The Hubbard model

IMPRS Focus Course, November 2018

Contents

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

Tutorials and active learning: I highly encourage participants to take part in the hands-on parts of this lecture. Basic knowledge of Mathematica, Matlab, Python, or higher-level programming required.

1 Introduction

- 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 & Metzner, Georges & 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 HH; here: basic introduction to get up to speed to learn more about advanced techniques and recent results

(2) Creation and annihilation operators

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

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

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

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

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

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

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

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

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

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

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

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

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

HH is also written with creation and annihilation operators. These are 'fermionic' 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 $\hat{x}, \hat{p}$!
They rather stand on their own.

<u>Technical differences:</u>

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

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

(iii) <u>anti</u> commutation relations

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

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

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

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

$\boxed{\text{Quiz 1:}}$ (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?

// end lecture 1 (90')

<u>Bookkeeping</u>: $|vac\rangle \equiv |0\,00\,000\,\ldots\rangle$

differ by a sign

$$|1\,0\,1\,000\ldots\rangle \equiv \hat{c}_1^{\dagger}\hat{c}_3^{\dagger}|vac\rangle$$

$$\widetilde{|1\,0\,1\,000\ldots\rangle} \equiv \hat{c}_3^{\dagger}\hat{c}_1^{\dagger}|vac\rangle$$

$$= -|1\,0\,1\,000\rangle$$

$\Rightarrow$ we have to define a <u>convention</u> for the order of application of creation operators when building the occupation number states.

Once defined: stick to your convention!

③ Hubbard Hamiltonian (HH)

<u>Goal:</u> A minimal model to study <u>competition</u> 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"]

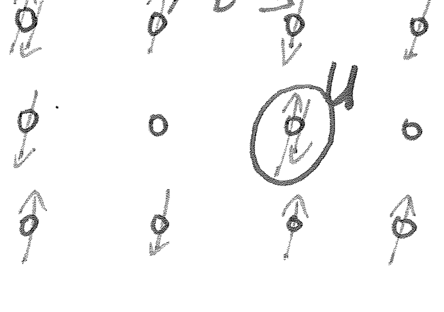
<u>Solids:</u> Consider cases with a single energy band near the Fermi energy

$\Longrightarrow$ Hubbard model provides effective <u>low-energy description</u>

Hubbard Hamiltonian for the single-band Hubbard model:

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

$$+ U \sum_{j} n_{j\uparrow} n_{j\downarrow} - \mu \sum_{j} \left(n_{j\uparrow} + n_{j\downarrow} \right).$$



t nearest-neighbor $\langle j,\ell \rangle$ hopping

U Hubbard on-site repulsion

μ chemical potential

4 Symmetries

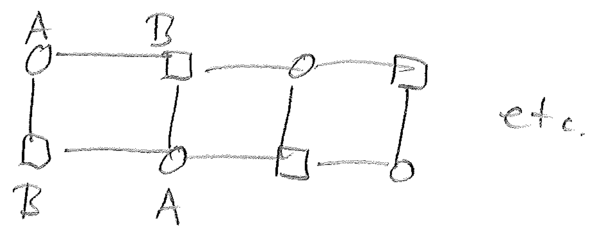
Symmetries help simplifying the solution of a problem. For example, one can block-diagonalize the Hamiltonian by choosing an appropriate basis with good quantum numbers.

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

PHS is secured by allowing for only 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 $d^{+}_{\ell\sigma} \equiv (-1)^{\ell} c_{\ell\sigma}$

where $(-1)^{\ell} = \begin{cases} +1 & \ell \in A \\ -1 & \ell \in B \end{cases}$

(PHT)

is a Particle-hole transformation because $d_{\ell\sigma}^\dagger d_{\ell\sigma} = 1 - c_{\ell\sigma}^\dagger c_{\ell\sigma}$

which means that if $\langle c_{\ell\sigma}^\dagger c_{\ell\sigma}\rangle = 1 \Rightarrow \langle d_{\ell\sigma}^\dagger d_{\ell\sigma}\rangle = 0$

and vice versa.

$\boxed{\text{Quiz 2:}}$ What happens to $\hat{H}$ under this particle-hole transformation?

// end lecture 2 75'

Kinetic energy: $c_{\ell\sigma}^\dagger c_{j\sigma} = \underbrace{(-1)^{j+\ell}}_{=-1 \text{ for nearest-neighbor hopping}} d_{\ell\sigma} d_{j\sigma}^\dagger = d_{\ell\sigma}^\dagger d_{j\sigma}$

Interaction energy: $U\left(\hat{n}_{j\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{j\downarrow} - \frac{1}{2}\right)$ is unchanged as well

$$= U \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} - \frac{U}{2}\left(n_{j\downarrow} + n_{j\uparrow}\right) + \frac{U}{4}$$

shift of μ trivial offset

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

$$\boxed{\hat{H} = -t \sum_{\langle j,\ell\rangle\sigma} \left(c_{\ell\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{\ell\sigma}\right) + U\sum_j \left(n_{j\uparrow} - \tfrac{1}{2}\right)\left(n_{j\downarrow} - \tfrac{1}{2}\right) - \mu \sum_{j\sigma} n_{j\sigma}}$$

How do observables transform under the PHT?

