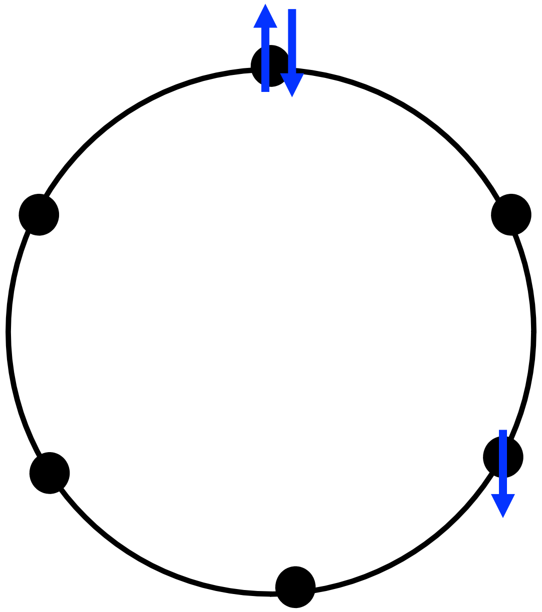
6-site Hubbard model

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

Large Fock space: dim 2^{12}

Use conservation of S_z: (s1, s2) sectors of dim $\binom{6}{s_1}\binom{6}{s_2}$

For example a **basis** function from (1,2) sector:



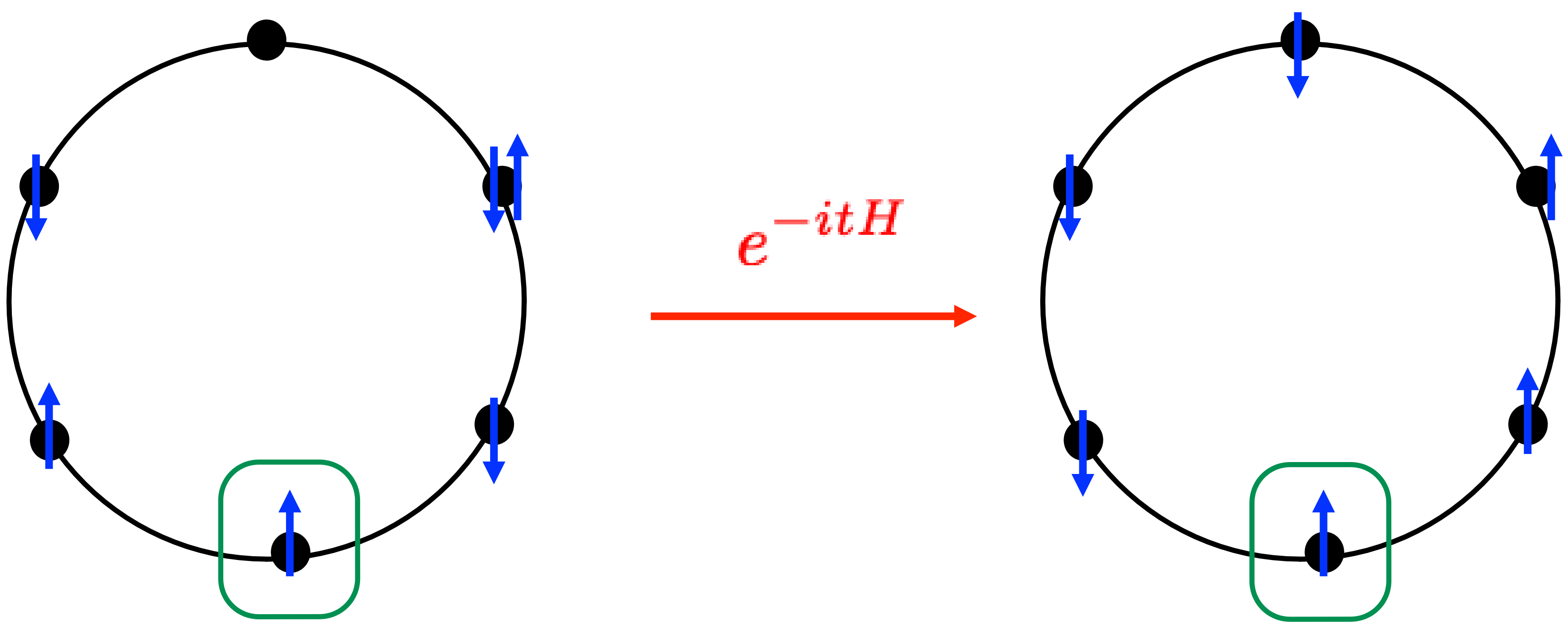
in binary code (10000|101000)

