1.7 Introduction to exact diagonalization: the two-site HH

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

noninteracting HH $\rightarrow$ band structure

but: <u>no interplay</u> of t and U.

The interesting physics in the HH arises because the kinetic and potential energy terms due not commute $\Rightarrow$ they prefer different groundstates that "compete" with each other for the lowest total energy.

Minimal extension to single-site HH where full exact diagonalization is still possible: two-site HH.

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

Dimension of Hilbert space: $2^4 = 16$

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

to divide Hilbert space into sectors:

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

dimensions of these sectors: 1, 2, 1, 2, 4, 2, 1, 2, 1

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

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

Answer:

Choose a basis $\underset{|1\rangle}{|\uparrow,\downarrow\rangle}, \underset{|2\rangle}{|\downarrow,\uparrow\rangle}, \underset{|3\rangle}{|\uparrow\downarrow,0\rangle}, \underset{|4\rangle}{|0,\uparrow\downarrow\rangle}$:

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

in the above basis:

$$\hat{H} = \begin{bmatrix} -\frac{U}{2} & 0 & -t & -t \\ 0 & -\frac{U}{2} & -t & -t \\ -t & -t & \frac{U}{2} & 0 \\ -t & -t & 0 & \frac{U}{2} \end{bmatrix}$$

check:

$-t\, c_{1\uparrow}^\dagger c_{2\uparrow} |0,\uparrow\downarrow\rangle = -t\,|\uparrow,\downarrow\rangle \rightarrow H_{14}$

$-t\, c_{1\downarrow}^\dagger c_{2\downarrow} |0,\uparrow\downarrow\rangle = -t\,|\downarrow,\uparrow\rangle \rightarrow H_{24}$

$-t\, c_{2\downarrow}^\dagger c_{1\downarrow} |\uparrow\downarrow,0\rangle = -t\,|\uparrow,\downarrow\rangle \rightarrow H_{13}$

$-t\, c_{2\uparrow}^\dagger c_{1\uparrow} |\uparrow\downarrow,0\rangle = -t\,|\downarrow,\uparrow\rangle \rightarrow H_{23}$

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

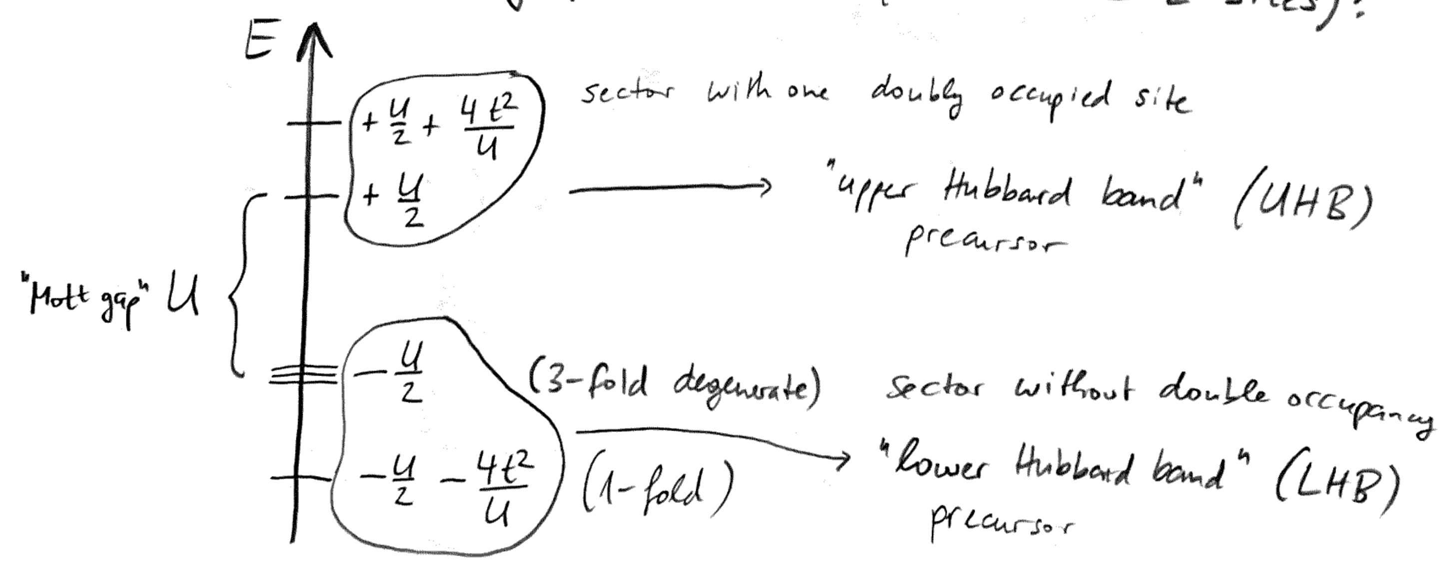
Eigenvalues of $\hat{H}$: $\underset{\substack{\equiv \\ E_t}}{-\frac{U}{2}}, \ \frac{U}{2}, \ \pm\sqrt{4t^2 + \frac{U^2}{4}}$
(see below)