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

$L = \#$ sites

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

$$\rho \xrightarrow{PHT} 2 - \rho \qquad (2 \text{ for spin} = \uparrow,\downarrow)$$

chemical potential term:

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

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

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

"half-filling"

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

$\Rightarrow$ relevant to high-T_c Cuprate superconductors (2D square lattice); there a diagonal next-nearest-neighbor hopping t' breaks PHS making the phase diagram asymmetric

(5) Single-site limit

We can set $t = 0$ in the HH and have L independent sites.

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

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

$\Rightarrow$ drop site index

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

$\boxed{\text{Quiz 3}}$ (A) What is the partition function $Z = \mathrm{Tr}[e^{-\beta \hat{H}}]$?

(B) What is the occupation $\rho = \langle n_\uparrow + n_\downarrow \rangle$?

(C) Plot $\rho(\mu)$ for $t = 0$, $U = 4$, $T \equiv \frac{1}{\beta} \in \begin{Bmatrix} 2.00 \\ 0.50 \\ 0.25 \end{Bmatrix}$ and an interval $\mu \in [-6, 6]$

(D) Plot the compressibility $\varkappa \equiv \frac{\partial \rho}{\partial \mu}$ for the same parameters as in (C)

//

end lecture 3 (90 min)

Answer: $\hat{H} = U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right) - \mu\left(n_\uparrow + n_\downarrow\right)$

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

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

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

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

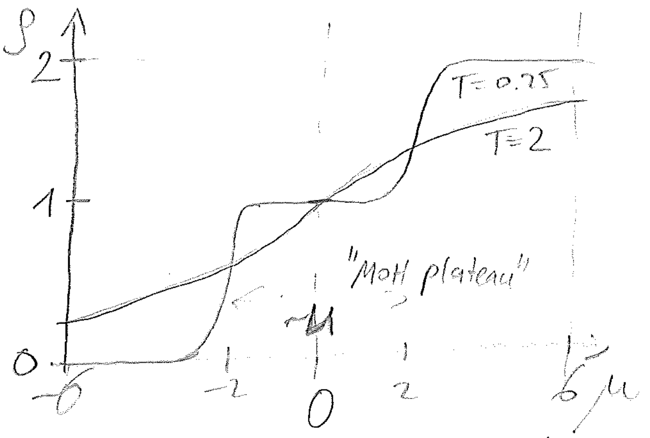
$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \mathrm{Tr}\begin{bmatrix} e^{-\beta \frac{U}{4}} & & & \\ & e^{-\beta\left(-\frac{U}{4}-\mu\right)} & & \\ & & e^{-\beta\left(-\frac{U}{4}-\mu\right)} & \\ & & & e^{-\beta\left(\frac{U}{4}-2\mu\right)} \end{bmatrix}$$

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

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

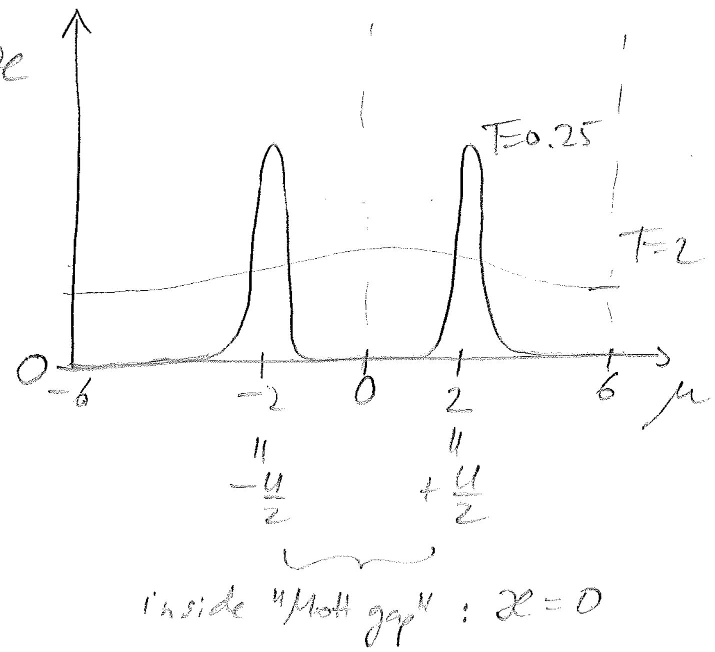
$$= Z^{-1}\left(2e^{-\beta\left(-\frac{U}{4}-\mu\right)} + 2e^{-\beta\left(\frac{U}{4}-2\mu\right)}\right)$$

$\mu = 0$; $\rho = 1$ (true even for $t \neq 0$)



$t = 0$
$U = 4$

Compressibility $\varkappa$



- high temperature : thermal fluctuations wash out sharp jumps in $\rho(\mu)$

at $T=0$, $t \neq 0$: quantum fluctuations due to hopping can play a "similar role" destroying the Mott plateau — much more complicated than in this simple single-site limit though.

