Computational Many-Body Physics

1. Introduction

1.1 many-particle systems in solid state theory

starting point: the general solid state Hamiltonian

$$H = \underbrace{T_e + T_a}_{\text{kinetic energies}} + \underbrace{V_{e\text{-}e} + V_{a\text{-}a} + V_{e\text{-}a}}_{\text{interactions}}$$

e: electrons
a: atoms/ions

$$\xrightarrow[\text{approximation}]{\text{adiabatic}} \boxed{H_e = T_e + V_{e\text{-}e} + V_{e\text{-}a}}$$

purely electronic problem for fixed positions of the ions

- kinetic energy: $T_e = \sum_{i=1}^{N_e} \frac{\vec{p}_i^{\,2}}{2m}$ $\quad N_e$: number of electrons

- interactions between the electrons:

$$V_{e\text{-}e}(\{\vec{r}\}) = \sum_{i<j} \underbrace{v_{ee}(\vec{r}_i - \vec{r}_j)}_{= \frac{e^2}{|\vec{r}_i - \vec{r}_j|}} \quad \text{Coulomb interaction}$$

- interactions between electrons and ions:

$$V_{e\text{-}a}(\{\vec{r}\},\{\vec{R}\}) = \sum_{i,k} \underbrace{v_{e\text{-}a}(\vec{r}_i - \vec{R}_k)}_{= -\frac{Z_k e^2}{|\vec{r}_i - \vec{R}_k|}} \quad Z_k e: \text{ charge of the ion } k$$

$\longrightarrow$ many-particle Schrödinger equation

$$H_e \, \Psi(\vec{r}_1, \dots, \vec{r}_{N_e}) = E \, \underbrace{\Psi(\vec{r}_1, \dots, \vec{r}_{N_e})}_{\text{the many-particle wave function}}$$

E: the corresponding many-particle (eigen) energie

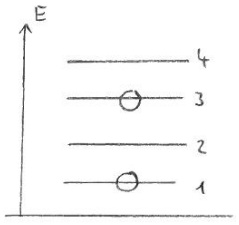
a (more) convenient way to deal with the many-particle problem

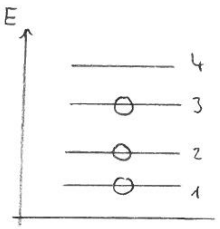
$\longrightarrow$ second quantization

define creation and annihilation operators $C^+_{k_\alpha}$, C_{k_α}

$C^+_{k_\alpha}$: creates a particle in the state $|k_\alpha\rangle$

example:

$|4\rangle \hat{=}$ 

$\rightarrow \quad C^+_2 |4\rangle \hat{=}$ 

the Hamiltonian H_e can be rewritten in second quantized form:

$$H_e = \sum_{\alpha,\beta} \langle k_\alpha | T_e + V_{e\text{-}a} | k_\beta \rangle C^+_{k_\alpha} C_{k_\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle k_\alpha | \langle k_\beta | V_{e\text{-}e} | k_\gamma \rangle | k_\delta \rangle C^+_{k_\alpha} C^+_{k_\beta} C_{k_\gamma} C_{k_\delta} \qquad (*)$$

[derivation, see lecture solid state theory]

the form of H_e follows from: – the basis $\{|k_\alpha\rangle\}$

– the lattice $\{\vec{R}\}$ via the interaction $V_{e\text{-}a}$

in the following: reduce the complexity of H_e

$\rightarrow$ specific assumptions and approximations

1.2 strongly correlated electron systems: the basic models

a) Hubbard model

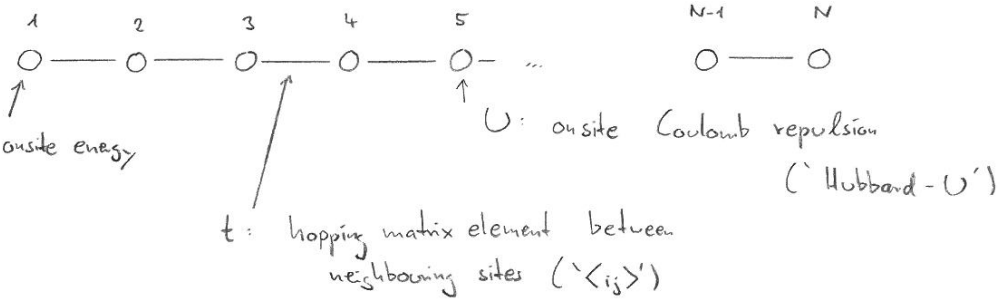
starting from H_e eq. (*) we now:

- consider a single band only
- use a basis of Wannier state, localized at each lattice site
- take into account only:
  - $\rightarrow$ local matrix elements for two-particle terms
  - $\rightarrow$ local and nearest neighbour (n.n.) matrix elements for single-particle terms

and we arrive at the following form of the Hubbard model:

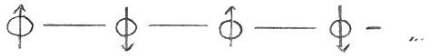
$$H = \sum_{i\sigma} \varepsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{\langle ij\rangle\sigma} t\, c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}$$

example : 1d lattice of N sites , $i = 1, 2, .. N$



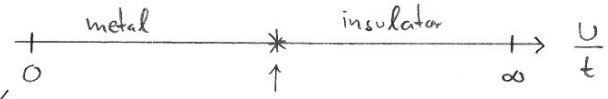
what is the Hubbard model supposed to describe ?

- magnetism :



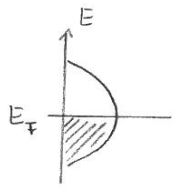
e.g. : antiferromagnetic order at large U and half filling

- Mott metal-insulator transition (at half filling)



set $U = 0$, $t \neq 0$

→ give rise to a single half-filled band :



=> metallic behavior

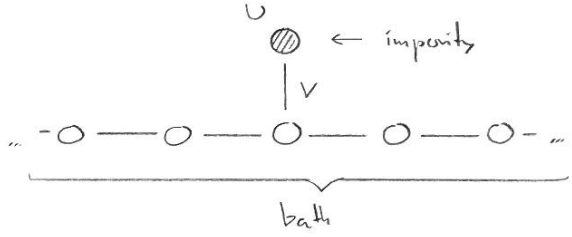
set $U > 0$, $t = 0$

→ no hopping of electrons

=> no charge transport

insulating behaviour

b) single-impurity Anderson model



a single correlated site, coupled to a band of non-interacting conduction electrons

$$H = H_{imp} + H_{imp-bath} + H_{bath}$$

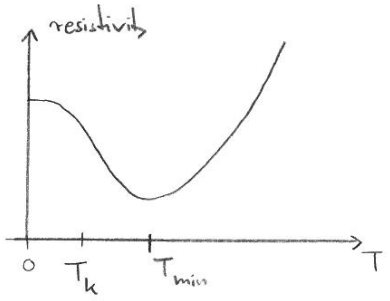
$$H_{imp} = \sum_\sigma \varepsilon_f f_\sigma^\dagger f_\sigma + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow$$

$$H_{imp-bath} = V \sum_\sigma \left(f_\sigma^\dagger c_{o\sigma} + c_{o\sigma}^\dagger f_\sigma \right)$$

H_{bath} : tight-binding model ($\hat{=}$ Hubbard model with $U = 0$)

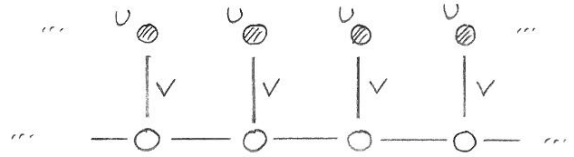
what is the siAm supposed to describe?

$\longrightarrow$ Kondo effect



T_k : Kondo temperature

c) periodic Anderson model



$\rightarrow$ periodic arrangement of "impurities"

associated with "heavy-fermion" physics

d) Heisenberg model

$$\boxed{H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j}$$

in $d = 1$: 

- spin on each lattice site with spin operator $\vec{S}_i = \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix}$
- spin originates from localized electrons
  $\hookrightarrow$ no hopping term as in the Hubbard model

anisotropic Heisenberg model :

$$H = -J_\parallel \sum_{\langle ij \rangle} S_i^z S_j^z - J_\perp \sum_{\langle ij \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right)$$

e, Ising model

set $J_\perp = 0$, $J_\parallel = J$ and add a magnetic field h

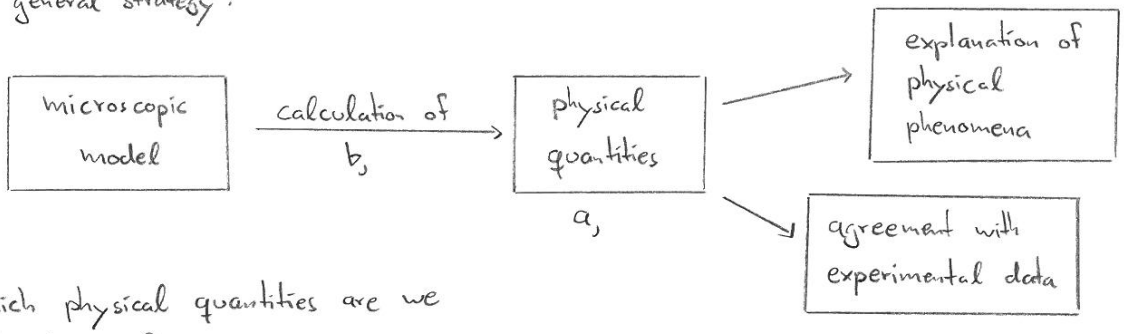
$$\rightarrow \quad \boxed{H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^z}$$

note that: operators S_i^z commute with H

$\Rightarrow$ H is the classical Hamilton function with the classical spin variables $S_i^z = \pm 1$

1.3 physical quantities

the general strategy:



a, which physical quantities are we interested in?

- eigenenergies E_n $\longrightarrow$ thermodynamics
- Green functions / correlation functions (see Sec. 2.2)
  $\longrightarrow$ dynamic quantities
- the wave function $|\Psi\rangle$ itself $\longrightarrow$ entanglement

b, how to calculate these quantities?

$\rightarrow$ solution of the Schrödinge equation $H|\Psi_n\rangle = E_n|\Psi_n\rangle$

or

$\rightarrow$ direct calculation of Green functions (without knowledge of $E_n, |\Psi_n\rangle$)

Using

$\longrightarrow$ analytical approaches, such as petrubation theory

or

$\longrightarrow$ numerical approaches $\Rightarrow$ the topic of this lecture

2. Quantum Many-Particle Systems: Basics

2.1 single-particle and many-particle spectra

in the following: solution of the Schrödinger equation for simple fermionic quantum systems

A, a single level

$$\boxed{H = \varepsilon\, c^\dagger c} \quad \hat{=} \quad \overset{\varepsilon}{\circ}$$

- a single site / level
- 'spinless' fermion

basis: $\{|i\rangle\} = \{|0\rangle, |1\rangle\}$ → the Hilbert space is two-dimensional

$|0\rangle$: the level/site is empty

$|1\rangle = c^\dagger |0\rangle$: the level/site is filled with one fermion

here we have: $H|i\rangle = E_i |i\rangle \qquad i = 0,1$

with $E_0 = 0$, $E_1 = \varepsilon$ — this means: we have chosen a basis of eigenstates

the Hamilton matrix → matrix elements $H_{ij} = \langle i|H|j\rangle$

here: 2×2 matrix $\{H_{ij}\} = \begin{pmatrix} 0 & 0 \\ 0 & \varepsilon \end{pmatrix}$ diagonal!

B, many levels

$$\boxed{H = \sum_{i=1}^{N} \varepsilon_i\, c_i^\dagger c_i} \quad \hat{=} \quad \underset{\varepsilon_1}{\overset{1}{\circ}} \quad \underset{\varepsilon_2}{\overset{2}{\circ}} \quad \underset{\varepsilon_3}{\overset{3}{\circ}} \quad \cdots \quad \underset{\varepsilon_{N-1}}{\overset{N-1}{\circ}} \quad \underset{\varepsilon_N}{\overset{N}{\circ}}$$

- again: 'spinless' fermions
- no hopping t

basis: $\{|0\rangle_1, |1\rangle_1\} \otimes \{|0\rangle_2, |1\rangle_2\} \otimes \cdots \otimes \{|0\rangle_N, |1\rangle_N\}$

$\hat{=} |n_1\rangle_1 |n_2\rangle_2 \cdots |n_N\rangle_N \qquad n_i = 0,1$

$\hat{=} \; |n_1, n_2, \dots, n_N\rangle = |\ell\rangle \qquad \text{with } \ell = 1, \dots 2^N$

$\rightarrow \; 2^N$ basis states

convention: $|1,1,1,\dots,1\rangle = c_N^\dagger c_{N-1}^\dagger \dots c_2^\dagger c_1^\dagger |0,0,\dots,0\rangle$

$\rightarrow \; \underset{n_1\, n_2\, n_3 \quad n_N}{\langle 1,1,1,\dots,1|} = \langle 0,0,\dots 0 | c_1 c_2 \dots c_N$

as in A_1: the basis $|\ell\rangle$ is a basis of eigenstates!

$$\boxed{H|\ell\rangle = E_\ell |\ell\rangle \;, \quad \ell = 1, \dots 2^N \;, \quad \text{with } E_\ell = \sum_{i=1}^{N} n_i \varepsilon_i}$$

proof $\rightarrow$ exercises

careful: write $H = \sum_{i=1}^{N} \left[\prod_{j \neq i} \mathbb{1}_j \right] H_i \qquad \text{with } H_i = \varepsilon_i c_i^\dagger c_i$

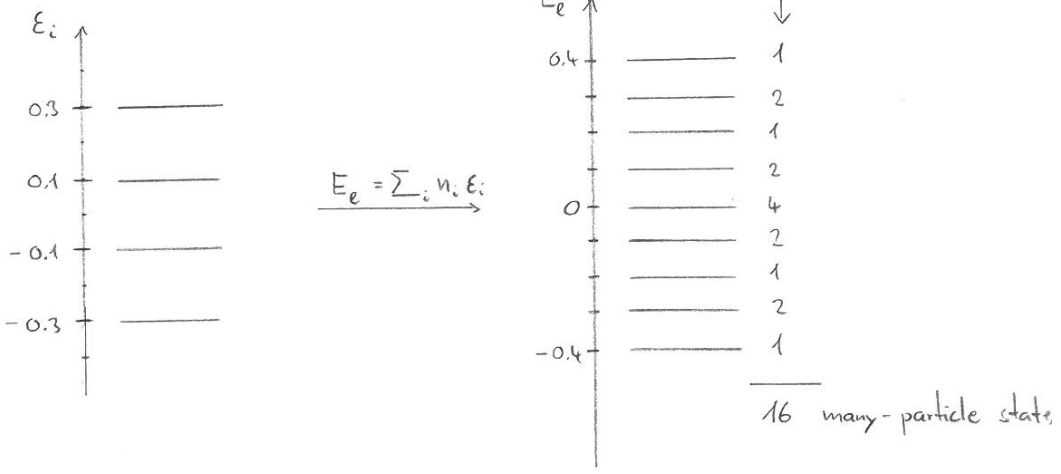
<u>single-particle and many-particle spectra</u>

$\rightarrow$ note the difference between the set of energies $\{\varepsilon_i\}$ and $\{E_\ell\}$!

$\{\varepsilon_i\}$: single-particle spectrum $\rightarrow$ exists only if the Hamiltonian can be mapped onto the form $H = \sum_i \varepsilon_i c_i^\dagger c_i$
(orthogonal transformation, see below)

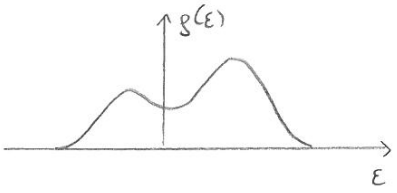
$\{E_\ell\}$: many-particle spectrum $\rightarrow$ exists always as the set of eigenenergies of the Hamiltonian

example: $\{\varepsilon_i\} = (-0.3, -0.1, 0.1, 0.3)$



- some numerical methods calculate $\{\varepsilon_i\}$

  → the density of states $g(\varepsilon)$ $\hat{=}$ continuous version of the single-particle spectrum



  → density functional theory (DFT)
  + local density approximation (LDA)

- some numerical methods calculate $\{E_e\}$
  - Exact Diagonalization (ED) → Sec. 3.1
  - Numerical Renormalization Group (NRG) → Sec. 3.2

- in some cases:

  $\{E_e\} \xrightarrow[\text{to}]{\text{mapping}} \{\varepsilon_i\}$ example → flow to fixed points (see Sec 3.2)

<u>now</u>: how to calculate numerically the many-particle spectrum from a given set of $\{\varepsilon_i\}$?

→ use an integer number j to label the many-particle states:

$$j = \sum_{i=1}^{N} n_i \, 2^{i-1} = n_1 + n_2 \cdot 2 + n_3 \cdot 4 + \dots$$

j goes from 0 to $2^N - 1$

this means: we have to convert j into the sequence

$n_1, n_2, \dots, n_N$ (bit pattern)

$7 \rightarrow 111$

$77 \rightarrow 10110010$ etc.