Time-dependent (dynamical) correlations

Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations

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



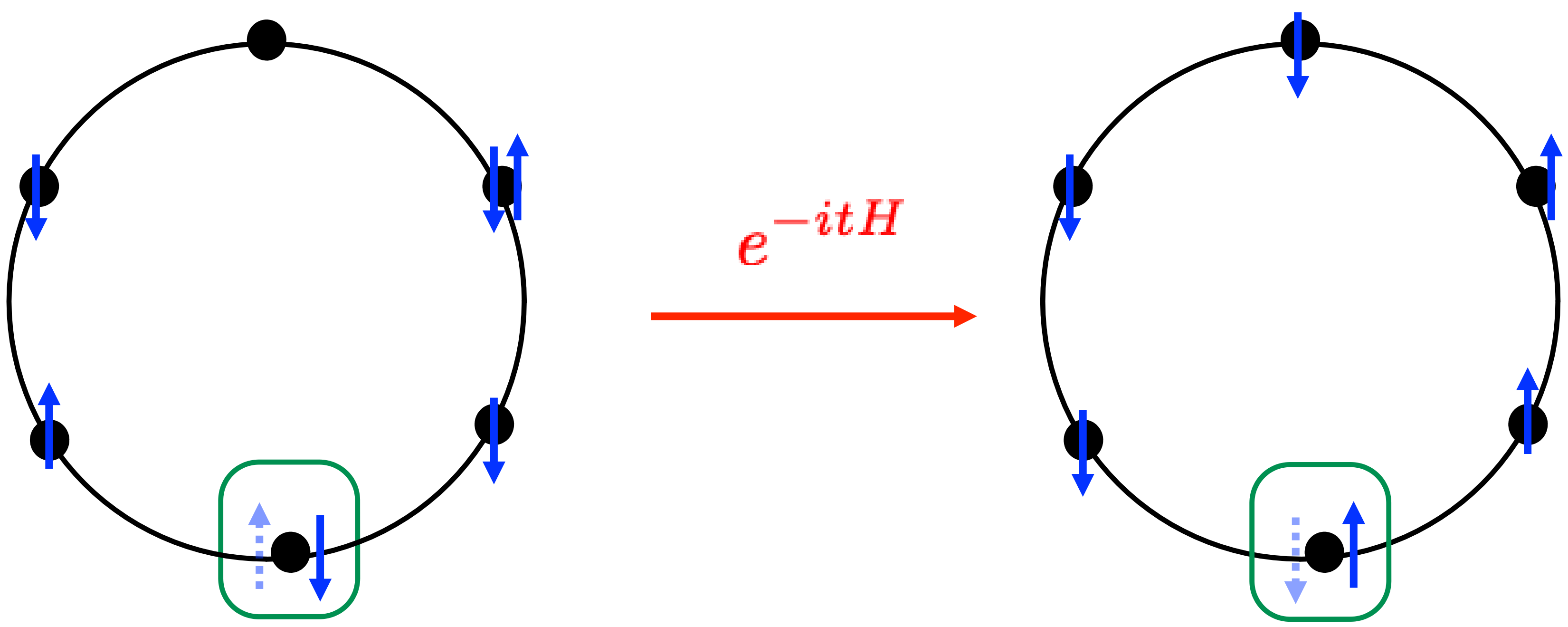
$$\langle S_{iz}(t) S_{iz}(0) \rangle \equiv \langle \psi_g | e^{itH} S_{iz} e^{-itH} S_{iz} | \psi_g \rangle$$

Time-dependent (dynamical) correlations

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

Why correlation functions?