Consider the strong-coupling limit $\frac{U}{t} \gg 1$:

$$\pm\sqrt{4t^2 + \frac{U^2}{4}} = \pm\frac{U}{2}\sqrt{1 + 16\frac{t^2}{U^2}} \approx \pm\frac{U}{2}\left(1 + 8\frac{t^2}{U^2}\right)$$

$$= \begin{cases} -\frac{U}{2} - \frac{4t^2}{U} \equiv E_s \quad \text{(see below)} \\ +\frac{U}{2} + \frac{4t^2}{U} \end{cases}$$

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



Eigenstates in the lower sector in the $\frac{U}{t} \gg 1$ limit:

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

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

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

→ Mapping of the Hubbard model to the $S=\frac{1}{2}$-Heisenberg model in the large-U limit

→ no hopping of charges, spin physics only with 1 spin ($\uparrow$ or $\downarrow$) on each site. "charges are frozen" for $\frac{U}{t} \gg 1$ (Mott insulator)

Heisenberg model on two sites: $\hat{H} = J \vec{S}_1 \cdot \vec{S}_2$

Trick to obtain spectrum:

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

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

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

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

$S_{tot}(S_{tot}+1)$ with $S_{tot} \in \{0,1\}$

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

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

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

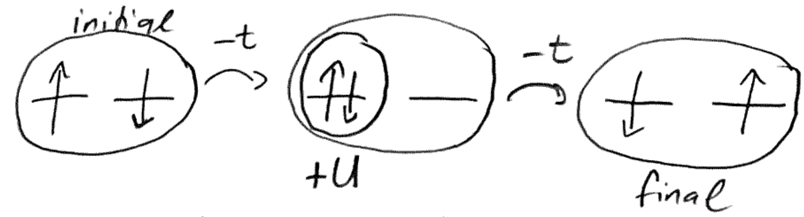
~ because of different reference energy compared to Hubbard model

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

Comparison with Hubbard:

$$\boxed{J = \frac{4t^2}{U}}$$

pictorially:



"magnetic exchange coupling"

$$\frac{(-t)\cdot(-t)}{U} = \frac{t^2}{U} \; ; \quad J = 4\,\frac{t^2}{U}$$

exchange of spins via virtual intermediate state

Combinatorial prefactor

1.8 Mott gap and spectral function

In chapter 2 we will learn that spectroscopy allows us to measure spectral functions, which can be computed used Green's functions.

Example: single-particle Green's function (G) contains information about single-particle excitations (energies and lifetimes). We will compute G's in the two simple limits $U=0$ and $t=0$.

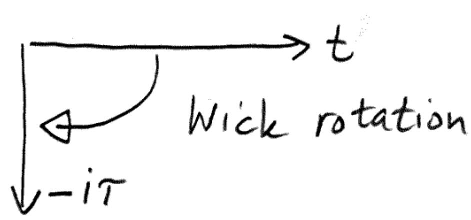
1.8.1 Green's functions at $U=0$

Definition: $G_{jn}(\tau) := -\langle c_j(\tau)\, c_n^+(0)\rangle$ for $\tau \in [0,\beta]$

with $c_j(\tau) = e^{\hat{H}\tau}\, c_j(0)\, e^{-\hat{H}\tau}$

Heisenberg picture time evolution with imaginary time $-i\tau$ $(\tau \in \mathbb{R})$. Compare with real-time evolution

$$c_j(t) = e^{i\hat{H}t}\, c_j\, e^{-i\hat{H}(t)} \qquad \boxed{t \to -i\tau}$$



What is $c_k(\tau)$? And what is $G_k(\tau) \equiv G_{kk'}(\tau)\,\delta_{kk'}$

for $U=0$, use momentum space

We know that $\dfrac{\partial c_k(\tau)}{\partial \tau} = [\hat{H}, c_k(\tau)]$ and $\hat{H} = \sum_{k'} \epsilon_{k'} c^+_{k'} c_{k'}$