<u>C, a single site with interaction</u>

$$\boxed{H = \sum_{\sigma} \varepsilon \, c_\sigma^\dagger c_\sigma + U \, c_\uparrow^\dagger c_\uparrow \, c_\downarrow^\dagger c_\downarrow} \quad \hat{=} \quad \begin{matrix} \varepsilon, U \\ 0 \end{matrix}$$

→ corresponds to a single site in the Hubbard model

basis: $\{|i\rangle\} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$

with the convention: $|\uparrow\downarrow\rangle = c_\downarrow^\dagger c_\uparrow^\dagger |0\rangle$

again we have $H|i\rangle = E_i|i\rangle$ with $E_1 = 0$

$E_2 = E_3 = \varepsilon$

$E_4 = 2\varepsilon + U$

$\rightarrow \{E_e\} = \{0, \varepsilon, \varepsilon, 2\varepsilon + U\}$

and the Hamilton matrix: $\{H_{ij}\} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon & 0 & 0 \\ 0 & 0 & \varepsilon & 0 \\ 0 & 0 & 0 & 2\varepsilon + U \end{pmatrix}$

as an exercise: show that $H|\uparrow\downarrow\rangle = (2\varepsilon + U)|\uparrow\downarrow\rangle$

particle - hole symmetry:

consider the Hamiltonian $H' = H(c^\dagger \to c, c \to c^\dagger)$

$\rightarrow H' = \sum_\sigma \varepsilon c_\sigma c_\sigma^\dagger + U c_\uparrow c_\uparrow^\dagger c_\downarrow c_\downarrow^\dagger$

- note that, in general, $H' \neq H$, since the operators c_σ and $c_\sigma^\dagger$ do not commute
- but we can use $[c_\sigma, c_\sigma^\dagger]_+ = 1$ and rewrite H' as follows:

$$H' = \sum_\sigma \varepsilon (1 - c_\sigma^\dagger c_\sigma) + U (1 - c_\uparrow^\dagger c_\uparrow)(1 - c_\downarrow^\dagger c_\downarrow)$$

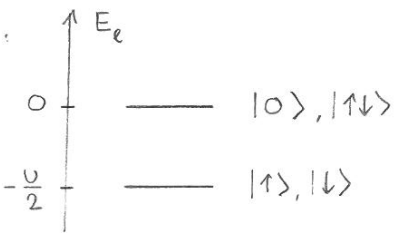
$$= 2\varepsilon + U + \sum_\sigma (-\varepsilon - U) c_\sigma^\dagger c_\sigma + U c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow$$

particle - hole symmetry means: $H' \stackrel{!}{=} H$

this is the case for $2\varepsilon + U = 0 \quad (\hat{=} -\varepsilon - U = \varepsilon)$

$\rightarrow \varepsilon = -\frac{U}{2}$ and $\{0, -\frac{U}{2}, -\frac{U}{2}, 0\}$

many-particle spectrum for $U > 0$ (and ph-symmetry):



D, a two-site model

$$\boxed{H = \sum_{i=1}^{2} \varepsilon_i c_i^\dagger c_i - t\,(c_1^\dagger c_2 + c_2^\dagger c_1)} \quad \hat{=} \quad \underset{1}{\overset{\varepsilon_1}{\circ}} \!\!-\!\!\!-\!\!\!- \underset{2}{\overset{\varepsilon_2}{\circ}} \quad t$$

- a two-site tight binding chain
- spinless fermions

basis: $\{|i\rangle\} = \{|0\rangle_1, |1\rangle_1\} \otimes \{|0\rangle_2, |1\rangle_2\}$

$\hat{=} \{|n_1, n_2\rangle\}$ with $n_i = 0, 1$

$= \{|0,0\rangle, |1,0\rangle, |0,1\rangle, |1,1\rangle\}$

note that this time, the basis $\{|i\rangle\}$ is not a basis of eigenstates!

$$\longrightarrow \quad H|1,0\rangle = \varepsilon_1 c_1^\dagger c_1 |1,0\rangle - t\, c_2^\dagger c_1 |1,0\rangle$$

$$= \varepsilon_1 |1,0\rangle - t|0,1\rangle \neq E|1,0\rangle$$

this means: we have to actually solve the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$

$\hat{=}$ we have to find a basis $|\bar{\ell}\rangle$ such that $H|\bar{\ell}\rangle = E_\ell |\bar{\ell}\rangle$

$|\bar{\ell}\rangle$ and $|i\rangle$ are related by an orthogonal transformation U (4×4 matrix)

$$\longrightarrow \quad |\bar{\ell}\rangle = \sum_{i=1}^{4} U_{\ell i} |i\rangle \qquad \text{with} \qquad U_{\ell i} = \langle i|\bar{\ell}\rangle$$

$$|i\rangle = \sum_{\ell=1}^{4} U_{\ell i} |\bar{\ell}\rangle \qquad (U^{-1} = U^t)$$

now consider the Hamilton matrix $\bar{H}_{\ell m} := \langle \bar{\ell}|H|\bar{m}\rangle$

i, $\{|\bar{\ell}\rangle\}$ is a basis of eigenstates

$$\Rightarrow \quad \bar{H}_{\ell m} = E_m \langle \bar{\ell}|\bar{m}\rangle = E_m \delta_{\ell m}, \quad \{\bar{H}_{\ell m}\} \text{ is diagonal}$$

ii, insert the unity operator $\mathbb{1} = \sum_i |i\rangle\langle i|$

$$\longrightarrow \quad \langle \bar{\ell}|H|\bar{m}\rangle = \sum_{ij} \underbrace{\langle \bar{\ell}|i\rangle}_{= U_{\ell i}} \underbrace{\langle i|H|j\rangle}_{= H_{ij}} \underbrace{\langle j|\bar{m}\rangle}_{= U_{mj}}$$

$$= \sum_{ij} U_{\ell i} H_{ij} (U^+)_{jm} = (UHU^+)_{\ell m} \overset{!}{=} E_m \delta_{\ell m}$$

$\Rightarrow$ the calculation proceeds in two steps:

i) calculate the matrix elements H_{ij} $\rightarrow$ the Hamilton matrix

ii) diagonalize $\{H_{ij}\}$ $\rightarrow$ this gives the eigenstate $|\bar{\ell}\rangle$ and the eigenenergies E_ℓ

in this example:

i) $$\{H_{ij}\} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \varepsilon_1 & -t & 0 \\ 0 & -t & \varepsilon_2 & 0 \\ 0 & 0 & 0 & \varepsilon_1+\varepsilon_2 \end{pmatrix}$$

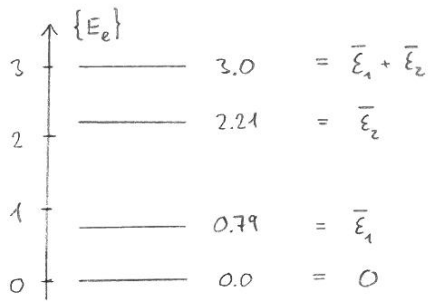
ii) numerical calculation for:

$\varepsilon_1 = 1$

$\varepsilon_2 = 2$

$t = 0.5$

$\Rightarrow$



in this case: $\{E_\ell\}$ can be constructed from a single-particle spectrum!

(explanation $\rightarrow$ see E, 1d tight-binding model)

$\longrightarrow$ note the block structure of the Hamilton matrix!

$$\begin{pmatrix} \cdot & 0 & 0 & 0 \\ 0 & \cdot & \cdot & 0 \\ 0 & \cdot & \cdot & 0 \\ 0 & 0 & 0 & \cdot \end{pmatrix}$$

$\longrightarrow$ $\langle i | H | j \rangle = 0$ when $|j\rangle, |i\rangle$ have different particle number

the total particle number is conserved: $\boxed{[H, \hat{N}]_- = 0}$

with $\hat{N} = \sum_{i=1}^{2} c_i^+ c_i$ $\Rightarrow$ the Hilbert space can be divided into subspaces with different particle numbe

$N = 0$: $|0,0\rangle \longrightarrow E_1 = 0$

$N = 1$: $|1,0\rangle, |0,1\rangle \longrightarrow$ diagonalize the matrix $\begin{pmatrix} \varepsilon_1 & -t \\ -t & \varepsilon_2 \end{pmatrix}$

$$\Rightarrow E_{2/3} = \frac{1}{2}(\varepsilon_1 + \varepsilon_2) \pm \frac{1}{2}\sqrt{(\varepsilon_1 - \varepsilon_2)^2 + 4t^2}$$

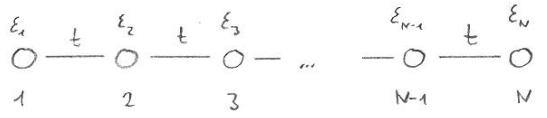
$N = 2$: $|1,1\rangle \longrightarrow E_4 = \varepsilon_1 + \varepsilon_2$

in general : symmetries of the Hamiltonian reduce the dimension of the matrices to be diagonalized !

E, tight-binding chain

$$\boxed{H_{tb} = -t \sum_{i=1}^{N-1} \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + \sum_{i=1}^{N} \varepsilon_i c_i^\dagger c_i} \qquad \longrightarrow \text{spinless fermions}$$

$\hat{=}$



open boundary conditions

for periodic boundary conditions, add : $-t\left(c_N^\dagger c_1 + c_1^\dagger c_N\right)$

the Hamiltonian H_{tb} belongs to a class of Hamiltonians of the form :

$$H = \sum_{ij=1}^{N} t_{ij} c_i^\dagger c_j = \vec{c}^{\,\dagger} T \vec{c}$$

with $\vec{c}^{\,\dagger} = (c_1^\dagger c_2^\dagger \dots c_N^\dagger)$, $\vec{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$, $T = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ t_{21} & \ddots & & \\ \vdots & & & \\ t_{N1} & & & t_{NN} \end{pmatrix}$

for $H = H_{tb}$, the matrix T has the following form :

$$T = \begin{pmatrix} \varepsilon_1 & -t & 0 & & \times \\ -t & \varepsilon_2 & -t & & \\ 0 & -t & \varepsilon_3 & \ddots & \\ \vdots & & \ddots & \ddots & -t \\ \times & & & -t & \varepsilon_N \end{pmatrix} \qquad \text{with} \quad \times = \begin{cases} 0 & : \text{ open bc} \\ -t & : \text{ periodic bc} \end{cases}$$

now: diagonalization of the Hamiltonian (not of the Hamilton matrix!)

→ orthogonal transformation of the operators:

$$\boxed{\begin{aligned} c_i &= \sum_k a_{ik} b_k \\ c_i^+ &= \sum_k a_{ik} b_k^+ \end{aligned}} \quad \hat{=} \quad \vec{c} = A\vec{b}$$

with $A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & \ddots & & \\ \vdots & & & \\ a_{N1} & & & a_{NN} \end{pmatrix}$

$$\Rightarrow \sum_{ij=1}^{N} t_{ij} c_i^+ c_j = \sum_{ij} t_{ij} \sum_k a_{ik} b_k^+ \sum_\ell a_{j\ell} b_\ell$$

$$= \sum_{k\ell} \underbrace{\sum_{ij} a_{ik} t_{ij} a_{j\ell}}\, b_k^+ b_\ell = \dots$$

$$= \underbrace{(A^t T A)_{k\ell}}_{\stackrel{!}{=} \varepsilon_\ell \delta_{k\ell}}$$

: this means → choose an orthogonal matrix A which diagonalizes the matrix T

$$\dots = \sum_{k=1}^{N} \varepsilon_k b_k^+ b_k \quad \rightarrow \text{ diagonal form of the Hamiltonian}$$

$$\boxed{H = \sum_k \varepsilon_k b_k^+ b_k}$$

as in B): $\{\varepsilon_k\}$ is the single-particle spectrum of the Hamiltonian

⇒ we do not have to diagonalize the $(2^N \times 2^N)$-matrix $\langle i|H|j\rangle$ to obtain the many-particle spectrum $\{E_\ell\}$

instead: i) diagonalize the $(N \times N)$-matrix T

$\rightarrow \{\varepsilon_k\}$

ii) $\{E_\ell\}$ follows from $E_\ell = \sum_{k=1}^{N} n_k \varepsilon_k \quad : n_k = 0,1$

2.2 Green functions

2.2.1 basic definitions

→ imaginary-time Green function:

$$\boxed{G(\tau) = -\langle A[\tau]\, B\rangle} \qquad 0 \leq \tau < \beta = \frac{1}{k_B T}$$

↳ 'imaginary time'

with:

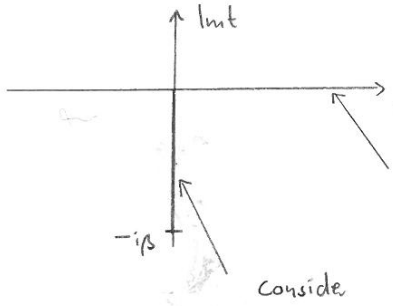
- A, B operators, for example $A = c_{i\sigma}$, $B = c_{i\sigma}^{\dagger}$
- $A[\tau] := e^{\tau H} A\, e^{-\tau H}$, H : the Hamiltonian
- $\langle x\rangle := \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} x\right]$, Tr : Trace
  $= \frac{1}{Z} \sum_i \langle i | e^{-\beta H} x | i\rangle$, $\{|i\rangle\}$: basis of the Hilbert space of the Hamiltonian
- $Z = \mathrm{Tr}\left[e^{-\beta H}\right]$: partition function

→ real-time correlation functions:

$$\boxed{\begin{aligned} C^{>}(t) &= \langle A(t)\, B\rangle \\ C^{<}(t) &= \langle B\, A(t)\rangle \end{aligned}} \qquad t \in \mathbb{R}$$

$$A(t) = e^{iHt} A\, e^{-iHt}$$

generalize the definition of $C^{>}(t)$ to $t \in \mathbb{C}$:



real-time correlation function defined on the real axis

consider $C^{>}(t = -i\tau)$ with $0 \leq \tau < \beta$

τ : imaginary time

→ $C^{>}(t = -i\tau) = \langle \underbrace{A(-i\tau)}\, B\rangle = \langle A[\tau]\, B\rangle = -G(\tau)$

$= e^{\tau H} A\, e^{-\tau H}$

now define :

$$\boxed{\begin{aligned} X(t) &= -i\,\Theta(t)\left[C^{>}(t) + C^{<}(t)\right] \\ &= -i\,\Theta(t)\left\langle [A(t), B]_{+} \right\rangle \end{aligned}}$$

the Laplace transform of $X(t)$ is defined as :

$$\boxed{X(z) = \int_0^\infty dt\; e^{izt}\, X(t) \equiv \langle\langle A, B \rangle\rangle_z}$$

↳ Zhubarev notation

$X(z)$ is defined in the whole upper complex plane : $z \in \{ \mathbb{C} \mid \mathrm{Im}\, z > 0 \}$

$$\rightarrow \quad e^{izt} = e^{i(\mathrm{Re}\, z)t} \underbrace{e^{-(\mathrm{Im}\, z)t}}$$

$\rightarrow$ convergence of the integral

spectral function

$$\boxed{A(\omega) = -\frac{1}{\pi} \lim_{\delta \to 0} \mathrm{Im}\, X(\omega + i\delta)}$$

now assume we have already solved the Schrödinger equation

$\rightarrow H|i\rangle = E_i |i\rangle$ with $\{|i\rangle\}$ a complete basis of eigenstates

$$\Rightarrow \quad C^{>}(t) = \frac{1}{Z} \sum_i \langle i | \underbrace{e^{-\beta H} e^{iHt}} A e^{-iHt} B | i \rangle$$

insert $\mathbb{1} = \sum_j |j\rangle\langle j|$

$$= \frac{1}{Z} \sum_{ij} \langle i|A|j\rangle \langle j|B|i\rangle\, e^{-\beta E_i}\, e^{i(E_i - E_j)t}$$

Fourier transform of $C^{>}(t)$:

$$C^{>}(\omega) = \int_{-\infty}^{\infty} dt\; e^{i\omega t}\, C^{>}(t)$$

$$= \frac{1}{Z} \sum_{ij} \langle i|A|j\rangle \langle j|B|i\rangle\, e^{-\beta E_i}\, 2\pi\, \delta(\omega + E_i - E_j)$$

with $A(\omega) = \frac{1}{2\pi}\left[C^{>}(\omega) + C^{<}(\omega)\right]$ (proof see exercises) and the analogous calculation for $C^{<}(\omega)$, we arrive at :

$$A(\omega) = \frac{1}{Z} \sum_{ij} \langle i|A|j\rangle\langle j|B|i\rangle \cdot \left(e^{-\beta E_i} + e^{-\beta E_j}\right) \delta(\omega + E_i - E_j)$$

→ Lehmann representation of the spectral function $A(\omega)$

example: $H = \varepsilon c^\dagger c$, $A = c$, $B = c^\dagger$

→ $\{|i\rangle\} = \{|0\rangle, |1\rangle\}$

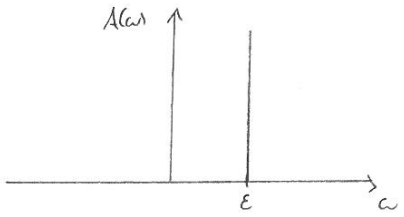
$\{E_i\} = \{0, \varepsilon\}$ → $Z = 1 + e^{-\beta\varepsilon}$

matrix elements: $\langle i|A|j\rangle\langle j|B|i\rangle = \langle i|c|j\rangle \underbrace{\langle j|c^\dagger|i\rangle}_{= (\langle i|c|j\rangle)^*} = |\langle i|c|j\rangle|^2$

here: $|\langle i|c|j\rangle|^2 = \begin{cases} 1 : (i,j) = (0,1) \\ 0 : (i,j) = (0,0), (1,0), (1,1) \end{cases}$

$$\Rightarrow A(\omega) = \frac{1}{1+e^{-\beta\varepsilon}} \left(1 + e^{-\beta\varepsilon}\right) \delta(\omega + 0 - \varepsilon)$$

$$\boxed{A(\omega) = \delta(\omega - \varepsilon)}$$



→ a single δ-peak at $\omega = \varepsilon$

2.2.2 analytic continuation

what is the relation between $X(\tau)$ (or the spectral function $A(\omega)$) and the imaginary-time Green function $G(\tau)$?