- Local spin moment :

$$\langle m^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n_\uparrow + n_\downarrow \rangle - 2 \underbrace{\langle n_\uparrow n_\downarrow \rangle}_{\equiv D}$$

$$= \rho - 2D$$

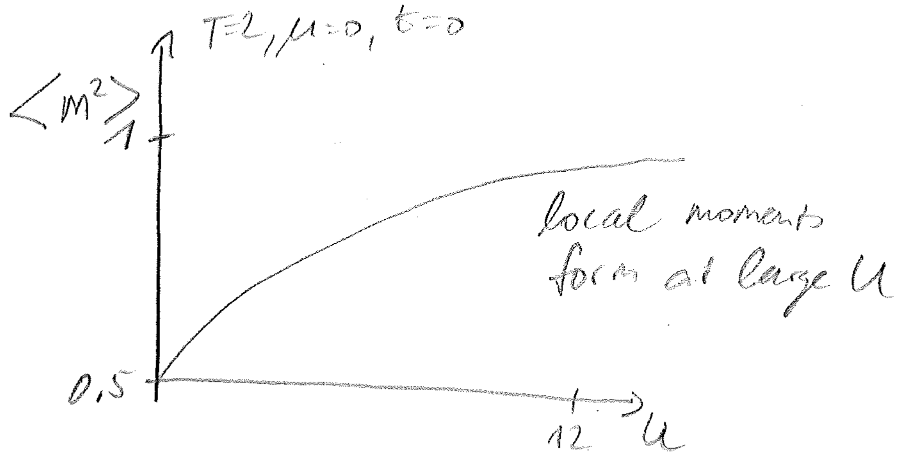
double occupancy

$\Rightarrow$ local moment is zero for $|0\rangle$ and $|\uparrow\downarrow\rangle$ but takes maximal value $(=1)$ for either $|\uparrow\rangle$ or $|\downarrow\rangle$

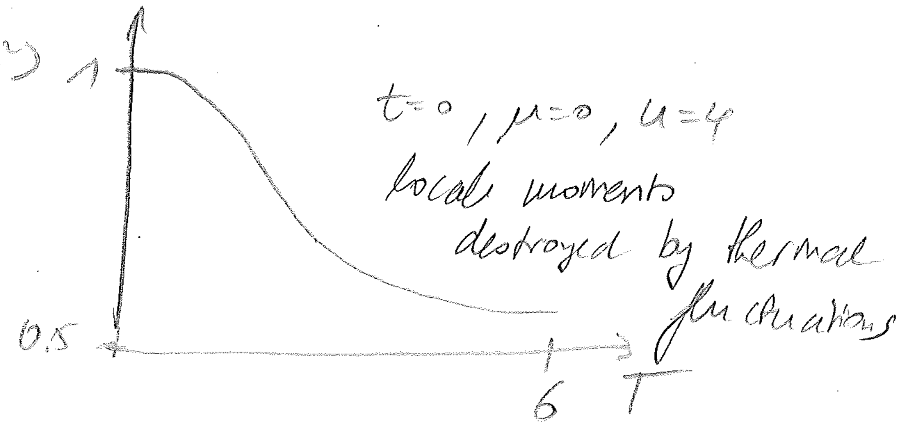
$\boxed{\text{Quiz 4:}}$ A) Plot $\langle m^2 \rangle$ as a function of $U \in [0,12]$ for $T=2$, $\mu=0$

B) —— " —— $T \in [0,6]$ for $U=4$, $\mu=0$

Answer: (A)



(B)



(6) Noninteracting limit → band picture

Starting point: $U=0$ HH

$$\hat{H} = -t \sum_{\langle i,j \rangle \sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + h.c. \right) - \mu \sum_{j\sigma} \hat{n}_{j\sigma}$$

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

(i) real space:

$$\left[\hat{H}, \hat{N}_{\uparrow} \right] = 0 , \quad \left[\hat{H}, \hat{N}_{\downarrow} \right] = 0 \qquad \text{(show!)}$$

$$\hat{N}_{\sigma} = \sum_{j} \hat{n}_{j\sigma}$$

How to see this? use a link $i-j$

$$\Rightarrow \left[c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} , n_{i\sigma'} + n_{j\sigma'} \right] = 0$$

Which can be shown using $[AB, C]$

$$= A \underbrace{\{B, C\}}_{\text{anticommutator } BC+CB} - \{A, C\} B$$

Another way to understand it: $c_{i\sigma}^{\dagger} c_{j\sigma}$ does have as many annihilation as creation operators

$\Rightarrow$ does not change the particle number for either spin, and does not flip a spin

Upshot: sectors of total $N_\uparrow$, $N_\downarrow$ can be considered separately (even for $U \neq 0$)

Example: $N_\uparrow = 1$, $N_\downarrow = 0$

Basis: $\underbrace{\{ |10000\ldots\rangle, |01000\ldots\rangle, |00100\ldots\rangle, \ldots \}}_{\dim = L \text{ for } L\text{-site chain}}$

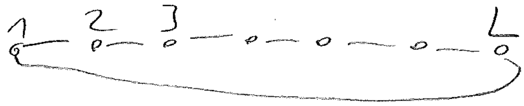
// end lecture 4 (75 min)

$$\hat{H} |01000\ldots\rangle = -\mu |01000\ldots\rangle - t |10000\ldots\rangle - t |00100\ldots\rangle$$

