rangle = -\frac{u}{4} \]

\[ \Rightarrow G_\tau (\tau) = Z^{-1} \left[ e^{\frac{u \tau}{2}} \begin{bmatrix} e^{-\beta \frac{u}{4}} & -e^{\beta \frac{u}{4}} \\ -e^{-\beta \frac{u}{4}} & e^{\beta \frac{u}{4}} \end{bmatrix} \right] \] \hspace{1cm} (***)

will \( \tau \) as \( \tau \in (***). \)

Def.: Spectral function \( A(\omega) \) can be defined as
\[ G(\omega) = \int_0^\infty d\omega \ A(\omega) \frac{e^{-\omega \tau}}{1 + e^{-\beta \omega}} \]

or alternatively
\[ A(\omega) \equiv -\frac{1}{\Pi} \text{Im} G^R (\omega) \]
\[ G^R (\omega) \equiv G(i\omega_n) \bigg|_{i\omega_n \rightarrow \omega + i0^+} \]

E.g., for the noninteracting case in 8.1: \[ G^R_k (\omega) = \frac{1}{\omega - E_k + i0^+} \]

Note: \[ \frac{1}{L} \sum_k A_k (\omega) = \frac{1}{L} \sum_k \delta (\omega - E_k) = N(\omega) = \text{Nos for randomized case} \]
Here: \[ A_f(\omega) = \frac{4}{z} \left( \delta(\omega - \frac{u}{2}) + \delta(\omega + \frac{u}{2}) \right) \]

Check: \[ G(\tau) = \int_{-\infty}^{\infty} \frac{4}{z} \left( \delta(\omega - \frac{u}{2}) + \delta(\omega + \frac{u}{2}) \right) \frac{e^{-\omega \tau}}{1 + e^{-\beta \omega}} \]

\[ = \frac{4}{z} \left[ \frac{e^{-\beta \frac{u}{2}}}{1 + e^{-\beta \frac{u}{2}}} + \frac{e^{\beta \frac{u}{2}}}{1 + e^{\beta \frac{u}{2}}} \right] = (x\text{x\text{x}) \checkmark \]

\[ A_0(\omega) \uparrow = A_f(\omega) \]

\[ \delta \text{-function peak width} \]

\[ \text{light \( \frac{1}{2} \)} \]

For the \( \frac{U}{t} \gg 1 \) Hubbard model, we expect a Mott insulator with a Mott gap \( \sim U \)

but what happens on an actual lattice with \( t/\sigma \) is nontrivial!
Ferromagnetism

Both ferromagnetism and antiferromagnetism occur in the Hubbard model.

Ferromagnetism: cf. Miello & Tasaki 1993

- Stoner criterion

\[ \Delta N = N(E_F) \delta E \]

\[ \Rightarrow U N(E_F) > 1 \]

Favors unequal \( \uparrow \) and \( \downarrow \) populations and thus a ferromagnetic polarization.

Very rough estimate (cf. Scalloba notes for the derivation)

Blue point towards regions in parameter space in which ferromagnetism may be found.

\[ \Rightarrow \text{large } U \text{ is good} \]
\[ \Rightarrow \text{large } N(E_F) \text{ is good} \Rightarrow \text{`flat bands'} \]

Another important thing: there should be no other competing and more dominant instability.

- Rigorous result: Nagaoka theorem (also derived by Thouless), Nagaoka 1965:

Certain Hubbard models at \( U = \infty \) and with exactly one hole have ferromagnetic ground states.

* In general still topic of ongoing research
9.2 Antiferromagnetism

(a) strong coupling picture

We already encountered kinetic exchange

\[ J = \frac{4t^2}{U} > 0 \] (antiferromagnetic exchange)

in the two-site H\_H

This expression is valid at \( U/t \gg 1 \),
in which case one can derive the Heisenberg model from the Hubbard model using a Schrieffer-Wolff transformation. (Actually: one can derive the t-J model.)

Hubbard model at half-filling (1 electron per site)

and \( U/t \gg 1 \) \( \Rightarrow \) \( H_{\text{Heisenberg}} = \sum_{\langle ij \rangle} J \mathbf{S}_i \cdot \mathbf{S}_j \).

The Heisenberg model itself can be solved approximately using mean-field theory. You will encounter MFT in the exercise for the antiferromagnetic instability at small \( U/t \ll 1 \) in the itinerant, band-electron limit.
Exercise Sheet 1: Mean-field

- Anti-ferromagnetism in the Hubbard Model (AF)

- Half-filled bipartite lattice has instability towards AF ordering.

- In particular:
  - 3D cubic lattice $T > 0$ (beyond MFT)
  - 2D square lattice at $T = 0$ (Moiré-Legnoz theorem)
  - 1D chain has algebraically decaying AF correlations but no true long-range order

Overall picture for AF order in the HUT (at $n = 1$, superlattice)