→ define the Fourier transform of $G(\tau)$:

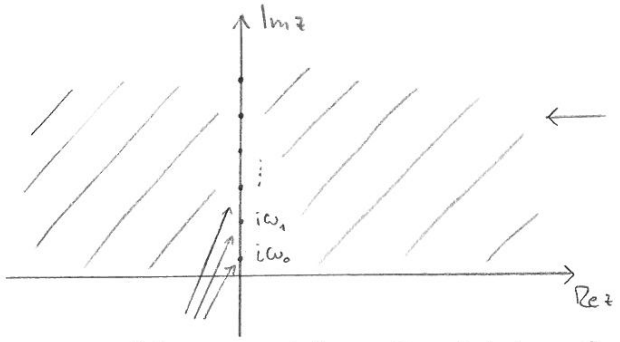
$$\boxed{G(i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n \tau} G(\tau)} \quad (*)$$

with the Matsubara frequencies

$i\omega_n = i\frac{\pi}{\beta}(2n+1)$, $n = 0, 1, 2, \ldots$

it turns out that: $\boxed{G(i\omega_n) = X(z = i\omega_n)}$

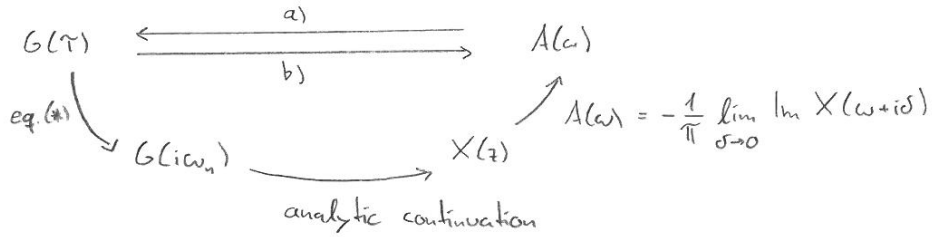
⇒ analytic continuation here means: obtain $X(z)$ for all values of $z \in \mathbb{C}$ from $X(z = i\omega_n)$



← $X(z)$ is defined in the whole upper complex plane

$G(i\omega_n)$ is defined for Matsubara frequencies only

<u>the general scheme</u> :



a, (without proof)

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

b, numerical inversion of this integral transformation (see below)

→ also termed 'analytic continuation'

<u>example</u> : as above → $H = \varepsilon c^\dagger c$

$A = c \;,\; B = c^\dagger$

$$\rightarrow \quad G(\tau) = -\langle c[\tau]c^\dagger\rangle =$$

$$= -\frac{1}{Z}\sum_{ij}\langle i|e^{-\beta H}e^{\tau H}\,c\,e^{-\tau H}|j\rangle\langle j|c^\dagger|i\rangle$$

$$= -\frac{1}{Z}\sum_{ij} e^{(\tau-\beta)E_i}e^{-\tau E_j}\,|\langle i|c|j\rangle|^2 = -\frac{e^{-\tau\varepsilon}}{1+e^{-\beta\varepsilon}}$$

Fourier transformation :

$$G(i\omega_n) = -\frac{1}{1+e^{-\beta\varepsilon}}\underbrace{\int_0^\beta d\tau\, e^{i\omega_n\tau}e^{-\tau\varepsilon}}$$

$$= \frac{1}{i\omega_n-\varepsilon}\left[e^{(i\omega_n-\varepsilon)\tau}\right]_0^\beta = -\frac{1}{i\omega_n-\varepsilon}\left(1+e^{-\beta\varepsilon}\right)$$

$$\Rightarrow \quad G(i\omega_n) = \frac{1}{i\omega_n-\varepsilon}$$

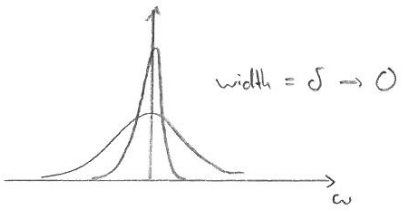
analytic continuation: replace $i\omega_n$ by z to obtain $X(z)$

$$\longrightarrow \boxed{X(z) = \frac{1}{z-\varepsilon}}$$

spectral function:

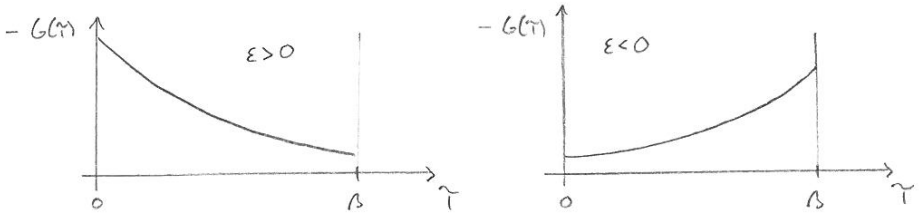
$$A(\omega) = -\frac{1}{\pi} \lim_{\delta \to 0} \mathrm{Im}\left(\frac{1}{\omega + i\delta - \varepsilon}\right) \overset{!}{=} \delta(\omega - \varepsilon) \quad \text{as in Sec. 2.2.1}$$

reminder: representation of δ-functions



and finally:

$$G(\tau) = -\int_{-\infty}^{\infty} d\omega \, \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} \, \delta(\omega - \varepsilon) = -\frac{e^{-\tau\varepsilon}}{1+e^{-\beta\varepsilon}} \qquad \text{ok}$$



<u>now</u>: what are we interested in? $G(\tau)$ or $A(\omega)$?

→ physical quantities are related to Green functions on the <u>real</u> (frequency/time) axis, such as the spectral function $A(\omega)$

direct calculation (Lehmann representation) → ED, NRG

via $G(\tau)$ and analytic continuation → Q.MC

<u>the problem</u>: the kernel for the inverse integral transformation $K_\beta^{-1}(\tau,\omega)$ does not exist!

$$G(\tau) = \int_{-\infty}^{\infty} d\omega \, K_\beta(\tau,\omega) \, A(\omega)$$

$G(\tau)$ ⟷ $A(\omega)$

$$A(\omega) = \int_0^\beta d\tau \, K_\beta^{-1}(\tau,\omega) \, G(\tau)$$

how to extract numerically the spectral function from a given $G(\tau)$?

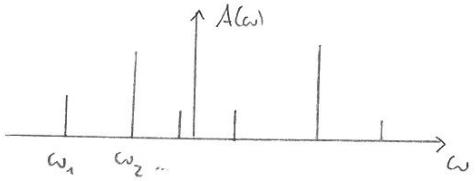
a) matrix inversion

we assume that • $G(\tau)$ is known for N values τ_j

$$g_j = G(\tau_j) \quad , \quad j = 1, \dots N$$

• $A(\omega)$ is given by $\quad A(\omega) = \sum_{i=1}^{N} a_i \, \delta(\omega - \omega_i)$

with $\{\omega_i\}$ fixed and $\{a_i\}$ to be determined



$$\Rightarrow \quad -g_j = \sum_{i=1}^{N} M_{ji} \, a_i \qquad \text{with} \qquad M_{ji} = \frac{e^{-\tau_j \omega_i}}{1 + e^{-\beta \omega_i}}$$

$$\hat{=} \quad -\vec{g} = M \vec{a} \qquad \Rightarrow \qquad \boxed{\vec{a} = -M^{-1} \vec{g}}$$

looks fine, but : • how to select the ω_i ?

• how to enforce $a_i \geq 0$?

↳ $|\langle i | c | j \rangle|^2 \geq 0$

b) optimization

choose a specific form for the spectral function

→ $A(\omega; x_1, x_2, \dots, x_M)$

for example : • x_i given by the position and weights of $\frac{M}{2}$ δ-peaks

$$A = \sum \delta\text{-peaks}$$

• x_i given by the position, weight, and width of $\frac{M}{3}$ Lorentzians

$$A = \sum \text{Lorentzians}$$

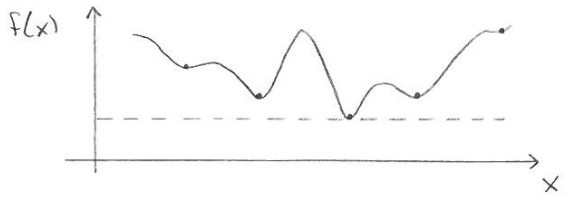
$G(\tau)$ again given for N values τ_j : $g_j = G(\tau_j)$

calculate $\bar{G}(\tau_j, \vec{x}) = -\int_{-\infty}^{\infty} d\omega \, \frac{e^{-\tau_j \omega}}{1+e^{-\beta\omega}} \, A(\omega; \vec{x})$

and determine $f(\vec{x}) = \sum_{j=1}^{N} \left[\bar{G}(\tau_j, \vec{x}) - g_j \right]^2$ or any other measure of the distance between $\bar{G}(\tau)$ and $G(\tau)$

$\Rightarrow$ the optimal $\vec{x}$, and the optimal $A(\omega)$, follow from minimization of the function $f(\vec{x})$

the usual problem: many local minima



c, Pade approximation

the Pade approximant of order (m,n) is given by the rational function

$$P(z) = \frac{p_0 + p_1 z + \dots + p_m z^m}{1 + q_1 z + \dots + q_n z^n}$$

in our case: $P(z)$ is known for $z = i\omega_n$

$\rightarrow P(z = i\omega_n) = X(z = i\omega_n)$

there exist fast algorithms to generate the coefficients p_i, q_i

but the resulting $P(z)$ might have poles in the upper complex plane

d, maximum entropy

the general idea:

we have a, the data $\rightarrow g_i = G(\tau_j)$

possibly with error bars (from QMC calculations)

b, prior knowledge about $A(\omega)$

$\rightarrow A(\omega) > 0$, sum rules, asymptotic form, etc.

how to combine the prior knowledge with the data to obtain the best estimate for $A(\omega)$?

$\rightarrow$ use probability theory : 'Bayesian logic'

2.2.3 equation of motion

consider the correlation function $X(z) = \langle\langle A, B \rangle\rangle_z$

$\rightarrow$ $$\boxed{z \langle\langle A, B \rangle\rangle_z + \langle\langle \mathcal{L}A, B \rangle\rangle_z = \langle [A, B]_+ \rangle}$$ (*) with the Liouville - Operator $\mathcal{L} \cdot = [H, \cdot]_-$

the proof works as follows :

- start with $\frac{d}{dt}\left[e^{izt} X(t) \right] = \dots$
- on both side of the resulting equation, take $\int_{-\infty}^{\infty} dt \dots$

example : $H = \varepsilon c^\dagger c$, $A = c$, $B = c^\dagger$

$\rightarrow$ calculate $\mathcal{L}A = [H, c]_- = \varepsilon \underbrace{[c^\dagger c, c]_-}_{= -c} = -\varepsilon c$

$\rightarrow$ $[A, B]_+ = [c, c^\dagger]_+ = 1$

and $\langle 1 \rangle = \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} \right] = 1$

$\overset{(*)}{\Rightarrow}$ $z \langle\langle c, c^\dagger \rangle\rangle_z - \varepsilon \langle\langle c, c^\dagger \rangle\rangle_z = 1 \quad \Rightarrow \quad \boxed{\langle\langle c, c^\dagger \rangle\rangle_z = \frac{1}{z - \varepsilon}}$

ok, see Sec. 2.2.2

the equation of motion seems to be very efficient in calculating correlation functions, but :

$\rightarrow$ this example is special since $\mathcal{L}A \propto A$

in general : $\mathcal{L}A = \sum_i C_i$ with operators C_i

$\hookrightarrow$ $\langle\langle \mathcal{L}A, B \rangle\rangle_z = \sum_i \underbrace{\langle\langle C_i, B \rangle\rangle_z}$

try to calculate these correlation functions again using the equation of motion

$$\rightarrow \quad \mathcal{L} C_i = \sum_j D_{ij}$$

$$\rightarrow \quad \mathcal{L} D_{ij} = \sum_k E_{ijk}$$

and so on

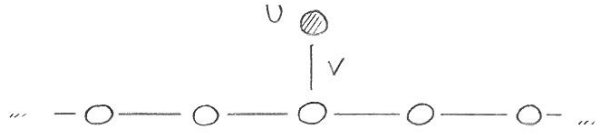
<u>this means</u> : prolifaation of operators and corresponding correlation function

→ system of equations of motion cannot be closed in geneal

furthermore : how to calculate $\langle [C_i, B] \rangle_t$ etc ?

2.2.4 example : Green functions for the single-impurity Anderson model

in Sec 1.2 b) : siAm in the 'site-representation'



<u>now</u>: mapping onto the 'k-representation'

→ write H_{bath} as $H_{bath} = \sum_\sigma \vec{C}_\sigma^+ \, T \, \vec{C}_\sigma \stackrel{!}{=} \sum_{\sigma k} \varepsilon_k b_{k\sigma}^+ b_{k\sigma}$

↳ diagonalization of the matrix T

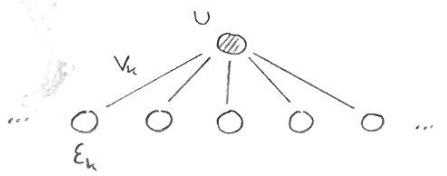
with $c_{i\sigma} = \sum_k a_{ik} b_{k\sigma}$

→ impurity-bath coupling :

$$H_{imp-bath} = V \sum_\sigma \left(f_\sigma^+ c_{o\sigma} + c_{o\sigma}^+ f_\sigma \right)$$

$$= \sum_{k\sigma} V_k \left(f_\sigma^+ b_{k\sigma} + b_{k\sigma}^+ f_\sigma \right) \qquad \text{with } V_k = V a_{ok}$$

$\Rightarrow$



no direct coupling between the bath degrees of freedom

<u>in the following</u> : use equations of motion for the calculation of the impurity Green function $G_\sigma(z) = \langle\langle f_\sigma, f_\sigma^+ \rangle\rangle_z$

first step: equation of motion for $\langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z$

$\rightarrow A = f_\sigma \,, \quad B = f_\sigma^\dagger$

$$\mathcal{L} f_\sigma = [H_{imp} + H_{bath} + H_{imp\text{-}bath}, f_\sigma]_-$$

$$= \varepsilon_f \underbrace{[\sum_{\sigma'} f_{\sigma'}^\dagger f_{\sigma'}, f_\sigma]_-}_{= -f_\sigma} + U \underbrace{[f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow, f_\sigma]_-}_{= -f_\sigma f_{\bar\sigma}^\dagger f_{\bar\sigma}}$$

$$+ \sum_{k\sigma'} \varepsilon_k \underbrace{[b_{k\sigma'}^\dagger b_{k\sigma'}, f_\sigma]_-}_{=0} + \sum_{k\sigma'} V_k \Big(\underbrace{[f_{\sigma'}^\dagger b_{k\sigma'}, f_\sigma]_-}_{= -b_{k\sigma}\delta_{\sigma\sigma'}} + \underbrace{[b_{k\sigma'}^\dagger f_{\sigma'}, f_\sigma]_-}_{=0} \Big)$$

$$\Rightarrow \underbrace{z \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z - \varepsilon_f \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z}_{= (z-\varepsilon_f) G_\sigma(z)} - \underbrace{U \langle\langle f_\sigma f_{\bar\sigma}^\dagger f_{\bar\sigma}, f_\sigma^\dagger \rangle\rangle_z}_{=: F_\sigma(z)} - \sum_k V_k \langle\langle b_{k\sigma}, f_\sigma^\dagger \rangle\rangle_z = 1$$

$\rightarrow$ equation of motion generate two new correlation functions!

second step: equation of motion for $\langle\langle b_{k\sigma}, f_\sigma^\dagger \rangle\rangle_z$

$\rightarrow A = b_{k\sigma} \,, \quad B = f_\sigma^\dagger$

$$\mathcal{L} b_{k\sigma} = -\varepsilon_k b_{k\sigma} - V_k f_\sigma \,, \quad [b_{k\sigma}, f_\sigma^\dagger]_+ = 0$$

$$\Rightarrow z \langle\langle b_{k\sigma}, f_\sigma^\dagger \rangle\rangle_z - \varepsilon_k \langle\langle b_{k\sigma}, f_\sigma^\dagger \rangle\rangle_z - V_k \underbrace{\langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle_z}_{= G_\sigma(z)} = 0$$

$$\boxed{\langle\langle b_{k\sigma}, f_\sigma^\dagger \rangle\rangle_z = \frac{V_k}{z-\varepsilon_k} G_\sigma(z)}$$

insert this into the equation of the first step

$$\rightarrow (z-\varepsilon_f) G_\sigma(z) - U F_\sigma(z) - \underbrace{\sum_k \frac{V_k^2}{z-\varepsilon_k}}_{=: \Delta(z) \text{ hybridization function}} G_\sigma(z) = 1$$

rewrite this equation as

$$G_\sigma(z) \left(z - \varepsilon_f - \Delta(z) - U \frac{F_\sigma(z)}{G_\sigma(z)} \right) = 1$$

now define the self-energy $\Sigma_\sigma(z)$:

$$\boxed{\Sigma_\sigma(z) = \Delta(z) + \Sigma^U_\sigma(z)}$$

$\Delta(z)$: hybridization part of the self-energy

$\Sigma^U_\sigma(z)$: correlation part

with the correlation part given by:

$$\boxed{\Sigma^U_\sigma(z) = U \frac{F_\sigma(z)}{G_\sigma(z)}}$$

$\Rightarrow$ formal solution for the impurity Green function:

$$\boxed{G_\sigma(z) = \frac{1}{z - \varepsilon_f - \Sigma_\sigma(z)}}$$

<u>but</u>: $F_\sigma(z)$ not yet determined, therefore ...