$\Rightarrow$ in this basis we have

$$\hat{H} = \begin{bmatrix} -\mu & -t & & & & -t \\ -t & -\mu & -t & & & \\ & -t & -\mu & -t & & \\ & & -t & -\mu & \ddots & \\ & & & \ddots & \ddots & -t \\ -t & & & & -t & -\mu \end{bmatrix}$$

periodic boundary conditions
$\Rightarrow$ hopping between sites 1 and L



$\Rightarrow$ $L \times L$ tridiagonal matrix with 'a' as diagonal and 'b' as upper/lower diagonal element has eigenvalues

$$\boxed{\begin{aligned} \lambda_n &= a + 2b\cos(k_n) \\ k_n &= \frac{2\pi n}{L}, \quad n = 1, \dots, L \end{aligned}}$$

How to see this?
Ansatz $v_\ell = e^{ik\ell}$ into eigenvalue eq.

$$a v_\ell + b v_{\ell-1} + b v_{\ell+1} = \lambda v_\ell$$

together with periodicity $v_0 = v_L$
$v_1 = v_{L+1}$

$\Rightarrow$ enforces discrete values of k

$\Rightarrow$ 1D chain has eigenvalues

$$\varepsilon(k) = -2t \cos(k) - \mu$$

and eigenvectors

$$\underbrace{(\vec{v}_k)_\ell}_{} = e^{ik\ell}$$

ℓ-th 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) <u>momentum space</u>

) Simpler way to solve $U=0$ HH:
Canonical transformation of operators:

$$c^\dagger_{k\sigma} = \frac{1}{\sqrt{L}} \sum_\ell e^{ik\ell} c^\dagger_{\ell\sigma}$$

orthogonality:

$$\frac{1}{L} \sum_\ell e^{i(k_n - k_m)\ell} = \delta_{n,m}$$

$$\frac{1}{L} \sum_n e^{ik_n(\ell-j)} = \delta_{\ell,j}$$

$\boxed{\text{Quiz 5:}}$ (A) Prove that $c^+_{\ell\sigma} = \frac{1}{\sqrt{L}} \sum_k e^{-ik\ell} c^+_{k\sigma}$

("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: $\hat{N} = \sum_{j\sigma} \hat{n}_{j\sigma} = \sum_{k\sigma} \hat{n}_{k\sigma}$

$$\hat{n}_{k\sigma} \equiv c^+_{k\sigma} c_{k\sigma}$$

$\boxed{\text{Quiz 6:}}$ Derive the $U=0$ HH in momentum space

Answer: $\hat{H} = \sum_{k\sigma} (\epsilon_k - \mu) c^+_{k\sigma} c_{k\sigma} = \sum_{k\sigma} (\epsilon_k - \mu) \hat{n}_{k\sigma}$

$$\epsilon_k = -t \sum_\ell e^{i\vec{k}\vec{a}_\ell}$$

$\vec{a}_\ell$ = real space vectors connecting a site with each nearest neighbor ℓ

1D chain: $\vec{a}_\ell = \pm\hat{x}$

$$\epsilon_k = -2t\cos k$$

(lattice constant = 1)

$\Rightarrow$ the noninteracting HH (and multiband/multiorbital generalizations) is determined by the <u>single-particle energy dispersion</u> ("band structure") ε_k

<u>Useful quantity:</u> density of states (DOS)

$$N(E) \equiv \frac{1}{L} \sum_k \delta(E - \varepsilon_k)$$

Continuum limit (on hypercubic lattice) $L \to \infty$: $\displaystyle \frac{1}{L} \sum_k \longrightarrow \int_{-\pi}^{\pi} \frac{d^d k}{(2\pi)^d}$

d = spatial dimension

$\boxed{\text{Quiz 7:}}$ Compute and plot $N(E)$ for 1D chain, $\varepsilon_k = -2t \cos k$.

<u>Answer:</u> $\displaystyle N(E) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \; \delta(E + 2t \cos k) = \ldots$

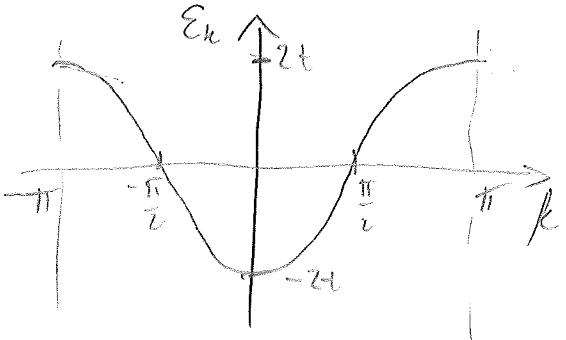
$x = -2t \cos k$, $dx = 2t \sin k \, dk = 2t \sqrt{1-\cos^2 k} \, dk$

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

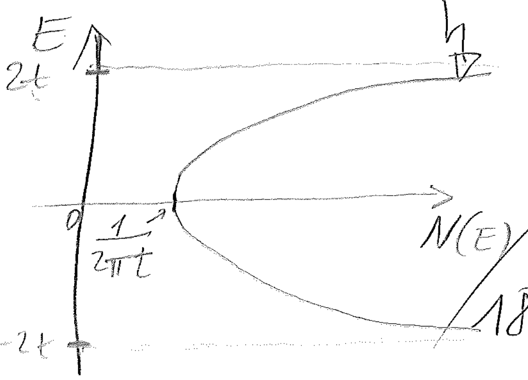
$$\ldots = \frac{1}{\pi} \int_{-2t}^{2t} \frac{dx}{\sqrt{4t^2 - x^2}} \, \delta(E - x)$$

$$N(E) = \begin{cases} \dfrac{1}{\pi \sqrt{4t^2 - E^2}} & |E| \leq 2t \\ 0 & |E| > 2t \end{cases} \quad (t > 0)$$

("van Hove singularity") divergence!