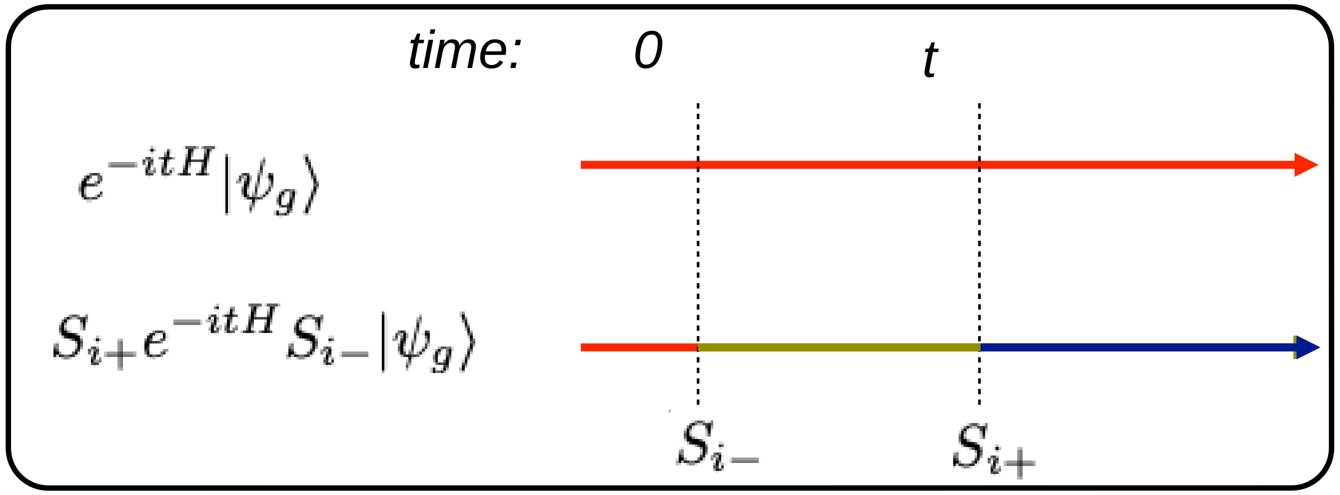
- Contributions to interaction energy of the system
- Response to small perturbations