<u>third step</u>: equation of motion for $\langle\langle f_\sigma f^\dagger_{\bar\sigma} f_{\bar\sigma}, f^\dagger_\sigma \rangle\rangle_z$

$\mathcal{L} f_\sigma f^\dagger_{\bar\sigma} f_{\bar\sigma} = \dots$ $\rightarrow$ equations of motion generated in this way get more and more complicated

possible approximation: $f_\sigma f^\dagger_{\bar\sigma} f_{\bar\sigma} \rightarrow f_\sigma \langle f^\dagger_{\bar\sigma} f_{\bar\sigma} \rangle$

2.2.5 broadening

spectral function of the impurity Green function (see previous subsection)

$\rightarrow \langle i|A|j\rangle\langle j|B|i\rangle = |\langle i|c_\sigma|j\rangle|^2$

Lehmann representation:

$$A(\omega) = \frac{1}{Z} \sum_{ij} |\langle i|c_\sigma|j\rangle|^2 \left(e^{-\beta E_i} + e^{-\beta E_j}\right) \delta\left(\omega + (E_i - E_j)\right)$$

$$= \sum_n a_n \delta(\omega - \omega_n)$$

'broadening' means: replace each δ-function in $\sum_n \dots$ by a suitable broadening function $P_b(\omega, \omega_n)$

↳ width

$\delta(\omega-\omega_n) \longrightarrow P_b(\omega,\omega_n)$ with the requirements

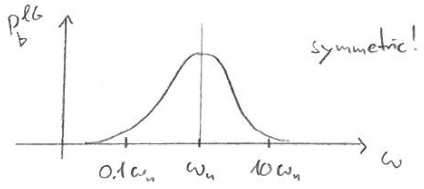
- $\int_{-\infty}^{\infty} d\omega\, P_b(\omega,\omega_n) = 1$
- $\lim_{b\to 0} P_b(\omega,\omega_n) = \delta(\omega-\omega_n)$

$\Rightarrow A_b(\omega) = \sum_n a_n P_b(\omega,\omega_n)$ $\quad A_b(\omega)$: the broadened spectral function

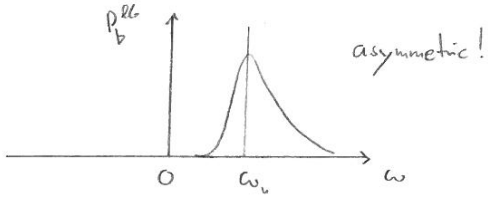
<u>examples</u> :

- Lorentzian: $P_b^L(\omega,\omega_n) = \frac{1}{\pi}\frac{b}{(\omega-\omega_n)^2+b^2}$
- Gaussian: $P_b^G(\omega,\omega_n) = \frac{1}{b\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\omega-\omega_n}{b}\right)^2\right]$
- logarithmic Gaussian: $P_b^{lG}(\omega,\omega_n) = \frac{e^{-b^2/4}}{b\omega_n\sqrt{\pi}} \exp\left[-\left(\frac{\ln\omega-\ln\omega_n}{b}\right)^2\right]$

$\hat{=}$ Gaussian on a logarithmic scale



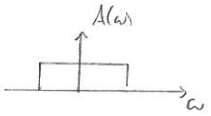
on a linear scale:



note that $P_b^{L,G}(\omega,\omega_n) > 0$ for all $\omega \in \mathbb{R}$

while $P_b^{lG}(\omega,\omega_n) = \begin{cases} 0 & : \omega \le 0 \\ \text{finite} & : \omega > 0 \end{cases}$

<u>in the following</u> : start with a continuous spectral function



↓ (artificial) discretization

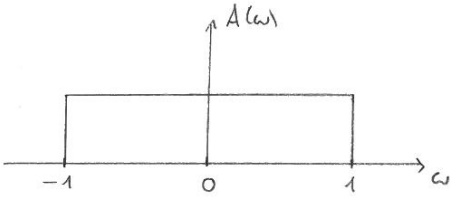
$A_d(\omega) = \sum_{n=1}^{N} a_n \delta(\omega-\omega_n)$

↓ broadening

try to recover $A(\omega)$ with the broadened $A_d(\omega)$

example:

$$A(\omega) = \begin{cases} \frac{1}{2} & : |\omega| \leq 1 \\ 0 & : |\omega| > 1 \end{cases}$$

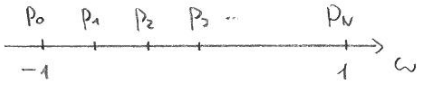


total spectral weight: $\int_{-\infty}^{\infty} d\omega\, A(\omega) = 1$

a, linear discretization

divide the interval $[-1,1]$ into N intervals $[p_i, p_{i+1}]$, $i = 0,1,\dots N-1$

with $p_i = -1 + i\,\frac{2}{N}$



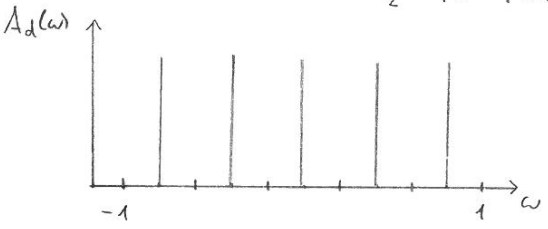
discretization means: the continuous spectral function $A(\omega)$ is replaced by a sum of δ-peaks

$$A(\omega) \longrightarrow A_d(\omega) = \sum_{n=1}^{N} a_n\, \delta(\omega - \omega_n)$$

with $\omega_n = \frac{1}{2}(p_{n-1} + p_n) = -1 + (n - \frac{1}{2})\frac{2}{N}$, $n = 1,2,\dots N$

$a_n = \int_{p_{n-1}}^{p_n} d\omega\, A(\omega)$ the spectral weight contained in this interval

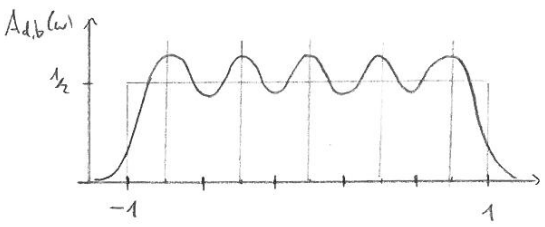
$= \frac{1}{2}(p_n - p_{n-1}) = \frac{1}{N}$



$$\longrightarrow \int_{-\infty}^{\infty} d\omega\, A_d(\omega) = \sum_{n=1}^{N} a_n = 1$$

broadening of $A_d(\omega)$:

$$A_d(\omega) \longrightarrow A_{d,b}(\omega) = \sum_{n=1}^{N} a_n\, P_b(\omega, \omega_n)$$



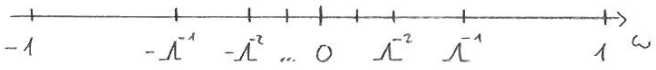
what is the optimal broadening parameta b?

↓

minimize $\int d\omega\, |A(\omega) - A_{d,b}(\omega)|^2$

$\longrightarrow$ b of the orde $\frac{2}{N}$

b) logarithmic discretization



→ divide the inteval $[-1,1]$ into : $[x_{n+1}, x_n]$ $(\omega>0)$, $[-x_n, -x_{n+1}]$ $(\omega<0)$ } $n = 0, 1, \dots, \infty$

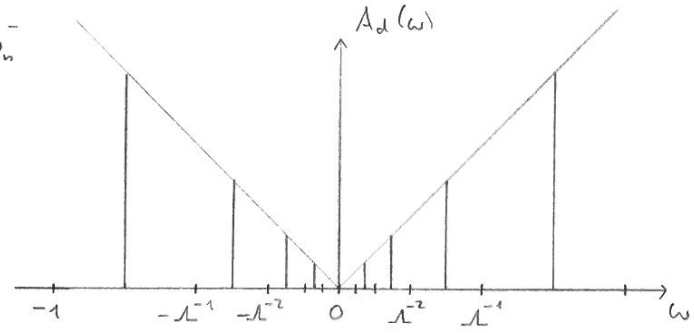
with $x_n = \Lambda^{-n}$ and the discretization parameter $\Lambda > 1$

discretization of $A(\omega)$ now gives :

$$A_d(\omega) = \sum_{n=1}^{N/2} a_n^- \, \delta(\omega - \omega_n^-) + \sum_{n=1}^{N/2} a_n^+ \, \delta(\omega - \omega_n^+)$$

with $\omega_n^+ = \frac{1}{2}\Lambda^{-n}(1+\Lambda) = -\omega_n^-$

$a_n^+ = \frac{1}{2}\Lambda^{-n}(\Lambda-1) = a_n^-$



broadening of $A_d(\omega)$:

i) Lorentzian with fixed width b

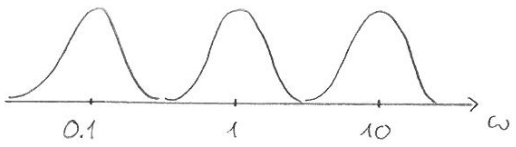
→ fine, but structure at small ω cannot be resolved (if present)

ii) Lorentzian with width $b \propto \omega_n$

→ artificial divergence for $\omega \to 0$ and $N \to \infty$

iii) logarithmic Gaussian with fixed width b

this means



→ same width on a log scale !

→ ok, see also Sec. 3.2 : broadening of discrete spectral functions calculated with the NRG

2.2.6 continued fractions

a real number $x \in \mathbb{R}$ can be written as a continued fraction:

$$x = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \dots}}}$$

a_0 : integer

$a_1, a_2, \dots$: positive integers

example: $\pi = 3 + \cfrac{1}{7 + \cfrac{1}{15 + \cfrac{1}{1 + \dots}}}$

$\longrightarrow$ this generates a sequence of rational approximations of π:

$$3 + \frac{1}{7} = \frac{22}{7} \quad ; \quad 3 + \cfrac{1}{7 + \cfrac{1}{15}} = \frac{333}{106} \quad ; \quad 3 + \cfrac{1}{7 + \cfrac{1}{15 + \cfrac{1}{1}}} = \frac{355}{113} \quad ; \dots$$

here: continued fraction representation of the Green function $G(z)$

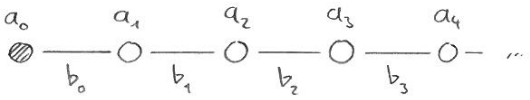
$$G(z) = \int_{-\infty}^{\infty} d\omega' \, \frac{A(\omega')}{z - \omega'} \qquad \text{with} \quad \int_{-\infty}^{\infty} d\omega \, A(\omega) = 1$$

for arbitary spectral functions $A(\omega)$, $G(z)$ can be written as

$$G(z) = \cfrac{1}{z - a_0 - \cfrac{b_0^2}{z - a_1 - \cfrac{b_1^2}{z - a_2 - \cfrac{b_2^2}{z - \dots}}}}$$

$a_n, b_n \in \mathbb{R}$

Green functions in a continued fraction form appear naturally for a tight-binding model on a semi-infinite chain



Hamiltonian:

$$H = \sum_{n=0}^{\infty} a_n \, c_n^{\dagger} c_n + \sum_{n=0}^{\infty} b_n \left(c_n^{\dagger} c_{n+1} + c_{n+1}^{\dagger} c_n \right)$$

$\longrightarrow$ calculate the Green function $G_0(z) = \langle\langle c_0, c_0^{\dagger} \rangle\rangle_z$ with the equation of motion method

define $G_n(z) = \langle\langle c_n, c_0^+ \rangle\rangle_z$

equation of motion: $z \langle\langle A, B \rangle\rangle_z + \langle\langle \mathcal{H} A, B \rangle\rangle_z = \langle [A, B]_+ \rangle$

i) $A = c_0$, $B = c_0^+$

$$\rightarrow \quad (z - a_0)\, G_0(z) - b_0\, G_1(z) = 1$$

$$\left(z - a_0 - b_0 \frac{G_1(z)}{G_0(z)}\right) G_0(z) = 1$$

$$\Rightarrow \quad \boxed{G_0(z) = \frac{1}{z - a_0 - b_0 \frac{G_1(z)}{G_0(z)}}} \qquad (0)$$

ii) $A = c_n$, $B = c_0^+$ $\quad (n = 1, 2, \ldots)$

$$\rightarrow \quad (z - a_n)\, G_n(z) - b_n\, G_{n+1}(z) - b_{n-1}\, G_{n-1}(z) = 0 \quad \Big| \cdot \frac{1}{G_n(z)}$$

$$z - a_n - b_n \frac{G_{n+1}(z)}{G_n(z)} - b_{n-1} \frac{G_{n-1}(z)}{G_n(z)} = 0$$

$$b_{n-1} \frac{G_{n-1}(z)}{G_n(z)} = z - a_n - b_n \frac{G_{n+1}(z)}{G_n(z)}$$

$$\Rightarrow \quad \boxed{\frac{G_n(z)}{G_{n-1}(z)} = \frac{b_{n-1}}{z - a_n - b_n \frac{G_{n+1}(z)}{G_n(z)}}} \qquad (n)$$

now: insert $\frac{G_1(z)}{G_0(z)}$ from eq. (1) into eq. (0)

$$G_0(z) = \frac{1}{z - a_0 - \frac{b_0^2}{z - a_1 - b_1 \frac{G_2(z)}{G_1(z)}}} \quad \longleftarrow \text{ insert } \frac{G_2(z)}{G_1(z)} \text{ from eq. (2) etc.}$$

examples

1. $a_n = a$, $b_n = b$ for all n

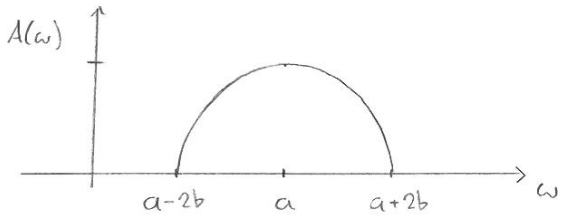
$$G(z) = \frac{1}{z - a - \frac{b^2}{z - a - \frac{b^2}{\ddots}}} \overset{!}{=} \frac{1}{z - a - b^2\, G(z)}$$

this gives a quadratic equation for $G(z)$

$$\Rightarrow \qquad G(z) = \frac{1}{2b^2}\left(z-a \pm \sqrt{(z-a)^2 - 4b^2}\right) =: T_{a,b}(z)$$

choose the sign such that the spectral function $A(\omega) \geq 0 \longrightarrow$ '$-$'

$$A(\omega) = \begin{cases} \frac{1}{2\pi b^2}\sqrt{4b^2 - (\omega-a)^2} & : \; -2b < \omega - a < 2b \\ 0 & : \text{ otherwise} \end{cases}$$



2. $a_n = a$, $b_n = b$ for all $n \geq N$

$$\longrightarrow \quad G(z) = \cfrac{1}{z - a_0 - \ddots \cfrac{b_{N-1}^2}{z - a - \cfrac{b^2}{z - a - \ddots}}}$$

$$= b_{N-1}^2 \, T_{a,b}(z)$$

↳ terminator

3. Quantum Many-Particle Systems: Methods

3.1 Exact Diagonalization

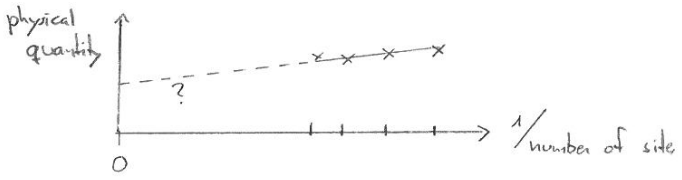
→ calculation of $E_n, |\Psi_n\rangle$ for a model of correlated electrons (such as the Hubbard model) on a finite cluster

e.g. for a 2d square lattice

3×3 lattice sites ; 4×4 , 5×5 ?