$\Rightarrow$



Knowledge of ε_k $\Rightarrow$ knowledge of all statistical properties:

partition function $Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \prod_k \prod_{n_k\in\{0,1\}} e^{-\beta(\varepsilon_k-\mu)}$

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

density $\rho = Z^{-1}\,\mathrm{Tr}\left[\sum_k \hat{n}_k e^{-\beta\hat{H}}\right] = \sum_k \left(1+e^{+\beta(\varepsilon_k-\mu)}\right)^{-1}$

$$\equiv \sum_k f(\varepsilon_k) \equiv \sum_k f_k$$

$$f(\varepsilon_k) \equiv \left(1+e^{\beta(\varepsilon_k-\mu)}\right)^{-1} \quad \text{Fermi function}$$

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

$$= \sum_k \varepsilon_k f_k$$

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

$$F = -\ln Z/\beta$$
$$E = F - TS$$

7 Introduction to exact diagonalization: the two-site HH

So far : Single-site HH → 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 spin

to divide Hilbert space into sectors:

$$(n_{1\uparrow}+n_{2\uparrow},\ n_{1\downarrow}+n_{2\downarrow}) = \left.\begin{matrix}(0,0),(1,0),(2,0),\\ (0,1),(1,1),(2,1)\\ (0,2),(1,2),(2,2)\end{matrix}\right\}\ 9 \text{ sectors}$$

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

- the 1d sectors are trivially diagonal, $E = \pm \frac{U}{2}$
- the 2d 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

$\boxed{\text{Quiz 8:}}$ Write H in the $(1,1)$ sector and compute its eigenvalues!

Answer:
Choose a basis $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle$:

$$\hat{H} = -t\sum_{\sigma}\left(c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}\right) + U\sum_{i=1,2}\left(\hat{n}_{i\uparrow}-\tfrac{1}{2}\right)\left(n_{i\downarrow}-\tfrac{1}{2}\right)$$

in the above basis:

$$(*)\quad H = \begin{bmatrix} -U/2 & 0 & -t & -t \\ 0 & -U/2 & -t & -t \\ -t & -t & U/2 & 0 \\ -t & -t & 0 & U/2 \end{bmatrix} \quad \begin{pmatrix} |\uparrow,\downarrow\rangle \\ |\downarrow,\uparrow\rangle \\ |\uparrow\downarrow,0\rangle \\ |0,\uparrow\downarrow\rangle \end{pmatrix} \text{ basis}$$

check:
$$-t\, c_{1\uparrow}^{\dagger}c_{2\uparrow}|0,\uparrow\downarrow\rangle = -t|\uparrow,\downarrow\rangle \quad \text{14-Element}$$
$$-t\, c_{1\downarrow}^{\dagger}c_{2\downarrow}|0,\uparrow\downarrow\rangle = -t|\downarrow,\uparrow\rangle \quad 24$$
$$-t\, c_{2\downarrow}^{\dagger}c_{1\downarrow}|\uparrow\downarrow,0\rangle = -t|\uparrow,\downarrow\rangle \quad 13$$
$$-t\, c_{2\uparrow}^{\dagger}c_{1\uparrow}|\uparrow\downarrow,0\rangle = -t|\downarrow,\uparrow\rangle \quad 23$$

Consistency: $c_{1\uparrow}^{\dagger}c_{2\uparrow}|0,\uparrow\downarrow\rangle \overset{!}{=} c_{2\downarrow}^{\dagger}c_{1\downarrow}|\uparrow\downarrow,0\rangle = |\uparrow,\downarrow\rangle$