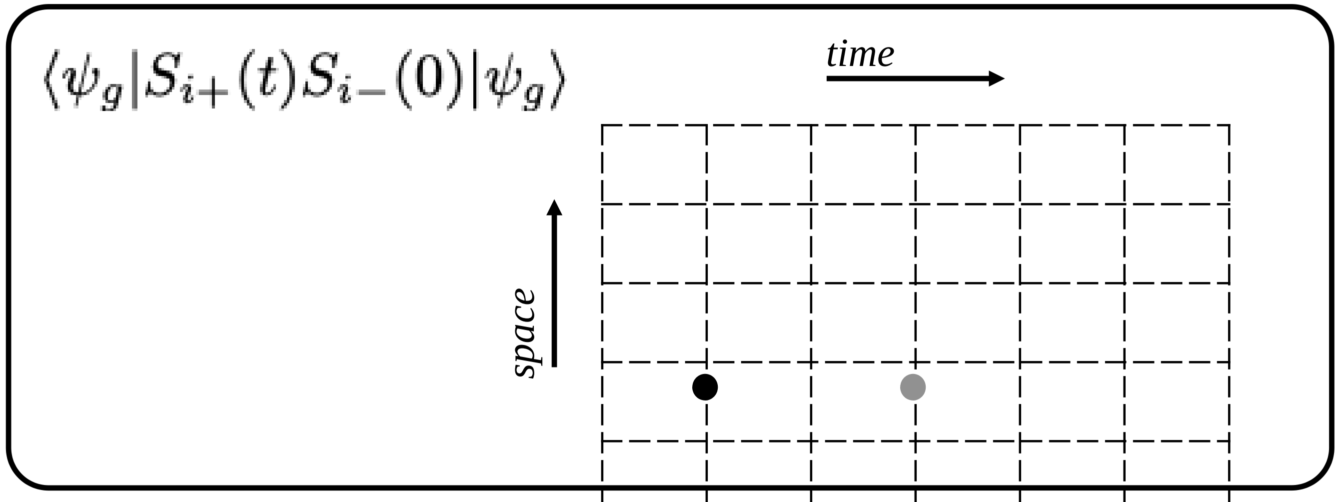


$$\langle S_{i+}(t) S_{i-}(0) \rangle \equiv \langle \psi_g | e^{itH} S_{i+} e^{-itH} S_{i-} | \psi_g \rangle$$

due to spin SU(2) symmetry is equivalent

Meaning?