measured relative to μ

$$\Rightarrow \frac{\partial c_k}{\partial \tau} = \sum_{k'} \epsilon_{k'} \underbrace{[c^+_{k'} c_{k'}, c_k]}_{c^+_{k'} c_{k'} c_k - c_k c^+_{k'} c_{k'} = \begin{cases} 0 & k \neq k' \\ -c_k & k = k' \end{cases}} = \ldots$$

$$\ldots = -\epsilon_k c_k \quad (*)$$

$$\Rightarrow \boxed{c_k(\tau) = e^{-\epsilon_k \tau} c_k(0)}$$

check that this fulfills the differential equation $(*)$

$$\Rightarrow G_k(\tau) = -\langle c_k(\tau) c^+_k(0)\rangle$$

$$= -e^{-\epsilon_k \tau} \underbrace{\langle c_k(0) c^+_k(0)\rangle}_{\langle 1 - c^+_k(0) c_k(0)\rangle \;=\; 1 - f(\epsilon_k)}$$

anticommutator

More precisely: $G_k(\tau) = -\mathcal{T}_\tau \langle c_k(\tau) c^+_k(0)\rangle$

with imaginary-time ordering (cf. Chapter 2)

$$\mathcal{T}_\tau\, A(\tau)\, B(0) \equiv \begin{cases} A(\tau) B(0) & \text{for } \tau > 0 \\ -B(0) A(\tau) & \text{for } \tau < 0 \end{cases}$$

fermionic

One can show that

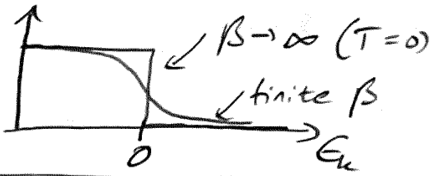
$$\boxed{G_k(\tau) = \begin{cases} -e^{-\epsilon_k \tau}(1 - f(\epsilon_k)) & \text{for } 0 < \tau < \beta \\ e^{-\epsilon_k \tau} f(\epsilon_k) & \text{for } -\beta < \tau < 0 \end{cases}} \quad (**)$$

different sign — no anticommutator needed

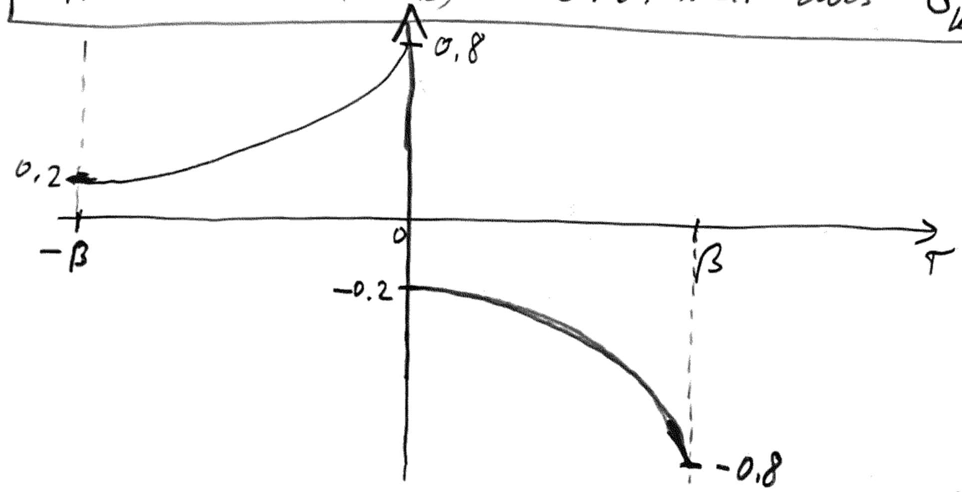
Fix some k (in Brillouin zone) $\Rightarrow$ $\epsilon_k \gtrless 0$ depending on whether we are below or above the Fermi energy.

The Fermi function $f(\epsilon_k)$ will take some value

$$f(\epsilon_k) = \frac{1}{e^{\beta\epsilon_k}+1}$$



Quiz: $\boxed{\text{Suppose that } f(\epsilon_k) = 0.8. \text{ What does } G_k(\tau) \text{ look like?}}$



$-(1-f(\epsilon_k)) = -0.2$ $\boxed{\tau \to 0^+}$

$$-e^{-\epsilon_k\beta}(1-f(\epsilon_k)) = -e^{-\epsilon_k\beta}\left(1-\frac{1}{e^{\beta\epsilon_k}+1}\right) = -e^{-\epsilon_k\beta}\left(\frac{e^{\beta\epsilon_k}}{e^{\beta\epsilon_k}+1}\right)$$

$$= -\frac{1}{e^{\beta\epsilon_k}+1} = -f(\epsilon_k) = -0.8 \qquad \boxed{\tau \to \beta^-}$$