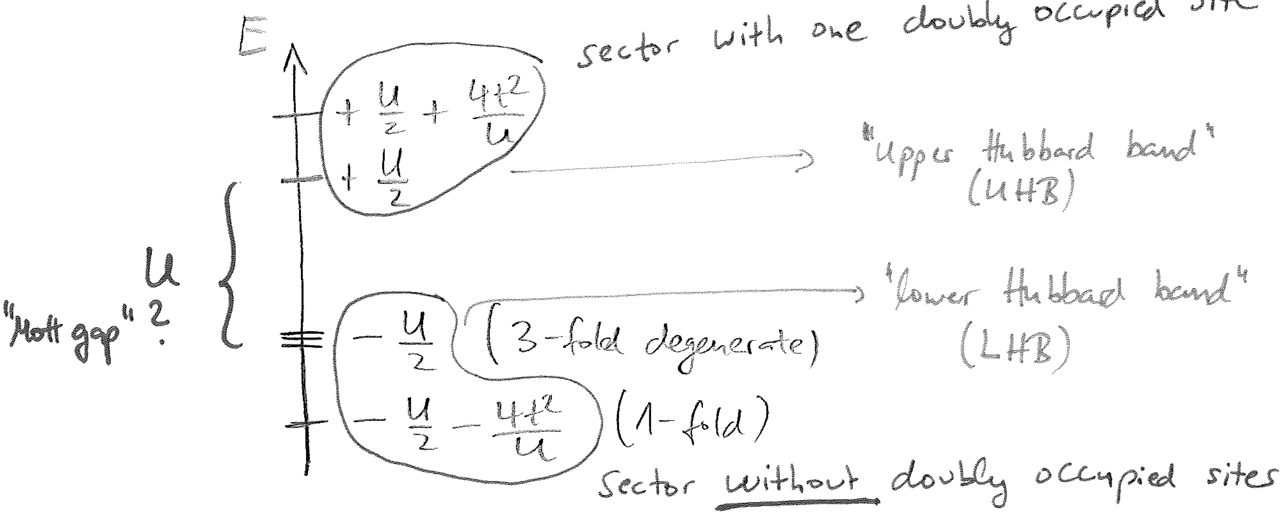
eigenvalues of $H\,(*)$: $\underset{\overset{|||}{E_t,\ \text{see below}}}{-U/2}, U/2, \pm\sqrt{4t^2+U^2/4}$

For $U/t \gg 1$ we can expand

$$\pm\sqrt{4t^2+U^2/4} = \pm\frac{U}{2}\sqrt{1+16t^2/U^2} \approx \pm\frac{U}{2}\left(1+8\frac{t^2}{U^2}\right)$$
$$= \begin{cases} -\frac{U}{2}-\frac{4t^2}{U} \equiv E_s, \text{ see below} \\ +\frac{U}{2}+\frac{4t^2}{U} \end{cases}$$

Together with the states $|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$, which both have energy $-\frac{U}{2}$, we have in the half-filled

Sector: $(N=2$ on $L=2$ sites$)$:



Eigenstates in the lower sector in limit $U/t \gg 1$:

singlet $\frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right)$ 1-fold

triplets
$$\left.\begin{array}{l} \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) \\ |\uparrow,\uparrow\rangle \\ |\downarrow,\downarrow\rangle \end{array}\right\} \text{3-fold}$$

Singlet-triplet splitting: $\boxed{\frac{4t^2}{U} = E_t - E_s}$

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

$\Rightarrow$ no hopping of charges, spin physics only
"charge degree of freedom is frozen" for $U/t \gg 1$

Heisenberg model on two sites:

$$\hat{H} = J\, \vec{S}_1 \cdot \vec{S}_2$$

Trick to obtain spectrum:

$$J\,(\vec{S}_1 \cdot \vec{S}_2) = \frac{J}{2}\left((\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^{\,2} - \vec{S}_2^{\,2}\right)$$

$$\vec{S}_1^{\,2} = \vec{S}_2^{\,2} = \frac{3}{4} \qquad [\text{cf. } \vec{S}^{\,2} = S(S+1)]$$

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

singlet triplet

$$\Rightarrow \vec{S}_{tot}^{\,2} = (\vec{S}_1 + \vec{S}_2)^2 = 0, 2$$

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

$$\frac{J}{2}\left(0 - \frac{3}{4} - \frac{3}{4}\right) = -\frac{3J}{4} \equiv \tilde{E}_S \quad \text{singlet}$$

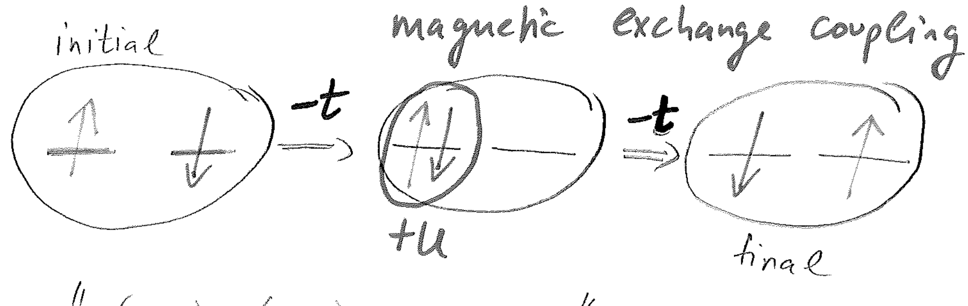
$$\frac{J}{2}\left(2 - \frac{3}{4} - \frac{3}{4}\right) = +\frac{J}{4} \equiv \tilde{E}_t \quad \text{triplet}$$

$$\Rightarrow \tilde{E}_t - \tilde{E}_S = J$$

Comparison with Hubbard: $\boxed{J = \frac{4t^2}{U}}$

magnetic exchange coupling

pictorial:



$$\text{"}\frac{(-t)\cdot(-t)}{U} = \frac{t^2}{U}\text{"}$$

exchange of spins via virtual intermediate state

8 Mott gap and Spectral function

Useful quantity for spectroscopy: Green's function

$\Rightarrow$ 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 $t=0$.