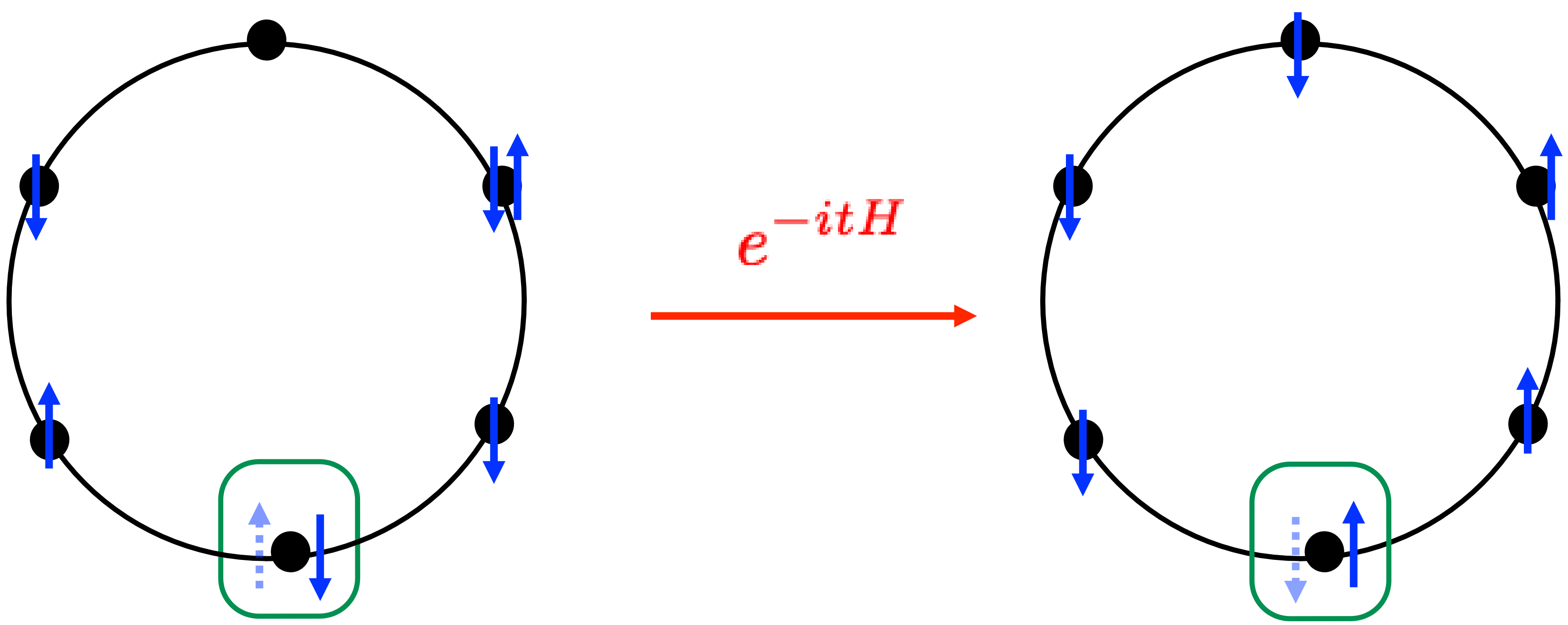


Time-dependent (dynamical) correlations

Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations

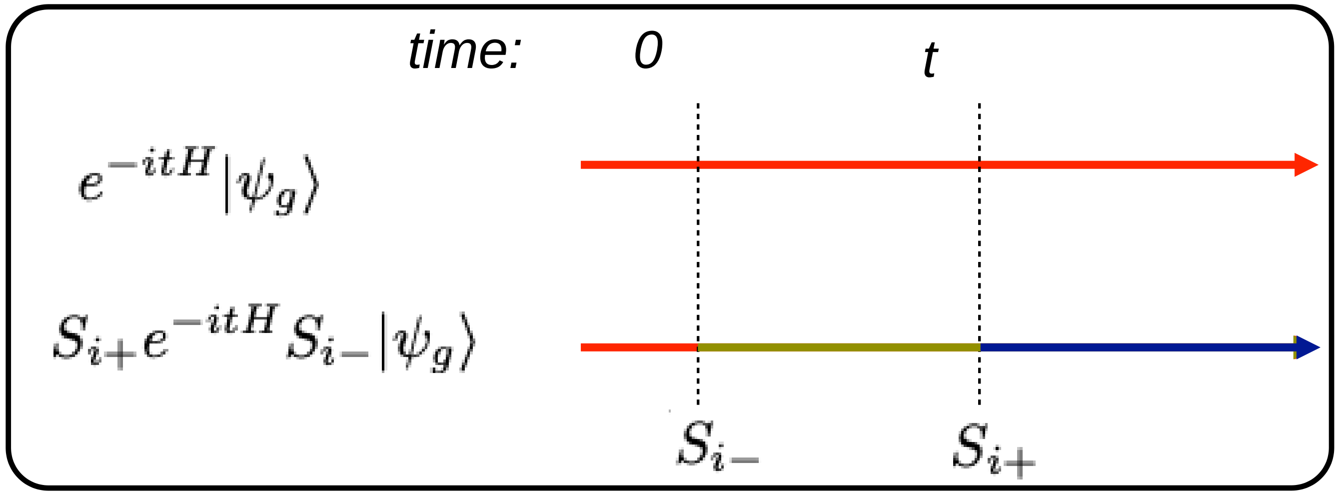
$$H = t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

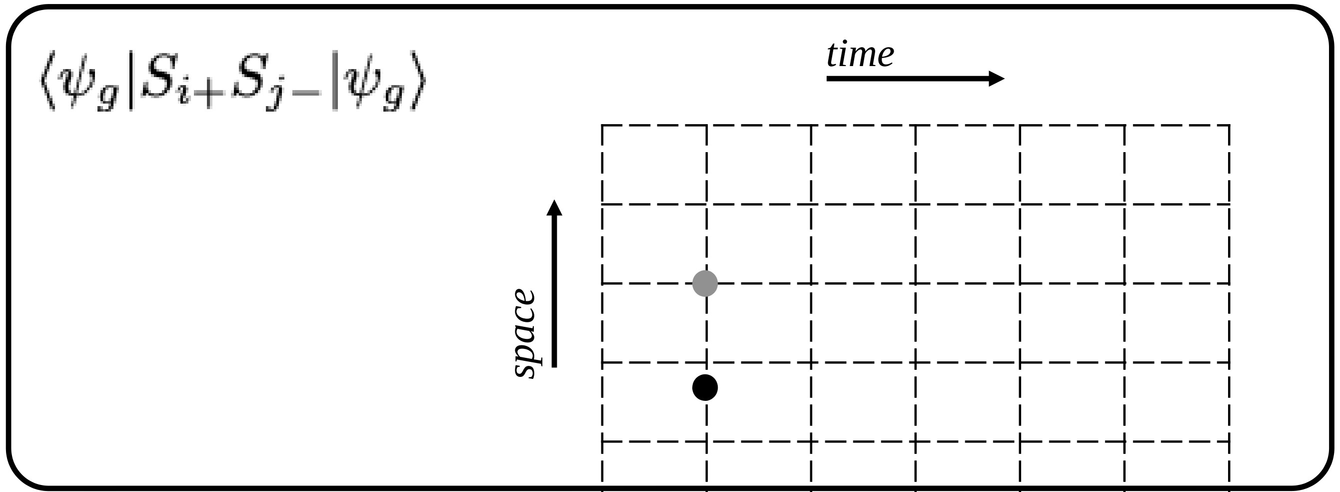


$$\langle S_{i+}(t) S_{i-}(0) \rangle \equiv \langle \psi_g | e^{itH} S_{i+} e^{-itH} S_{i-} | \psi_g \rangle$$

due to spin SU(2) symmetry is equivalent

Meaning?