disadvantages:

- severe size limitations
  → depending on the structure of the model, the limit is of the orde of 20-30 sites
- finite size extrapolation is problematic



- if used as an approximation of the model in the thermodynamic limit ($N \to \infty$):
  → poor resolution at low frequencies

advantages:

- direct access to energies and wave functions
- results are exact ⇒ benchmark for approximate methods
- Green functions on real frequency axis (no need for analytic continuation)

the strategy:

A:	set up the Hamilton matrices
B:	diagonalize the Hamilton matrices
C:	calculate physical properties

A, the Hamilton matrices

→ identify the symmetries of the Hamiltonian, i.e the operators $\hat{Q}_1, \hat{Q}_2, \ldots$

with $[H, \hat{Q}_\ell] = 0 \quad , \quad \ell = 1,2,\ldots$

→ find a suitable basis of the Hilbert space of the Hamiltonian, such that

$$\hat{Q}_\ell \, | \, i \, ; \underbrace{q_1, q_2, \ldots}_{\equiv \{q\}} \rangle = q_\ell \, | \, i \, ; q_1, q_2, \ldots \rangle$$

with $i = 1, \ldots, \dim_{\{q\}}$

$\dim_{\{q\}}$: dimension of the subspace $H(\{q\})$

$\sum_{\{q\}} \dim_{\{q\}}$ = dimension of the full Hilbert space

example : three-site Hubbard model → $\hat{Q}_1 = \hat{N}$: total particle number

O — O — O $\quad\quad$ $\hat{Q}_2 = \hat{S}_z$: z-component of total spin

for $q_1 = 2$, $q_2 = 1$:

$$\left.\begin{aligned} |1; 2,1\rangle &= |\uparrow,\uparrow,0\rangle \\ |2; 2,1\rangle &= |\uparrow,0,\uparrow\rangle \\ |3; 2,1\rangle &= |0,\uparrow,\uparrow\rangle \end{aligned}\right\} \quad \dim_{2,1} = 3$$

→ Hamilton matrix in each subspace :

$$H(\{q\})_{\ell m} = \langle \ell, \{q\} \, | \, H \, | \, m, \{q\} \rangle \qquad \ell, m = 1, \ldots, \dim_{\{q\}}$$

- for short range interactions / hoppings :

  numbe of <u>non-zero matrix elements</u> $\propto \dim_{\{q\}}$, not $\propto \dim_{\{q\}}^2$!

  → only these have to be stored

- determine the signs :

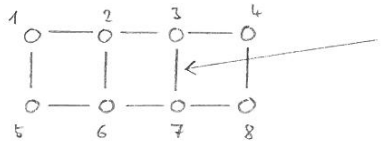
$$\langle n_1, n_2, \ldots, \underset{\uparrow n_i}{1}, \ldots, \underset{\uparrow n_j}{0}, \ldots, n_N \, | \, c_i^\dagger c_j \, | \, n_1, n_2, \ldots, \underset{\uparrow n_i}{0}, \ldots, \underset{\uparrow n_j}{1}, \ldots n_N \rangle = \qquad (j > i)$$

$$= \langle 0 | \, c_1 c_2 \ldots c_i \ldots c_N \, c_i^\dagger \, c_j \, c_N^\dagger \ldots c_j^\dagger \ldots c_2^\dagger c_1^\dagger \, | 0 \rangle =$$

$$p = \sum_{\substack{\ell = i+1 \\ (\ell \neq j)}}^{N} n_\ell \; + \sum_{\ell = j+1}^{N} n_\ell \quad : \text{ numbe of permutations}$$

$$\rightarrow \quad p = \underbrace{2\sum_{l=j+1}^{N} n_l}_{= \text{even}} + \underbrace{\sum_{l=i+1}^{j-1} n_l}_{= \begin{cases} 0 \text{ for } j = i+1 \rightarrow (-1)^p = 1 \\ \text{even} \rightarrow (-1)^p = 1 \\ \text{odd} \rightarrow (-1)^p = -1 \end{cases}}$$

enumeration of the sites for 2d clusters:



hopping between site $i = 3$ and $j = 7$

$\Rightarrow$ sign depends on the filling of sites 4, 5, and 6

B, diagonalization

i, full diagonalization $\rightarrow$ calculation of all $E_n, |\Psi_n\rangle$

computing time $\propto (\dim_{\{q\}})^3$

memory $\propto (\dim_{\{q\}})^2$

ii, Lanczos algorithm $\rightarrow$ calculation of $E_n, |\Psi_n\rangle$ for ground state and low-lying states

computing time $\propto (\dim_{\{q\}})^1$

memory $\propto (\dim_{\{q\}})^1$

with $\ln \dim_{\{q\}} \propto$ number of sites

$\rightarrow$ the Lanczos algorithm

- select an arbitrary vector $|\Phi_0\rangle$ in the relevant Hilbert space

  $\rightarrow$ basis $\{|i\rangle\}$: $|\Phi_0\rangle = \sum_i a_{0i} |i\rangle$

  we must have : $\langle \Phi_0 | \Psi_0 \rangle \neq 0$

  $\hookrightarrow$ the actual ground state

  $\Rightarrow$ select a random initial state (randomly chosen a_{0i})

- define

$$\boxed{|\Phi_1\rangle = H|\Phi_0\rangle - \frac{\langle \Phi_0 | H | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} |\Phi_0\rangle}$$

$$\rightarrow \quad \langle \Phi_0 | \Phi_1 \rangle = \langle \Phi_0 | H | \Phi_0 \rangle - \frac{\langle \Phi_0 | H | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} \langle \Phi_0 | \Phi_0 \rangle = 0$$

$|\Phi_1\rangle$ is orthogonal to $|\Phi_0\rangle$

$$\rightarrow \quad \langle \Phi_1 | \Phi_1 \rangle = \langle \Phi_1 | H | \Phi_0 \rangle \quad \rightarrow \quad \langle \Phi_0 | H | \Phi_1 \rangle = (\langle \Phi_1 | \Phi_1 \rangle)^* = \langle \Phi_1 | \Phi_1 \rangle \qquad (*)$$

- then define:

$$\boxed{|\Phi_2\rangle = H|\Phi_1\rangle - \frac{\langle \Phi_1 | H | \Phi_1 \rangle}{\langle \Phi_1 | \Phi_1 \rangle} |\Phi_1\rangle - \frac{\langle \Phi_1 | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} |\Phi_0\rangle}$$

$$\rightarrow \quad \langle \Phi_0 | \Phi_2 \rangle = \langle \Phi_0 | H | \Phi_1 \rangle - \langle \Phi_1 | \Phi_1 \rangle = 0 \quad (*)$$

$$\rightarrow \quad \langle \Phi_1 | \Phi_2 \rangle = \langle \Phi_1 | H | \Phi_1 \rangle - \langle \Phi_1 | H | \Phi_1 \rangle = 0$$

$\Big\}$ $|\Phi_2\rangle$ orthogonal to $|\Phi_0\rangle$ and $|\Phi_1\rangle$

$$\rightarrow \quad \langle \Phi_2 | \Phi_2 \rangle = \langle \Phi_2 | H | \Phi_1 \rangle$$

- iterate this procedure with:

$$\boxed{|\Phi_{n+1}\rangle = H|\Phi_n\rangle - \frac{a_n}{b_n}|\Phi_n\rangle - \frac{b_n}{b_{n-1}}|\Phi_{n-1}\rangle}$$

with $a_n = \langle \Phi_n | H | \Phi_n \rangle$

$b_n = \langle \Phi_n | \Phi_n \rangle$

M iterations generate a sequence of orthogonal states

$$\rightarrow \quad \{|\Phi_0\rangle, |\Phi_1\rangle, \dots, |\Phi_{M-1}\rangle\} \qquad \text{(not eigenstate of } H\text{!)}$$

now consider: $|\Psi_n\rangle = \sum_{i=0}^{\dim_H - 1} |\Phi_i\rangle\langle\Phi_i|\Psi_n\rangle$

$$\Rightarrow \quad \sum_{i=0}^{M-1} |\Phi_i\rangle\langle\Phi_i|\Psi_n\rangle$$ converges rapidly to $|\Psi_n\rangle$ for the ground and low lying states

truncate the Lanczos iterations at $M \ll \dim_H$!!

the Hamilton matrix in the basis $\{|\Phi_i\rangle\}$:

$$\langle \Phi_i | H | \Phi_j \rangle = \begin{pmatrix} a_0 & b_1 & & 0 \\ b_1 & a_1 & b_2 & \\ & b_2 & a_2 & \ddots \\ 0 & & \ddots & \ddots \end{pmatrix}$$

- $M \times M$ matrix
- tridiagonal!
  - ↳ there are efficient algorithms to diagonalize a tridiagonal matrix

C physical propeties

- static expectation values of the operator $\hat{A}$

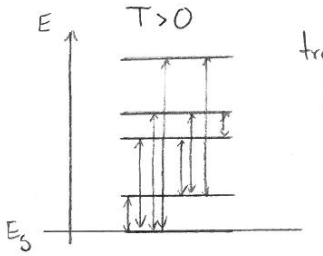
  $\rightarrow \langle \Psi_0 | \hat{A} | \Psi_0 \rangle$

  ↳ ground state obtained from the Lanczos procedure

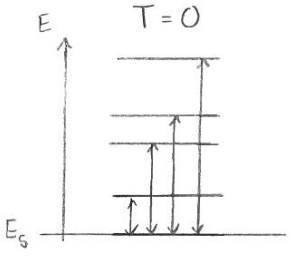
- dynamic quantities $\rightarrow$ Green functions / spectral functions

  • Lehmann representation :

$$A(\omega) = \frac{1}{Z} \sum_{ij} \langle i|A|j\rangle\langle j|B|i\rangle \left(e^{-\beta E_i} + e^{-\beta E_j}\right) \delta(\omega + E_i - E_j)$$



transitions between all state



transitions between ground state and all excited states

$\Rightarrow$ cannot be used with the $|i\rangle$, E_i from the Lanczos procedure !

• instead : Lanczos algorithm for the T=0 - Green function

write $G_{AB}(z) = \langle \Psi_0 | A \frac{1}{z - H} B | \Psi_0 \rangle$

$\rightarrow$ run a second Lanczos procedure with

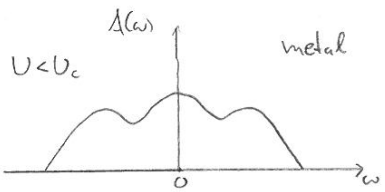
$|\tilde{\Phi}_0\rangle = B|\Psi_0\rangle$ this give $G_{AB}(z)$ in a continued fraction form !

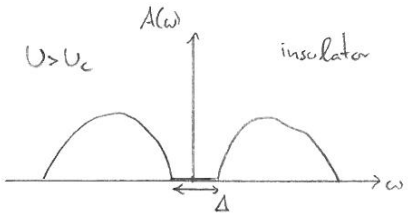
applications of the Exact Diagonalization method

a, Hubbard model

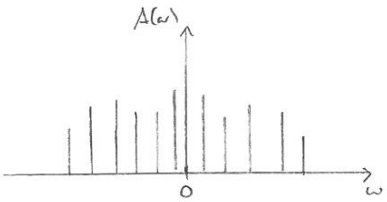
$\rightarrow$ how to locate the Mott metal-insulator transition ?

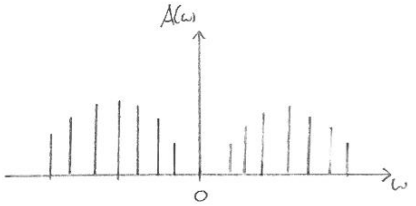
in the thermodynamic limit





for a small cluste





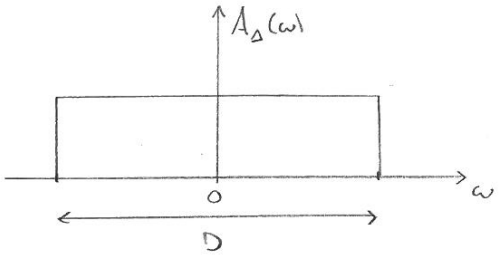
→ how to detect the vanishing / opening of a gap in a discrete spectrum?

b) single-impurity Anderson model

assume we are interested in the siAm with the number of bath sites $\to \infty$ (thermodynamic limit)

⇒ the hybridization function $A_\Delta(\omega) = -\frac{1}{\pi} \lim_{\delta \to 0} \operatorname{Im} \underbrace{\Delta(z = \omega + i\delta)}$ is continuous

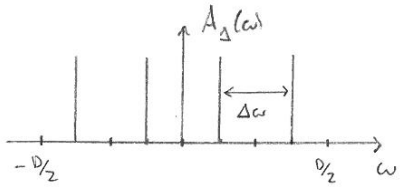
definition, see Sec. 2.2.4



D: bandwidth

to apply the Exact Diagonalization method (full or Lanczos) the continuous $A_\Delta(\omega)$ has to be discretized (see Sec. 2.2.5)

→ linear discretization:

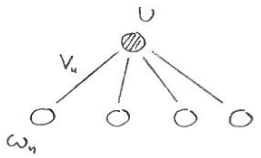


$\Delta\omega = \frac{D}{N}$

resolution in frequency / energy

$$\Rightarrow A_\Delta(\omega) = \sum_{n=1}^{N} V_n^2 \, \delta(\omega - \omega_n) \quad \hat{=} \quad \Delta_d(z) = \sum_{n=1}^{N} \frac{V_n^2}{z - \omega_n}$$

<u>this means</u>: the siAm is approximated by a model with N bath sites!



<u>but</u>: the physics of the siAm is characterized by an emergent low-energy scale

→ Kondo temperature $T_K \propto e^{-\gamma U/V^2}$

to resolve this scale, we must have $\Delta\omega \ll T_K$

$$\Rightarrow N \gg \frac{D}{T_K}$$

<u>therefore</u>: try other discretization scheme plus ideas from renormalization group

→ the following section

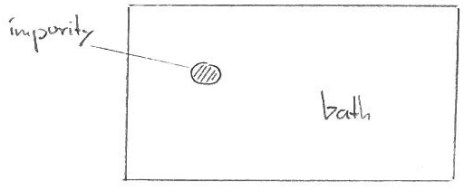
3.2 Numerical Renormalization Group (NRG)

review: R. Bulla, T. A. Costi, Th. Pruschke
Rev. Mod. Phys. 80, 395 (2008)

the NRG is designed to treat "quantum impurity systems"

$\rightarrow$ $H = H_{imp} + H_{imp-bath} + H_{bath}$

- H_{imp}: small system, the 'impurity'
- $H_{imp-bath}$: coupling between impurity and bath
- H_{bath}: large system: environment or bath



important: the bath has to be non-interacting

$\rightarrow$ the main disadvantage: the NRG cannot be generalized to other types of models (such as the Hubbard model)

the first quantum impurity problem:

$\rightarrow$ the Kondo model: magnetic impurities in nonmagnetic metals

other realizations: - artificial impurities: quantum dots
- dissipative systems: spin in a bosonic bath

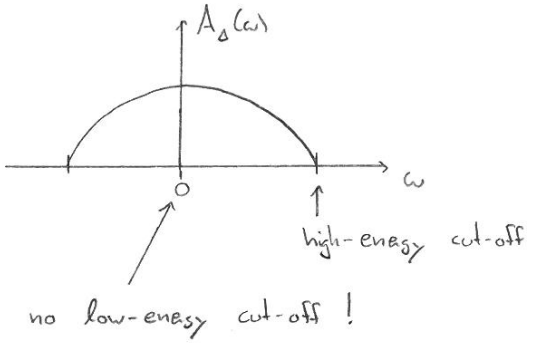
what are the difficulties?

- in many cases (and for a significant part of the parameter space) perturbative methods are not sufficient!