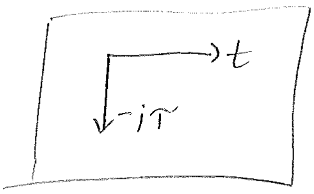
8.1 Green's functions at $U=0$

Definition: $$G_{jn}(\tau) := \langle c_j(\tau)\, c_n^\dagger(0)\rangle \qquad (\tau > 0)$$
with $$c_j(\tau) = e^{\hat{H}\tau} c_j(0)\, e^{-\hat{H}\tau} \qquad (*)$$

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

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

and $t \to -i\tau$ gives $(*)$



Complex-time plane

What is $c_k(\tau)$? We know that $\frac{\partial c_k(\tau)}{\partial \tau} = [\hat{H}, c_k(\tau)]$

and $\hat{H} = \sum_{k'} \varepsilon_{k'} c_{k'}^\dagger c_{k'}$, such that

$$\frac{\partial c_k(\tau)}{\partial \tau} = \sum_{k'} \varepsilon_{k'} \underbrace{[c_{k'}^\dagger c_{k'}, c_k]}_{c_{k'}^\dagger c_{k'} c_k - c_k c_{k'}^\dagger c_{k'} = \delta_{kk'} \cdot (-c_k)} = -\varepsilon_k c_k$$

$$\Rightarrow \quad \frac{\partial c_k}{\partial \tau} = -\varepsilon_k c_k \Rightarrow \boxed{c_k(\tau) = e^{-\varepsilon_k \tau} c_k(0)}$$

$$\Rightarrow \quad G_{jn}(\tau) = \frac{1}{N}\sum_k e^{ik(n-j)} \underbrace{(1-f_k)}_{\text{using } \langle c_k c_k^+\rangle = 1-f_k} e^{-\varepsilon_k \tau}$$

$$\Rightarrow \quad G_{jn} = G(j-n) \quad \text{for translationally invariant } \hat{H} \checkmark$$

More precisely: $G_k(\tau) := -\langle T_\tau c_k(\tau) c_k^+(0)\rangle$

with time ordering T_τ

$$T_\tau \, c_k(\tau) c_k^+(0) = \begin{cases} c_k(\tau) c_k^+(0) & \text{for } \tau > 0 \\ -c_k^+(0) c_k(\tau) & \text{for } \tau < 0 \end{cases}$$

$$\Rightarrow \quad G_k(\tau+\beta) = -G(\tau) \quad \text{for } -\beta < \tau < 0$$

$\Rightarrow$ define Fourier transform for discrete frequencies

$$G_k(\tau) = \frac{1}{\beta}\sum_n G_k(i\omega_n) e^{-i\omega_n \tau}$$

$$G_k(i\omega_n) = \int_0^\beta d\tau \, G_k(\tau) e^{i\omega_n \tau}$$

$$\omega_n = \frac{\pi}{\beta}(2n+1) \quad \text{fermionic Matsubara frequencies}$$

We have $$G_k(\tau) = \begin{cases} -e^{-\varepsilon_k \tau}(1-f_k) & \text{for } 0<\tau<\beta \\ e^{-\varepsilon_k \tau} f_k & \text{for } -\beta<\tau<0 \end{cases}$$

$$\Rightarrow \boxed{G_k(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_k}}$$

This noninteracting Green's function forms the basis of many-body perturbation theory and is also a central quantity for DMFT (cf. Chapter 11)

8.2 Green's functions at t=0

Consider again a single site with two spins. $\hat{H} = U(\hat{n}_\uparrow - \frac{1}{2})(\hat{n}_\downarrow - \frac{1}{2})$

Let us compute

$$G_\uparrow(\tau) = \langle c_\uparrow(\tau)\, c_\uparrow^\dagger(0)\rangle . \quad (*)$$

We need to consider only two states, namely $|00\rangle$ and $|01\rangle$. (why?)

$$c_\uparrow(\tau)\, c_\uparrow^\dagger(0)|00\rangle = e^{H\tau} c_\uparrow e^{-H\tau} c_\uparrow^\dagger |00\rangle$$

$$= e^{H\tau} c_\uparrow e^{-H\tau} |10\rangle$$

$$= e^{H\tau} c_\uparrow e^{+U\tau/4} |10\rangle$$

$$= e^{H\tau} e^{+U\tau/4} |00\rangle$$

$$= e^{+U\tau/2} |00\rangle$$

Quiz 9: Repeat the same for $|01\rangle$!
What is $G_\uparrow(\tau)$ in $(*)$?

Answer: $G_\uparrow(\tau) = Z^{-1} \, \mathrm{Tr}\left[e^{-\beta \hat{H}} \, c_\uparrow(\tau)\, c_\uparrow^\dagger(0)\right]$

$$= Z^{-1} \sum_n e^{-\beta E_n} \langle n | c_\uparrow(\tau)\, c_\uparrow^\dagger(0) | n \rangle$$

Where $n \in \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \}$

for the occupation number states $|n_\uparrow n_\downarrow\rangle$.