$\boxed{\tau \to 0^-}$: $f(\epsilon_k) = 0.8$

$\boxed{\tau \to -\beta^+}$: $e^{-\epsilon_k\beta} f(\epsilon_k) = e^{-\epsilon_k\beta}\left(\frac{1}{e^{\beta\epsilon_k}+1}\right) = 1 - f(\epsilon_k) = 0.2$

$G_k(\tau)$ is 2β-periodic and β-antiperiodic:

$$G_k(\tau+\beta) = -G_k(\tau)$$

$$G_k(\tau+2\beta) = -G_k(\tau+\beta) = +G_k(\tau)$$

$\Rightarrow$ define Fourier transform:

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

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

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

Quiz: $\boxed{\text{What is } G_k(i\omega_n) \text{ for the above noninteracting band-fermion } G_k(\tau) \ (**)\text{ ?}}$

Answer: $G_k(i\omega_n) = \int_0^\beta d\tau \left(-e^{-\epsilon_k \tau}(1-f(\epsilon_k))\right) e^{i\omega_n \tau} =$

$$= (f(\epsilon_k)-1) \underbrace{\int_0^\beta d\tau \, e^{(i\omega_n - \epsilon_k)\tau}}_{\frac{1}{i\omega_n - \epsilon_k}\left[e^{(i\omega_n-\epsilon_k)\tau}\right]_0^\beta} =$$

$$= \frac{1}{i\omega_n - \epsilon_k} (f(\epsilon_k)-1)\left[e^{(i\omega_n - \epsilon_k)\beta} - 1\right]$$

We know that $e^{i\omega_n \beta} = -1$ since $\omega_n = (2n+1)\frac{\pi}{\beta}$

$$\Rightarrow \quad = -(f(\epsilon_k)-1)\left(e^{-\epsilon_k \beta}+1\right) = \left(1 - \frac{1}{e^{\beta\epsilon_k}+1}\right)\left(1+e^{-\beta\epsilon_k}\right)$$

$$= 1 + \underbrace{e^{-\beta\epsilon_k}}_{\frac{1+e^{-\beta\epsilon_k}}{1+e^{\beta\epsilon_k}}} - \frac{1+e^{-\beta\epsilon_k}}{1+e^{\beta\epsilon_k}} = 1$$

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

The Matsubara Green's function $G_k(i\omega_n)$ contains information about the possible excitation energies at momentum k. Here that is only one energy, namely ϵ_k. In section 2 we will see that in the presence of interactions, this G will take the form $G_k(i\omega_n) = \frac{1}{i\omega_n - \epsilon_k - \Sigma_k(i\omega_n)}$ with the <u>self-energy</u> Σ that encodes an energy shift and quasiparticle lifetime.

1.8.2 Green's functions at $t=0$ (single-site)

Go back to $\hat{H} = U(\hat{n}_\uparrow - \frac{1}{2})(\hat{n}_\downarrow - \frac{1}{2})$ and compute

$$G_\uparrow(\tau) \equiv -\langle c_\uparrow(\tau)\, c_\uparrow^+(0)\rangle, \qquad (*)$$

the local imaginary-time Green's function.

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

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

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

$$= e^{\hat{H}\tau} e^{U\tau/4}|00\rangle = e^{U\tau/2}|00\rangle$$

Quiz: $\boxed{\text{Repeat the same for } |01\rangle\text{. Then compute } G_\uparrow(\tau).}$

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

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

Where $|n\rangle \in \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ for $|n_\uparrow n_\downarrow\rangle$ states.

We had in 1.5 $\boxed{Z \overset{\mu=0}{=} 2e^{-\beta\frac{U}{4}} + 2e^{\beta\frac{U}{4}}}$ $(**)$

and $\langle 00|\hat{H}|00\rangle = \frac{U}{4}$, $\langle 01|\hat{H}|01\rangle = -\frac{U}{4}$.