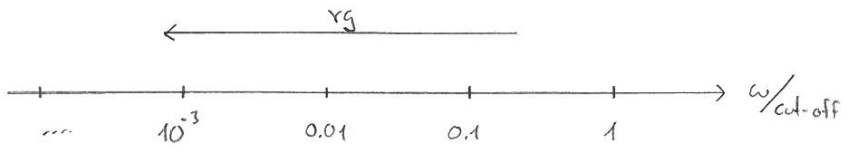
  why? $\rightarrow$ $T_K \propto e^{-\gamma U/V^2}$

  - slow convergence of perturbation theory in U
  - perturbation theory in V does not work

- the bath is continuous



on a logarithmic scale ($\omega > 0$ only)



a wide (infinite) range of energie, has to be coveed

→ use concepts from renormalization group (rg) theory !

applications / developments of the NRG

- Kondo model : 1975 - K.G. Wilson
- single-impurity Anderson model : 1980
- multi-channel impurity models : 1980
- multi-impurity models : 1987
- applications within DMFT : 1994
- quantum dot systems : 1998
- bosonic impurity models : 2003

siAm in the 'integral representation'

→ the actual starting point of the NRG-procedure

$$H_{bath} = \sum_{\sigma} \int_{-1}^{1} d\varepsilon \; g(\varepsilon)\, a^{\dagger}_{\varepsilon\sigma} a_{\varepsilon\sigma}$$

$$H_{imp\text{-}bath} = \sum_{\sigma} \int_{-1}^{1} d\varepsilon \; h(\varepsilon) \left(f^{\dagger}_{\sigma} a_{\varepsilon\sigma} + a^{\dagger}_{\varepsilon\sigma} f_{\sigma} \right)$$

→ continuous conduction band

H_{imp} as before

- band operators satisfy the fermionic commutation relations :

$$\left[a^{\dagger}_{\varepsilon\sigma}, a_{\varepsilon'\sigma'} \right]_{+} = \delta(\varepsilon - \varepsilon')\, \delta_{\sigma\sigma'}$$

- $g(\varepsilon)$: dispersion of the conduction band
  → band cut-offs are set to -1 and 1

- $h(\varepsilon)$: hybridization

→ hybridization function $\Delta(\omega) = \pi \int_{-1}^{1} d\varepsilon \; h(\varepsilon)^2\, \delta(\omega - g(\varepsilon)) = \ldots$

↳ defined as $\pi A_{\Delta}(\omega)$

$$\ldots = \pi\, h(g^{-1}(\omega))^2 \frac{d}{d\omega} g^{-1}(\omega) \qquad \text{(derivation: see exercises)}$$

with $g^{-1}(\omega)$ the inverse function of $g(\varepsilon) \longrightarrow g^{-1}(g(\varepsilon)) = \varepsilon$

now assume $\Delta(\omega)$ to be given

$\Rightarrow$ there are many ways to divide the ω-dependence between $g^{-1}(\omega)$ and $h(g^{-1}(\omega))^2$

$\hat{=}$ ——— " ——— ε-dependence between $g(\varepsilon)$ and $h(\varepsilon)$

Example:

set $g(\varepsilon) = \varepsilon \longrightarrow g^{-1}(\omega) = \omega$

$\Rightarrow \frac{d}{d\omega} g^{-1}(\omega) = 1$, $h(g^{-1}(\omega)) = h(\omega)$ and we obtain $\Delta(\omega) = \pi (h(\omega))^2$

the NRG proceeds as follows:

A. logarithmic discretization
B. mapping on a semi-infinite chain
C. iterative diagonalisation

A. logarithmic discretization

see also Sec. 2.2.5

$\longrightarrow$ discretization points $x_n = \pm \Lambda^{-n}$, $n = 0, 1, 2, \ldots$

$\hookrightarrow$ $\Lambda > 1$: discretization parameter

width of the intervals: $d_n = \Lambda^{-n}(1 - \Lambda^{-1})$

within each interval: introduce a complete set of orthonormal functions

$$f_{np}^{\pm}(\varepsilon) = \begin{cases} \frac{1}{\sqrt{d_n}} e^{\pm i \omega_n p \varepsilon} & : \; x_{n+1} < \pm\varepsilon < x_n \\ 0 & : \text{ outside this interval} \end{cases}$$

with $p \in \mathbb{Z}$ and $\omega_n = \frac{2\pi}{d_n}$

$\longrightarrow$ expand the conduction electron operators $a_{\varepsilon\sigma}$ in this basis

$$a_{\varepsilon\sigma} = \sum_{np} \left[a_{np\sigma}\, \psi^{+}_{np}(\varepsilon) + b_{np\sigma}\, \psi^{-}_{np}(\varepsilon) \right]$$

inverse transformation:

$$a_{np\sigma} = \int_{-1}^{1} d\varepsilon \left[\psi^{+}_{np}(\varepsilon) \right]^{*} a_{\varepsilon\sigma}$$

$$b_{np\sigma} = \int_{-1}^{1} d\varepsilon \left[\psi^{-}_{np}(\varepsilon) \right]^{*} a_{\varepsilon\sigma}$$

the $a_{np\sigma}$, $b_{np\sigma}$ are fermionic operators:

$$\left[a^{\dagger}_{np\sigma}, a_{n'p'\sigma'} \right]_{+} = \delta_{nn'} \delta_{pp'} \delta_{\sigma\sigma'} \; ; \quad \left[b^{\dagger}_{np\sigma}, b_{n'p'\sigma'} \right]_{+} = \delta_{nn'} \delta_{pp'} \delta_{\sigma\sigma'} \; ;$$

$$\left[a^{\dagger}_{np\sigma}, b_{n'p'\sigma'} \right]_{+} = 0 \; , \text{ etc.}$$

<u>the next step</u>: express the Hamiltonian (the siAm in the integral representation) in terms of the operators $a_{np\sigma}$, $b_{np\sigma}$

- H_{imp}: unchanged
- $H_{imp\text{-}bath}$: consider $\int_{-1}^{1} d\varepsilon\, h(\varepsilon)\, f^{\dagger}_{\sigma} a_{\varepsilon\sigma} =$

$$= f^{\dagger}_{\sigma} \sum_{np} \left[a_{np\sigma} \int^{+,n} d\varepsilon\, h(\varepsilon)\, \psi^{+}_{np}(\varepsilon) + b_{np\sigma} \int^{-,n} d\varepsilon\, h(\varepsilon)\, \psi^{-}_{np}(\varepsilon) \right]$$

with $\int^{+,n} d\varepsilon \equiv \int_{x_{n+1}}^{x_n} d\varepsilon$, $\int^{-,n} d\varepsilon \equiv \int_{-x_n}^{-x_{n+1}} d\varepsilon$.

$\longrightarrow$ set $h(\varepsilon) = h$, in this case:

$$\int^{+,n} d\varepsilon\, h(\varepsilon)\, \psi^{+}_{np}(\varepsilon) = h \underbrace{\int^{+,n} d\varepsilon\, \psi^{+}_{np}(\varepsilon)}_{= \sqrt{d_n}\, \delta_{p,0}}$$

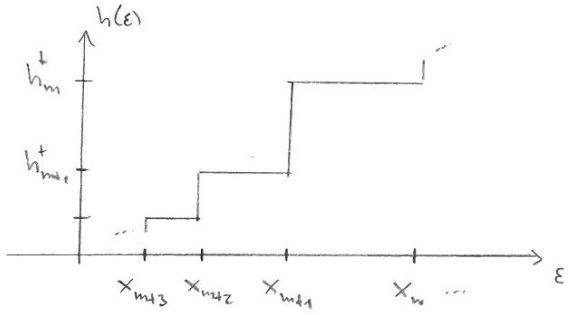
this means: the impurity couples to the $p=0$ components only!

$\longrightarrow$ to take advantage of this simplification, set

$$h(\varepsilon) = h^{\pm}_{n} \; , \quad x_{n+1} < \pm\varepsilon < x_n$$

this does not involve any approximations!

$\longrightarrow$ shift the remaining ε-dependence to $g(\varepsilon)$



set $h_n^{\pm 2} = \frac{1}{d_n} \int^{\pm,n} d\varepsilon \, \frac{1}{\pi} \Delta(\varepsilon)$

this leads to: $$\int_{-1}^{1} d\varepsilon \, h(\varepsilon) \, f_\sigma^\dagger \, a_{\varepsilon\sigma} = \frac{1}{\sqrt{\pi}} \, f_\sigma^\dagger \sum_n \left[\gamma_n^+ \, a_{n0\sigma} + \gamma_n^- \, b_{n0\sigma} \right]$$

with $$\left(\gamma_n^\pm\right)^2 = \int^{\pm,n} d\varepsilon \, \Delta(\varepsilon)$$

- H_{bath}: the conduction electron term transforms as follows:

$$\int_{-1}^{1} d\varepsilon \, g(\varepsilon) \, a_{\varepsilon\sigma}^\dagger \, a_{\varepsilon\sigma} = \sum_{np} \left(\xi_n^+ \, a_{np\sigma}^\dagger \, a_{np\sigma} + \xi_n^- \, b_{np\sigma}^\dagger \, b_{np\sigma} \right)$$
$$+ \sum_{n,p\neq p'} \left(\alpha_n^+(p,p') \, a_{np\sigma}^\dagger \, a_{np'\sigma} - \alpha_n^-(p,p') \, b_{np\sigma}^\dagger \, b_{np'\sigma} \right)$$

first term: → diagonal in p

→ $$\xi_n^\pm = \frac{\int^{\pm,n} d\varepsilon \, \Delta(\varepsilon)\varepsilon}{\int^{\pm,n} d\varepsilon \, \Delta(\varepsilon)} \overset{\uparrow}{=} \pm \frac{1}{2} \Lambda^{-n}(1+\Lambda^{-1})$$

for $\Delta(\varepsilon) = \Delta$ (constant)

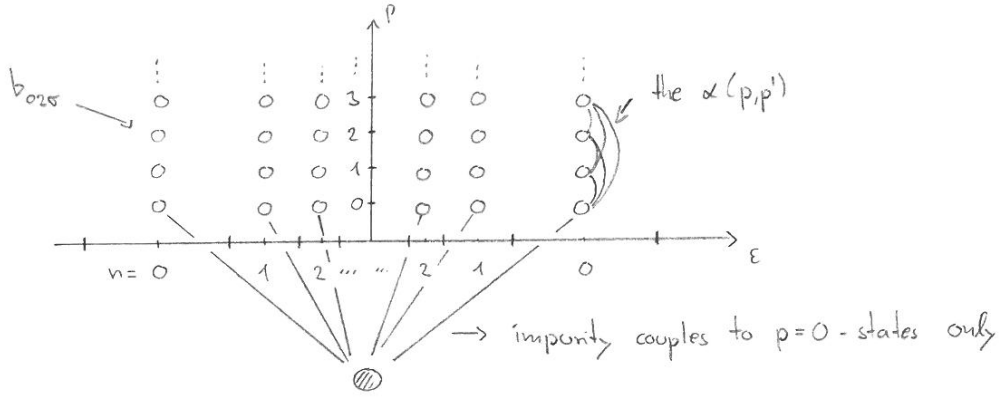
→ $\xi_n \propto \Lambda^{-n}$

second term: → couples states with $p \neq p'$

→ for $g(\varepsilon) = \varepsilon$ we obtain:

$$\alpha_n^\pm(p,p') = \frac{1-\Lambda^{-1}}{2\pi i} \, \frac{\Lambda^{-n}}{p'-p} \, \exp\left[\frac{2\pi i (p'-p)}{1-\Lambda^{-1}} \right] \qquad (*)$$

the Hamiltonian now has the following structure
(no approximations have been made so far)



now we perform the following approximation:

$\longrightarrow$ drop the $p \neq 0$ terms in H_{bath} $\hat{=}$ the actual discretization of H_{bath}

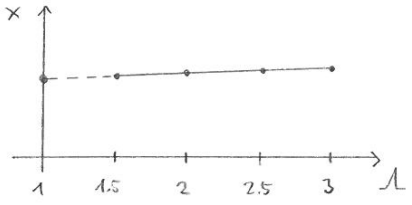
this might be a good approximation because:

- the $p \neq 0$ terms couple to the impurity only via the $a_{n\sigma}, b_{n\sigma}$
- the factor $\underbrace{(1-\Lambda^{-1})}$ in eq. (*)

  $\longrightarrow$ vanishes in the limit $\Lambda \to 1$!

  (the continuum is recovered in this limit)

later: extrapolation of the results (for a physical quantity x) for $\Lambda \to 1$



$\longrightarrow$ results turn out to depend only weakly on Λ!

$\Lambda \approx 2$ sufficient (in most cases)

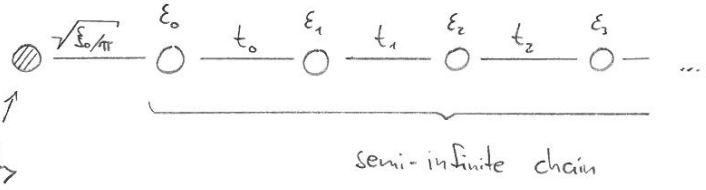
finally, with relabeling the operators $a_{n\sigma} \equiv a_{n\sigma}$, etc., we arrive at the discretized Hamiltonian:

$$H = H_{imp} + \sum_{n\sigma} \left[\xi_n^+ a_{n\sigma}^\dagger a_{n\sigma} + \xi_n^- b_{n\sigma}^\dagger b_{n\sigma} \right] + \frac{1}{\sqrt{\pi}} \sum_\sigma f_\sigma^\dagger \left[\sum_n \left(\gamma_n^+ a_{n\sigma} + \gamma_n^- b_{n\sigma} \right) \right] + h.c. \qquad (1)$$

B. mapping on a semi-infinite chain

$\longrightarrow$ orthogonal transformation of the operators $\{a_{n\sigma}, b_{n\sigma}\}$ to a new set of operators $\{c_{n\sigma}\}$ such that the discretized Hamiltonian takes the form:

$$H = H_{imp} + \sqrt{\frac{\xi_0}{\pi}} \sum_\sigma \left[f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma \right] + \sum_{\sigma, n=0}^{\infty} \left[\varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + t_n \left(c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma} \right) \right] \qquad (2)$$



- the hybridization term: → compare eqs. (1) and (2)

$$\Rightarrow \quad \frac{1}{\sqrt{\pi}} \sum_n \left(\gamma_n^+ a_{n\sigma} + \gamma_n^- b_{n\sigma} \right) = \sqrt{\frac{\xi_0}{\pi}}\, c_{0\sigma}$$

the $c_{n\sigma}^{(\dagger)}$ are fermionic operators → $[c_{n\sigma}^\dagger, c_{n\sigma}]_+ = 1$

$$\Rightarrow \quad \xi_0 = \sum_n \left((\gamma_n^+)^2 + (\gamma_n^-)^2 \right) = \int_{-1}^{1} d\varepsilon\, \Delta(\varepsilon)$$

↳ see the definition of the $\gamma_n^\pm$

- the mapping (1) → (2) is equivalent to the tridiagonalization of a matrix!

→ rewrite the Hamiltonians as

$$(1) \quad H = U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + \sum_\sigma \vec{d}_\sigma^{\,\dagger} M \vec{d}_\sigma$$

$$(2) \quad H = U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow + \sum_\sigma \vec{\tilde{d}}_\sigma^{\,\dagger} T \vec{\tilde{d}}_\sigma$$

with $\vec{d}_\sigma^{\,\dagger} = (f_\sigma^\dagger, a_{0\sigma}^\dagger, b_{0\sigma}^\dagger, a_{1\sigma}^\dagger, b_{1\sigma}^\dagger, \dots)$

$\vec{\tilde{d}}_\sigma^{\,\dagger} = (f_\sigma^\dagger, c_{0\sigma}^\dagger, c_{1\sigma}^\dagger, \dots)$

and $$T = \begin{pmatrix} \varepsilon_f & \sqrt{\xi_0/\pi} & & \\ \sqrt{\xi_0/\pi} & \varepsilon_0 & t_0 & 0 \\ & t_0 & \varepsilon_1 & t_1 \\ & 0 & t_1 & \ddots \\ & & \ddots & \end{pmatrix}$$

→ use standard tridiagonalization algorithms to calculate the $\{\varepsilon_n\}, \{t_n\}$

analytical result for $\Delta(\omega) = \Delta$:

$$\boxed{t_n = \frac{(1+\Lambda^{-1})(1-\Lambda^{-n-1})}{2\sqrt{1-\Lambda^{-2n-1}}\sqrt{1-\Lambda^{-2n-3}}}\, \Lambda^{-n/2}, \quad \varepsilon_n = 0}$$

in the large-n limit: $t_n \longrightarrow \frac{1}{2}(1+\Lambda^{-1})\,\Lambda^{-n/2}$

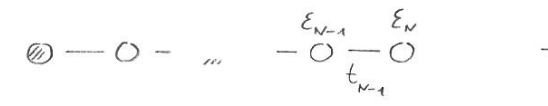
<u>this means</u>: in moving along the chain, we go from high energies to arbitrary low energie

high energies (U,V,D) $\xrightarrow[\text{rg!}]{}$ low energies

C. Herative diagonalization

the chain Hamiltonian eq. (2) can be viewed as a series of Hamiltonians H_N $(N = 0,1,2,\dots)$:

$$H_N = \Lambda^{(N-1)/2}\Big[H_{imp} + \sqrt{\xi_0/\pi}\sum_\sigma (f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma) + \sum_{\sigma,n=0}^{N} \varepsilon_n c_{n\sigma}^\dagger c_{n\sigma} + \sum_{\sigma,n=0}^{N-1} t_n (c_{n\sigma}^\dagger c_{n+1\sigma} + c_{n+1\sigma}^\dagger c_{n\sigma})\Big]$$