We had (cf. Chapter 5)

$$\boxed{Z \overset{\mu=0}{=} 2e^{-\beta\frac{U}{4}} + 2e^{\beta\frac{U}{4}}} \quad (**)$$

and $\langle 00 | H | 00 \rangle = \frac{U}{4}$

$\langle 01 | H | 01 \rangle = -\frac{U}{4}$

$$\Rightarrow \boxed{G_\uparrow(\tau) = Z^{-1}\left[e^{U\tau/2} e^{-\beta\frac{U}{4}} + e^{-U\tau/2} e^{\beta\frac{U}{4}}\right] \quad \text{with } Z \text{ as in } (**).} \quad (***)$$

Def.: Spectral function $A(\omega)$ can be defined as

$$G(\tau) = \int_{-\infty}^{\infty} d\omega \, A(\omega) \frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$$

or alternatively

$$A(\omega) \equiv -\frac{1}{\pi} \, \mathrm{Im}\, G^R(\omega)$$

$$G^R(\omega) \equiv G(i\omega_n)\Big|_{i\omega_n \to \omega + i0^+}$$

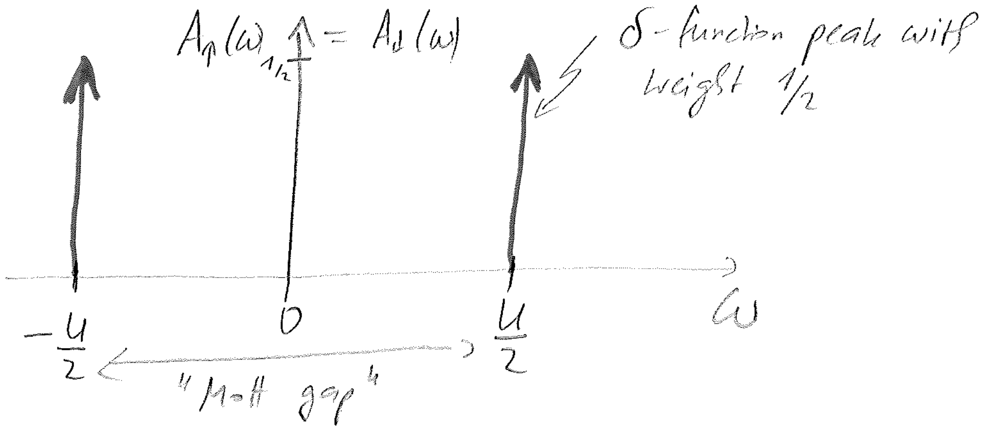
e.g., for the noninteracting case in 8.1: $G_k^R(\omega) = \dfrac{1}{\omega - \varepsilon_k + i0^+}$

Note: $\frac{1}{L}\sum_k A_k(\omega) = \frac{1}{L}\sum_k \delta(\omega - \varepsilon_k) = N(\omega) =$ DOS for noninteracting case

Here : $\boxed{A_\uparrow(\omega) = \frac{1}{2}\left(\delta\left(\omega-\frac{U}{2}\right)+\delta\left(\omega+\frac{U}{2}\right)\right)}$

Check: $G(\tau) = \int_{-\infty}^{\infty} d\omega \, \frac{1}{2}\left(\delta\left(\omega-\frac{U}{2}\right)+\delta\left(\omega+\frac{U}{2}\right)\right)\frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$

$$= \frac{1}{2}\left[\frac{e^{-\tau\frac{U}{2}}}{1+e^{-\beta\frac{U}{2}}} + \frac{e^{+\tau\frac{U}{2}}}{1+e^{+\beta\frac{U}{2}}}\right] = (***) \checkmark$$



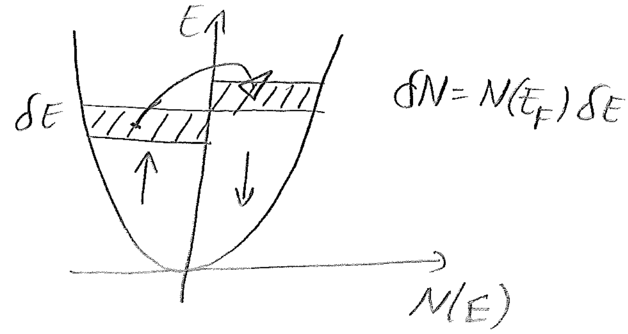
For the $U/t \gg 1$ Hubbard model we "expect" a Mott insulator with a Mott gap $\sim U$ — but what happens on an actual lattice with $t \neq 0$ is nontrivial!

(9) Magnetism

Both ferromagnetism and antiferromagnetism occur in the Hubbard model.

(9.1) Ferromagnetism : cf. Mielke & Tasaki 1993

- Stoner criterion



→ $\boxed{U N(E_F) > 1}$

favors unequal ↑ and ↓ populations and thus a ferromagnetic polarization.

Very rough estimate (cf. Scalettar notes for the derivation) but points towards regions in parameter space in which ferromagnetism may be found

→ large U is good

→ large $N(E_F)$ is good ⟺ "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

$$J = \frac{4t^2}{U} > 0 \quad \text{(antiferromagnetic exchange)}$$

in the two-site HH.

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 $U/t \gg 1$ $\Rightarrow$ $H_{\text{Heisenberg}} = \sum_{\langle ij \rangle} J\, \vec{S}_i \cdot \vec{S}_j$.

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

(b) weak-coupling picture

→ exercise Sheet 1 : Mean-field antiferromagnetism (AF) in the Hubbard model

→ half-filled bipartite lattice has instability towards AF ordering.

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

Overall picture for AF order in the HM (at $n=1$, simple AB lattice)