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

From this we compute $G_\uparrow(i\omega_n)$ as before via

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

Compute $\displaystyle\int_0^\beta d\tau\, e^{(i\omega_n+\frac{U}{2})\tau} = \frac{e^{(i\omega_n+\frac{U}{2})\beta}-1}{i\omega_n+\frac{U}{2}} = -\frac{(1+e^{\beta\frac{U}{2}})}{i\omega_n+\frac{U}{2}}$

$$\Rightarrow \boxed{G_\uparrow(i\omega_n)} = Z^{-1}\left[\frac{e^{\beta\frac{U}{4}}+e^{-\beta\frac{U}{4}}}{i\omega_n+\frac{U}{2}} + \frac{e^{\beta\frac{U}{4}}+e^{-\beta\frac{U}{4}}}{i\omega_n-\frac{U}{2}}\right] = \boxed{\frac{1}{2}\left[\frac{1}{i\omega_n+\frac{U}{2}} + \frac{1}{i\omega_n-\frac{U}{2}}\right]}$$

Definition: We define the spectral function $A(\omega)$ as

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

or equivalently via the retarded Green's function G^R as

$$\boxed{\begin{aligned} A(\omega) &\equiv -\frac{1}{\pi} \operatorname{Im} G^R(\omega) \\ G^R(\omega) &\equiv G(i\omega_n)\Big|_{i\omega_n \to \omega + i0^+} \end{aligned}}$$

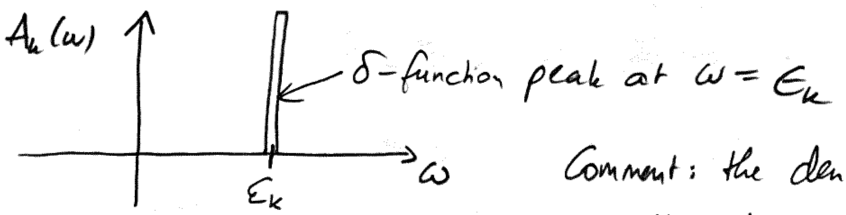
analytical continuation in complex frequency plane

Example 1: For the noninteracting case in 1.8.1 we had

$G_k(i\omega_n) = \frac{1}{i\omega_n - \epsilon_k}$. Therefore $G_k^R(\omega) = \frac{1}{i\omega_n - \epsilon_k}\Big|_{i\omega_n \to \omega + i0^+} =$

$= \frac{1}{\omega + i0^+ - \epsilon_k}$. The spectral function is $A_k(\omega) = -\frac{1}{\pi} \operatorname{Im}\left[\frac{1}{\omega + i0^+ - \epsilon_k}\right] =$

$= \delta(\omega - \epsilon_k)$ due to the Dirac identity $\frac{1}{x + i0^+} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$.

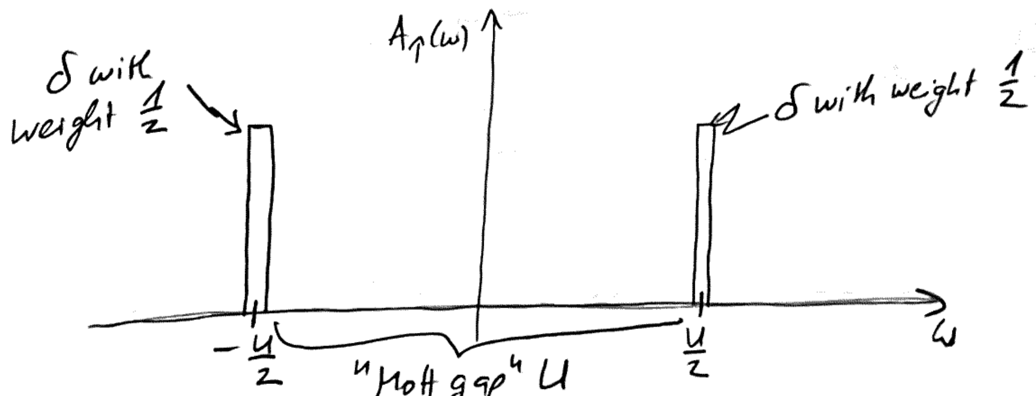


Comment: the density of states (DOS) is nothing but $N(\omega) \equiv \sum_k A_k(\omega)$.

Example 2: Back to local $G_\uparrow(i\omega_n)$ for $t=0$.

Here we have $A_\uparrow(\omega) = -\frac{1}{\pi} \operatorname{Im} G_\uparrow^R(\omega) = -\frac{1}{\pi} \operatorname{Im}\left[\frac{1}{2}\left(\frac{1}{i\omega_n + \frac{U}{2}} + \frac{1}{i\omega_n - \frac{U}{2}}\right)\right]_{i\omega_n \to \omega + i0^+} =$

$= \frac{1}{2}\left(\delta(\omega + \frac{U}{2}) + \delta(\omega - \frac{U}{2})\right)$. The same result for $A_\downarrow(\omega)$.



Compare to compressibility curve in 1.5