$\hat{=}$  → finite chain

→ we have: $H = \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N$

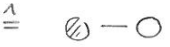
→ the factor $\Lambda^{(N-1)/2}$: will be useful later in the discussion of fixed points

two successive Hamiltonians are related by:

$$H_{N+1} = \sqrt{\Lambda}\, H_N + \Lambda^{N/2}\Big[\sum_\sigma \varepsilon_{N+1} c_{N+1\sigma}^\dagger c_{N+1\sigma} + \sum_\sigma t_N (c_{N\sigma}^\dagger c_{N+1\sigma} + c_{N+1\sigma}^\dagger c_{N\sigma})\Big]$$

the starting point

$$H_0 = \Lambda^{-1/2}\Big[H_{imp} + \sum_\sigma \varepsilon_0 c_{0\sigma}^\dagger c_{0\sigma} + \sqrt{\xi_0/\pi}\sum_\sigma (f_\sigma^\dagger c_{0\sigma} + c_{0\sigma}^\dagger f_\sigma)\Big]$$

$\hat{=}$ 

<u>now</u>: <u>the renormalization group concept</u>

Consider a Hamiltonian H, specified by a set of interaction parameters/couplings

$\vec{k} = (k_1, k_2, \dots) \longrightarrow H = H(\vec{k})$

the renormalization group is a mapping R of the Hamiltonian:

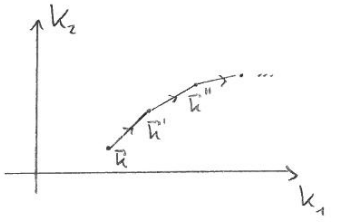
$$\boxed{R\{H(\vec{K})\} = H(\vec{K}')} \quad \hat{=} \quad R(\vec{K}) = \vec{K}'$$

↳ Hamiltonian of the same form !

a sequence of transformations:

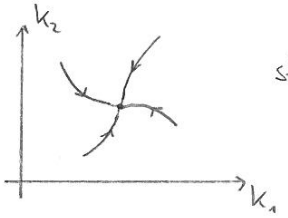
$$\vec{K} \xrightarrow{R} \vec{K}' \xrightarrow{R} \vec{K}'' \xrightarrow{R} \dots$$

→ results in a trajectory in parameta space



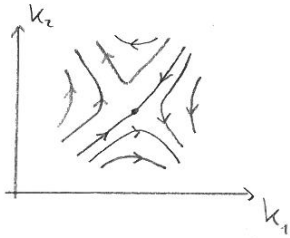
Key concepts of the rg:
- fixed points
- perturbations around fixed points

$\vec{K}^*$ is a fixed point if $\boxed{R(\vec{K}^*) = \vec{K}^*}$



stable fixed point

all perturbations are 'irrelevant'



unstable fixed point

there is at least one 'relevant' perturbation

back to the NRG

→ the rg transformation can be formally written as

$$\boxed{H_{N+1} = R(H_N)}$$

but, instead of $\vec{K}$, use the set of many-particle energies to characterize H_N

$$H_N |r\rangle_N = E_N(r) |r\rangle_N \quad , \quad r = 1, \dots, N_s$$

↳ dimension of H_N

now: set up an iterative scheme fo the diagonalization of H_N

starting point : assume we know the $\{|r\rangle_N\}$ for some value of N

a, construct a basis of H_{N+1} : $|r,s\rangle_{N+1} = |r\rangle_N \otimes |s(N+1)\rangle$

$|r;s\rangle_{N+1} = |r\rangle_N \otimes |s(N+1)\rangle$

basis of the added site

b, set up the Hamilton matrix for H_{N+1} :

$$H_{N+1}(rs,r's') = {}_{N+1}\langle r;s|\, H_{N+1}\, |r';s'\rangle_{N+1}$$

c, diagonalization of the Hamilton matrix gives the new eigenenegies $E_{N+1}(w)$ and eigenstates $|w\rangle_{N+1}$, with

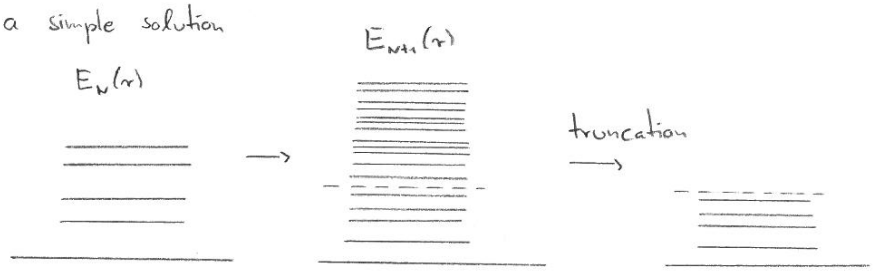
$$|w\rangle_{N+1} = \sum_{rs} U(w,rs)\, |r;s\rangle_{N+1}$$

then : continue with a, and $N \to N+1$

$\longrightarrow$ a), b, c, $\hat{=}$ one step of the iterative diagonalization

<u>the obvious problem</u> : dimension of H_N grows exponentially with N

here : a simple solution



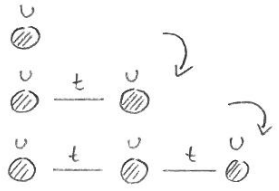
$\longrightarrow$ keep only the N_s eigenstates with the lowest E_{N+1} !
(this is an approximation)

- computation time now increases linearly with N
- why does the truncation work ?
  - $\rightarrow$ adding a site to the chain is a small petubation, since $t_N \propto \Lambda^{-N/2}$

3.3 Density-Matrix Renormalization Group (DMRG)

does the iterative diagonalization, together with the truncation scheme of Sec. 3.2, work if $t_n \approx$ const ?

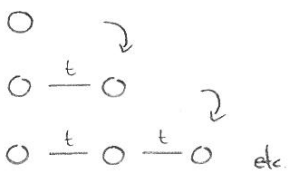
→ Hubbard model ($d=1$!)



if 'yes': the Hubbard model could be treated for much larger systems as in the ED method

but: as soon as the truncation sets in, the many-particle spectrum is incorrect

→ this can already be seen for a chain of spinless fermions



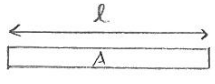
(see exercises)

DMRG solves this problem by keeping the advantage of iterative diagonalization

⇒ modify the truncation scheme

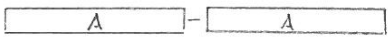
real-space renormalization group

→ the exponential growth prescription

1, 'block' A of length ℓ : 

→ Hamiltonian $\hat{H}_A$, dimension M

2, combine two blocks



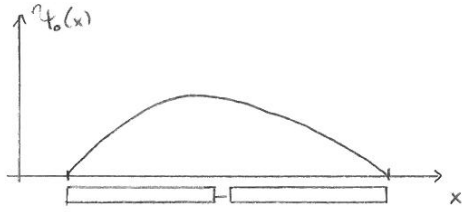
→ $\hat{H}_{AA}$ with dimension M^2

3, diagonalize $\hat{H}_{AA}$

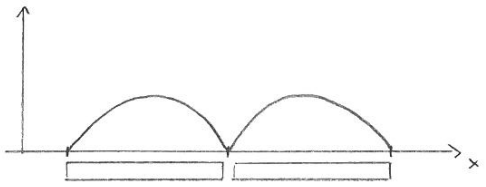
4, project $\hat{H}_{AA}$ onto the truncated space spanned by the M lowest-lying eigenstates $\hat{H}_{AA} \rightarrow \hat{H}_{AA}^{tr}$

set $AA \rightarrow A$
$2\ell \rightarrow \ell$
$\hat{H}_{AA}^{tr} \rightarrow \hat{H}_A$
and continue with 2,

now: consider the single-particle ground state of AA:



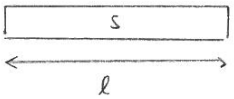
and try to represent $\psi_0(x)$ using the ground state of A



→ does not seem to be the appropriate choice!

the DMRG: works with a linear growth prescription

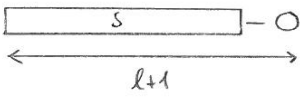
→ start with a block S (S = System)



basis of the Hilbert space: $\{|m_\ell^S\rangle\}$

→ dimension M^S, Hamiltonian $\hat{H}_\ell$

linear growth means: add one site in each iteration

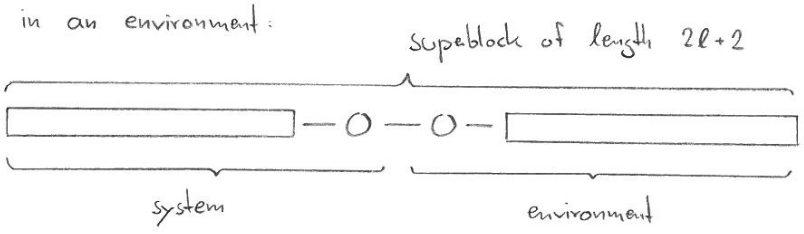


product basis $\{|m_\ell^S \sigma^S\rangle\} \equiv \{|m_\ell^S\rangle |\sigma^S\rangle\}$

$\{|\sigma^S\rangle\}$: basis of the added site

→ dimension N_{site}

important: try to mimick the thermodynamic limit by embedding the system in an environment:



diagonalization of the superblock Hamiltonian gives the ground state

$$|\psi\rangle = \sum_{m^S=1}^{M^S} \sum_{\sigma^S=1}^{N_{site}} \sum_{\sigma^E=1}^{N_{site}} \sum_{m^E=1}^{M^E} \psi_{m^S \sigma^S \sigma^E m^E} |m^S \sigma^S\rangle |m^E \sigma^E\rangle$$

$$= \sum_{i=1}^{N^S} \sum_{j=1}^{N^E} \psi_{ij} |i\rangle |j\rangle$$

with $|i\rangle = |m^S \sigma^S\rangle$, $N^S = M^S N_{site}$

$|j\rangle = |m^E \sigma^E\rangle$, $N^E = M^E N_{site}$

<u>now:</u> implement a truncation procedure on the system block, such that

$N^S \longrightarrow M^S$ $\Rightarrow$ same number of states in each iteration

$\longrightarrow$ define the operator

$$\boxed{\hat{\rho} = Tr_E |\psi\rangle\langle\psi| = \sum_j \langle j|\psi\rangle\langle\psi|j\rangle}$$

with the matrix elements

$$\rho_{ii'} = \langle i|\hat{\rho}|i'\rangle = \langle i| \sum_j \langle j|\psi\rangle\langle\psi|j\rangle |i'\rangle$$

$$= \sum_j \psi_{ij} \psi^*_{i'j}$$

the $N^S \times N^S$ matrix ρ (and also the operator $\hat{\rho}$) $\longrightarrow$ 'reduced density matrix'

diagonalization of ρ gives:

$$\boxed{\hat{\rho}\,|w_\alpha\rangle = w_\alpha |w_\alpha\rangle} \qquad \alpha = 1, \dots, N^S$$

properties of the eigenvalues w_α:

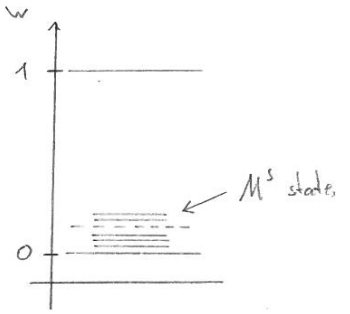
- $\sum_\alpha w_\alpha = 1$ follows from $\sum_i \rho_{ii} = \sum_{ij} \psi_{ij} \psi^*_{ij} =$

$$= \sum_{ij} |\psi_{ij}|^2 = 1$$

- $w_\alpha \geq 0$ $\Rightarrow$ all the eigenvalues are $\in [0,1]$

<u>the DMRG - truncation</u>

$\longrightarrow$ retain the M^S states with the largest eigenvalues w_α!



$\Rightarrow$ this should give the best description of the ground state of the system

Why is this approximation reasonable ?

Conside the expectation value $\langle \hat{A} \rangle$ of an operator $\hat{A}$ acting on the system (not on the environment)

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_{ij} \sum_{i'j'} \langle i' | \langle j' | \hat{A} | i \rangle | j \rangle \, \psi^*_{i'j'} \psi_{ij}$$

$$= \sum_{ii'} \sum_{jj'} \psi^*_{i'j'} \psi_{ij} \langle i' | \hat{A} | i \rangle \underbrace{\langle j' | j \rangle}_{= \delta_{jj'}}$$

$$= \sum_{ii'} \underbrace{\sum_{j} \psi^*_{i'j} \psi_{ij}}_{= \rho_{ii'}} \langle i' | \hat{A} | i \rangle = \sum_{ii'} \rho_{ii'} \langle i' | \hat{A} | i \rangle$$

$$= \sum_{i} \underbrace{\sum_{i'} \langle i | \hat{\rho} | i' \rangle \langle i' |}_{= \mathbb{1}} \hat{A} | i \rangle = \sum_{i} \langle i | \hat{\rho} \hat{A} | i \rangle$$

$$\Rightarrow \boxed{\langle \hat{A} \rangle = \mathrm{Tr}_S (\hat{\rho} \hat{A})}$$

Furthermore: the trace is invariant under orthogonal transformations

$$\Rightarrow \sum_{i} \langle i | \hat{\rho} \hat{A} | i \rangle = \sum_{\alpha=1}^{N_S} \langle w_\alpha | \hat{\rho} \hat{A} | w_\alpha \rangle$$

($|w_\alpha\rangle$ gives the eigenvalue w_α)

and we obtain $$\boxed{\langle \hat{A} \rangle = \sum_{\alpha=1}^{N_S} w_\alpha \langle w_\alpha | \hat{A} | w_\alpha \rangle}$$

with $w_1 \geq w_2 \geq w_3 \ldots$ the DMRG approximation reads:

$$\langle \hat{A} \rangle \longrightarrow \langle \hat{A} \rangle_{\text{approx}} = \sum_{\alpha=1}^{M_S} w_\alpha \langle w_\alpha | \hat{A} | w_\alpha \rangle$$

$\rightarrow$ error is of the orde of the truncated weight:

$$\varepsilon_S = 1 - \sum_{\alpha=1}^{M^S} w_\alpha$$

$\rightarrow$ a fast decay of the eigenvalue w_α is essential for this truncation scheme

3.4 Quantum Monte Carlo (QMC)

in this section: a) classical MC for the Ising model
→ Metropolis algorithm
b) quantum MC for the one-dimensional Heisenberg model
→ world-line QMC
c) quantum MC for correlated electrons
→ Hubbard-Stratonovich transformation

a) classical MC for the Ising model

Ising model

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^z$$

with the classical spin variables $S_i^z \equiv S_i = \pm 1$

→ spin configuration: $\{S_\ell\} = (S_1, S_2, \dots, S_N)$

→ energy of a given spin configuration:

$$E = H(\{S_\ell\})$$

statistical mechanics of the Ising model

we assume a canonical ensemble

→ the system is in the state $\{S_\ell\}$ with probability

$$w(\{S_\ell\}) = \frac{1}{Z} e^{-\beta H(\{S_\ell\})} \qquad \beta = \frac{1}{k_B T}$$

$$Z = \sum_{\{S_\ell\}} e^{-\beta H(\{S_\ell\})} \quad \rightarrow \text{partition function}$$

$\sum_{\{S_\ell\}}$: sum over all 2^N spin configurations (micro states)

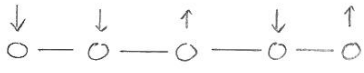
average magnetization $\langle m \rangle$ (for a given temperature T):

$$\langle m \rangle = \sum_{\{S_\ell\}} \frac{1}{Z} e^{-\beta H(\{S_\ell\})} m(\{S_\ell\}) = \sum_{\{S_\ell\}} w(\{S_\ell\}) m(\{S_\ell\})$$

with the magnetization of the spin configuration given by

$$m(\{s_e\}) = \sum_{i=1}^{N} s_i$$

example:



$\rightarrow N = 5$

$\rightarrow \{s_e\} = (-1, -1, 1, -1, 1)$

$$m(\{s_e\}) = -1 - 1 + 1 - 1 + 1 = -1$$

$$H(\{s_e\}) = \underbrace{-J + J + J + J}_{= 2J} - h \underbrace{m(\{s_e\})}_{= -1} = 2J + h$$

how to calculate $\langle m \rangle$? (as a function of T)

- analytical (only for a few special cases)
- numerical $\rightarrow$ computing time grows as 2^N !

therefore $\rightarrow$ Monte Carlo calculation of $\langle m \rangle$

idea: sampling of $\sum_{\{s_e\}} w(\{s_e\})\, m(\{s_e\})$ with $M \ll 2^N$ spin configurations $\{s_e\}^k$, $k = 1, \dots, M$

here: Markov-chain sampling

$\rightarrow$ create a sample $\{s_e\}^k$ according to the probability distribution $w(\{s_e\})$

$\rightarrow$ Metropolis algorithm

given a spin configuration $\{s_e\}^k$, iterate the following procedure:

- choose a random number $z \in \{1, \dots, N\}$
- flip the spin z $\rightarrow \{\bar{s}_e\} = (s_1^k, s_2^k, \dots, -s_z^k, \dots, s_N^k)$
- calculate

$$\alpha = \frac{w(\{\bar{s}_e\})}{w(\{s_e\}^k)} = e^{-\beta \underbrace{(H(\{\bar{s}_e\}) - H(\{s_e\}^k))}_{= \Delta E}} = e^{-\beta \Delta E}$$

- choose a random number $\gamma \in [0,1]$

  if $\alpha \geq \gamma$: the spin-flip is accepted $\Rightarrow \{S_e\}^{k+1} = \{\bar{S}_e\}$

  if $\alpha < \gamma$: the spin-flip is rejected $\Rightarrow \{S_e\}^{k+1} = \{S_e\}^{k}$

the Metropolis algorithm generates a Markov chain of spin configurations $\{S_e\}^k$

→ the average magnetization is given by:

$$\boxed{\langle m \rangle \approx \frac{1}{M} \sum_{k=1}^{M} m(\{S_e\}^k)}$$

note that this approach cannot be applied to quantum spin models !

→ the spin configurations are not eigenstates of the Hamiltonian

⇒ the probabilities cannot be calculated as $w = \frac{1}{Z} e^{-\beta H(\{S_e\})}$

b) quantum Monte-Carlo for the one-dimensional Heisenberg model

the model :

$$\boxed{H = -J \sum_{i=1}^{N-1} \vec{S}_i \cdot \vec{S}_{i+1}}$$

→ the general idea : mapping of the model onto a classical model in 1+1 dimensions

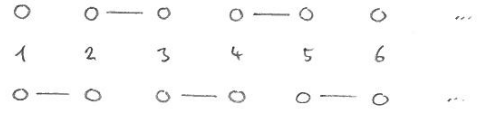
the first step :

write $H = \sum_i H_i$ with $H_i = -J \vec{S}_i \cdot \vec{S}_{i+1}$

and separate H into two parts : $H = H_A + H_B$

with $H_A = \sum_{i \text{ even}} H_i$

$H_B = \sum_{i \text{ odd}} H_i$



note that $[H_A, H_B] \neq 0$

but : $[H_i, H_j] = 0$ for ij both even or both odd

Suzuki - Trotter approximation

the partition function $Z = Tr\left(e^{-\beta H}\right)$

$$= Tr\left(\underbrace{e^{-\Delta\tau H} \cdot e^{-\Delta\tau H} \cdot \ldots \cdot e^{-\Delta\tau H}}_{= \left(e^{-\Delta\tau H}\right)^M}\right)$$

with $\Delta\tau = \frac{\beta}{M}$! this step is exact !

the approximation : $e^{-\Delta\tau H} = e^{-\Delta\tau (H_A + H_B)} = e^{-\Delta\tau H_A} e^{-\Delta\tau H_B} + O(\Delta\tau^2)$

$\rightarrow$ neglect the terms $O(\Delta\tau^2)$!

$$\Rightarrow \quad Z \overset{\uparrow}{=} Tr\left(e^{-\Delta\tau H_A} e^{-\Delta\tau H_B} e^{-\Delta\tau H_A} e^{-\Delta\tau H_B} \cdot \ldots \cdot e^{-\Delta\tau H_A} e^{-\Delta\tau H_B}\right)$$

within the Suzuki - Trotter approximation

now write for the trace

$$Tr(\ldots) = \sum_{\sigma^0} \langle\sigma^0| \ldots |\sigma^0\rangle$$ with $\{|\sigma^0\rangle\}$ the 2^N - dimensional basis of spin configurations of H

and insert unity operators of the form $\mathbb{1} = \sum_{\sigma^1} |\sigma^1\rangle\langle\sigma^1|$, $\mathbb{1} = \sum_{\sigma^2} |\sigma^2\rangle\langle\sigma^2|$, etc.

$$\rightarrow Tr\left(e^{-\Delta\tau H_A} e^{-\Delta\tau H_B} \cdot \ldots \cdot e^{-\Delta\tau H_A} \cdot e^{-\Delta\tau H_B}\right)$$

$$\uparrow \qquad \uparrow \qquad \uparrow$$

$$\mathbb{1} \qquad \mathbb{1} \qquad \mathbb{1}$$

with label $2M-1$ $\qquad 2 \qquad 1$

$$\Rightarrow \quad \boxed{Z = \underbrace{\sum_{\sigma^0} \sum_{\sigma^1} \ldots \sum_{\sigma^{2M-1}}}_{= \sum_{\{\sigma\}}} \langle\sigma^0| e^{-\Delta\tau H_A} |\sigma^{2M-1}\rangle \langle\sigma^{2M-1}| e^{-\Delta\tau H_B} |\sigma^{2M-2}\rangle \cdot \ldots \cdot \ldots \cdot \langle\sigma^1| e^{-\Delta\tau H_B} |\sigma^0\rangle}$$

$\rightarrow$ the Suzuki - Trotter decomposition of Z

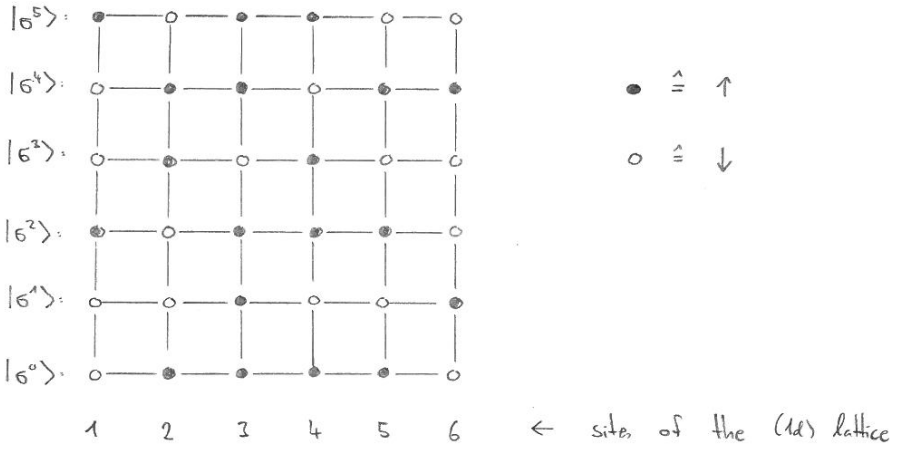
example: set $N = 6$, $M = 3$

→ count the number of terms in $\sum_{\{\sigma\}}$:

- dimension of the Hilbert space $2^N = 2^6$
- number of spin configurations $2M = 6$

$\Big\}$ $(2^N)^{2M} = 2^{2NM} = 2^{36}$ terms

now: visualize each contribution to $\sum_{\{\sigma\}}$ as a spin configuration on a two-dimensional lattice:



→ not all of the 2^{36} contributions to Z are actually possible

to see this, consider the individual matrix elements, for example

$$\langle \sigma^1 | e^{-\Delta\tau H_3} | \sigma^0 \rangle = \dots$$

write $|\sigma^0\rangle = |\sigma_1^0, \sigma_2^0, \sigma_3^0, \sigma_4^0, \sigma_5^0, \sigma_6^0\rangle$

$|\sigma^1\rangle = |\sigma_1^1, \sigma_2^1, \sigma_3^1, \sigma_4^1, \sigma_5^1, \sigma_6^1\rangle$

and $H_3 = H_1 + H_3 + H_5$

$$\dots = \langle \sigma_1^1, \sigma_2^1, \sigma_3^1, \sigma_4^1, \sigma_5^1, \sigma_6^1 | e^{-\Delta\tau H_1} e^{-\Delta\tau H_3} e^{-\Delta\tau H_5} | \sigma_1^0, \sigma_2^0, \sigma_3^0, \sigma_4^0, \sigma_5^0, \sigma_6^0 \rangle = \dots$$

H_1 acts on sites 1,2
H_3 — " — 3,4
H_5 — " — 5,6

$\Big\}$ ⇒ the matrix element can be split up:

$$\ldots = \underbrace{\langle \sigma_1^1, \sigma_2^1 | e^{-\Delta\tau H_1} | \sigma_1^0, \sigma_2^0 \rangle} \langle \sigma_3^1, \sigma_4^1 | e^{-\Delta\tau H_3} | \sigma_3^0, \sigma_4^0 \rangle \langle \sigma_5^1, \sigma_6^1 | e^{-\Delta\tau H_5} | \sigma_5^0, \sigma_6^0 \rangle$$

$= M_{ij}$ → matrix element of a 4×4 - matrix with

$\{|i\rangle\} = \{|\sigma_1^1, \sigma_2^1\rangle\} = \{|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$

($\{|j\rangle\}$ accordingly)

with $H_1 = -J\,\vec{S}_1 \cdot \vec{S}_2$ → $M_{ij} = \langle i | e^{\Delta\tau J \vec{S}_1 \cdot \vec{S}_2} | j \rangle$

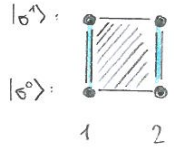
the matrix M can be evaluated analytically :

$$M = e^{-\Delta\tau J/4} \begin{pmatrix} e^{\frac{1}{2}\Delta\tau J} & 0 & 0 & 0 \\ 0 & \cosh\left(\frac{1}{2}\Delta\tau J\right) & \sinh\left(\frac{1}{2}\Delta\tau J\right) & 0 \\ 0 & \sinh\left(\frac{1}{2}\Delta\tau J\right) & \cosh\left(\frac{1}{2}\Delta\tau J\right) & 0 \\ 0 & 0 & 0 & e^{\frac{1}{2}\Delta\tau J} \end{pmatrix}$$

<u>this means</u>: only the following transitions are allowed

a) diagonal → $|\uparrow,\uparrow\rangle$ → $|\uparrow,\uparrow\rangle$ etc.

this can be visualized as



‖ for spin ↑

| for spin ↓

and for the other diagonal terms:

the double and dashed lines will be part of the world lines for the up and down spins

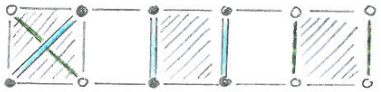
b) there are only two non-diagonal terms:

$|\uparrow\downarrow\rangle \longrightarrow |\downarrow\uparrow\rangle$ $\qquad$ $|\downarrow\uparrow\rangle \longrightarrow |\uparrow\downarrow\rangle$

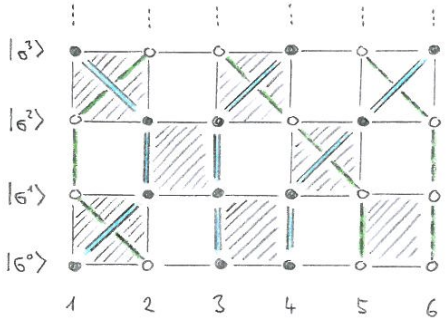
$\hat{=}$  $\qquad$ $\hat{=}$ 

→ these are the allowed shaded plaquette configurations

the full matrix element $\langle \sigma' | e^{-\Delta\tau H_0} | \sigma \rangle$:



and a single valid contribution to the partition function:



- 'checkerboard decomposition'
- 'world lines' for up and down spins

comparison with the partition function of the two-dimensional Ising model

$$Z_{2d\,\mathrm{I}} = \sum_{\{\sigma\}} \underbrace{e^{-\beta H(\{\sigma\})}}_{\text{the Boltzmann weight}}$$

$\uparrow$ sum over all spin configurations

$\rightarrow$ similar structure as the Suzuki-Trotter decomposition of Z for the 1d Heisenberg model

$\Rightarrow$ 'quantum-to-classical' mapping

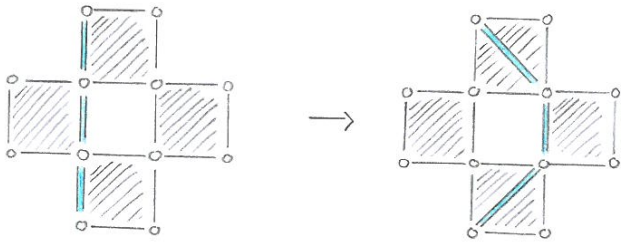
1d $\rightarrow$ 2d

difference: - not all spin configurations are allowed

- weight = product of the matrix elements M_{ij}

<u>how to generate a new spin configuration?</u>

$\rightarrow$ local updates, such as



<u>but</u> local updates are not efficient

$\Rightarrow$ global updates

'loop algorithm'

C, quantum Monte Carlo for correlated electrons

again: how to avoid solving the Schrödinger equation?

→ introduce auxiliary fields $\{s_\ell\}$ for each step in imaginary time

→ Hubbard-Stratonovich transformation

≙ mapping on a classical model in d+1 dimensions

the starting point:

functional integral representation of the partition function

$$\boxed{Z = \int D\psi^\dagger D\psi \; e^{S(\psi,\psi^\dagger)}}$$

$\psi^\dagger, \psi$: Grassmann variables

$S(\psi^\dagger,\psi)$: action

examples:

1. $H = \varepsilon c^\dagger c$

$$S(\psi,\psi^\dagger) = \sum_{n=1}^{N} \psi_n^\dagger (\psi_{n-1} - \psi_n) - \Delta\tau \sum_{n=1}^{N} \underbrace{H(c^\dagger \to \psi_n^\dagger, c \to \psi_{n-1})}_{= \varepsilon \psi_n^\dagger \psi_{n-1}}$$

with $\Delta\tau = \frac{\beta}{N}$

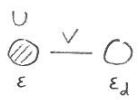
in this case, the action can be written as

$$S(\psi,\psi^\dagger) = -\sum_{ij} \psi_i^\dagger M_{ij} \psi_j$$

and the evaluation of the functional integral gives $Z = \det M$

2. two-site siAm

$$H = H_{imp} + \sum_\sigma \varepsilon_d d_\sigma^\dagger d_\sigma + \sum_\sigma V (c_\sigma^\dagger d_\sigma + d_\sigma^\dagger c_\sigma)$$

≙ 

$$S(\psi,\psi^+) = S_{imp}(\psi_c,\psi_c^+) + S_d(\psi_d,\psi_d^+) + S_v(\psi_c,\psi_c^+,\psi_d,\psi_d^+)$$

with $$S_{imp}(\psi_c,\psi_c^+) = \sum_{n=1}^{N}\sum_{\sigma} \psi^+_{n\sigma}(\psi_{n-1\sigma} - \psi_{n\sigma})$$

$$- \Delta\tau \sum_{n=1}^{N}\left[\sum_{\sigma} \varepsilon\, \psi^+_{n\sigma}\psi_{n-1\sigma} + U\psi^+_{n\uparrow}\psi_{n-1\uparrow}\psi^+_{n\downarrow}\psi_{n-1\downarrow}\right]$$

$\Rightarrow$ the action cannot be written as $\sum_{ij} \psi_i^+ M_{ij} \psi_j$!

discrete Hubbard-Stratonovich transformation

$$\exp\left[\frac{1}{2}\Delta\tau U(\psi^+_{e\uparrow}\psi_{e'\uparrow} - \psi^+_{e\downarrow}\psi_{e'\downarrow})^2\right] = \frac{1}{2}\sum_{s_e=\pm 1}\exp\left[\lambda s_e(\psi^+_{e\uparrow}\psi_{e'\uparrow} - \psi^+_{e\downarrow}\psi_{e'\downarrow})\right]$$

with: $\cosh\lambda = \exp\left(\frac{1}{2}\Delta\tau U\right)$

$\rightarrow$ the interactions between the electrons is replaced by the inteaction with an auxiliary binary field $\{s_e\}$

the partition function can now be written in the form

$$Z = \sum_{\{s_i\}} \int D\psi^+ D\psi\, e^{S(\psi,\psi^+,\{s_i\})} = \sum_{\{s_i\}} \det M(\{s_i\})$$

$\hookrightarrow$ sum ove all 'spin' configurations

similar expressions for: - expectation values $\langle\hat{A}\rangle$

- imaginary Green function $G(\tau)$

$\rightarrow$ use the Metropolis algorithm to generate a Markov chain of auxiliary spin configurations $\{s_i\}^k$

$\Rightarrow$ instead of an exact solution, QMC gives a controlled approximation which converges towards the exact solution with arbitrary precision

the errors in QMC

1. discretization error
2. statistical MC error

1. discretization errors

→ discretization of the imaginary time axis $[0,\beta]$

$$\Delta\tau = \frac{\beta}{N}$$

errors are due to the Trotter decomposition:

$$e^{-\beta(H_1+H_2)} = \left(e^{-\Delta\tau H_1} e^{-\Delta\tau H_2}\right)^N + \mathcal{O}(\text{energy}\cdot\Delta\tau)^2$$

set energy = U

$$\Rightarrow \quad U\Delta\tau \ll 1 \qquad \text{this means} \qquad \boxed{N \gg \frac{U}{k_B T}}$$

↳ determines the size of the matrices to be diagonalized

this limits the applicability of the QMC method in the large U/small T regime!

2. statistical Monte Carlo errors

already present in classical MC simulations

in addition:

→ fermion sign problem (minus sign problem)

for the expectation value $\langle A\rangle$ we have

$$\langle A\rangle = \sum_i a_i \underbrace{\det M_i}_{\text{can be negative}} \Rightarrow \text{split up the sum}$$

$$= \underbrace{\sum_{i^+} a_{i^+} \underbrace{\det M_{i^+}}_{>0}}_{=\langle A\rangle^+} + \underbrace{\sum_{i^-} a_{i^-} \underbrace{\det M_{i^-}}_{<0}}_{=\langle A\rangle^-}$$

problematic if $\langle A\rangle^+ \approx -\langle A\rangle^-$

as a consequence: statistical errors grow exponentially with system size

(details depend on the model)