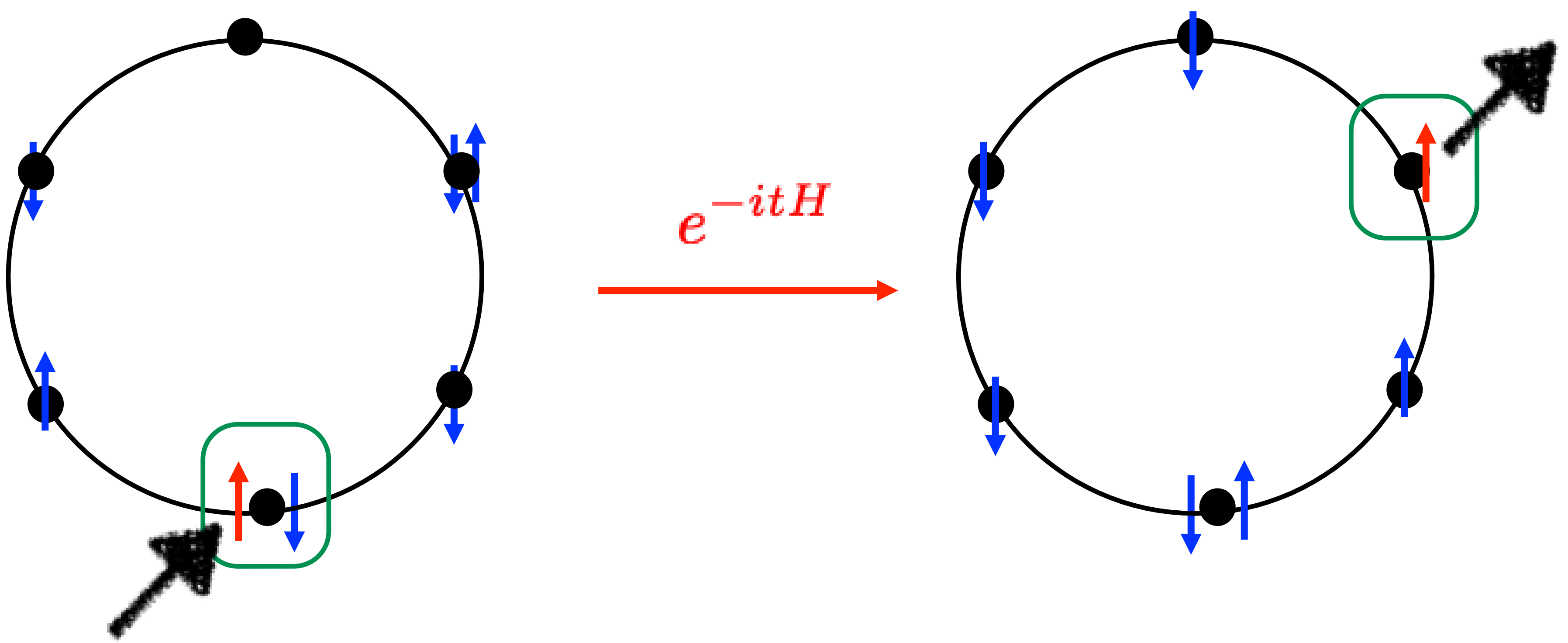


Time-dependent (dynamical) correlations

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

Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations



$$\langle c_{j\uparrow}(t) c^\dagger_{i\uparrow}(0) \rangle \equiv \langle \psi_g | e^{itH} c_{j\uparrow} e^{-itH} c^\dagger_{i\uparrow} | \psi_g \rangle$$

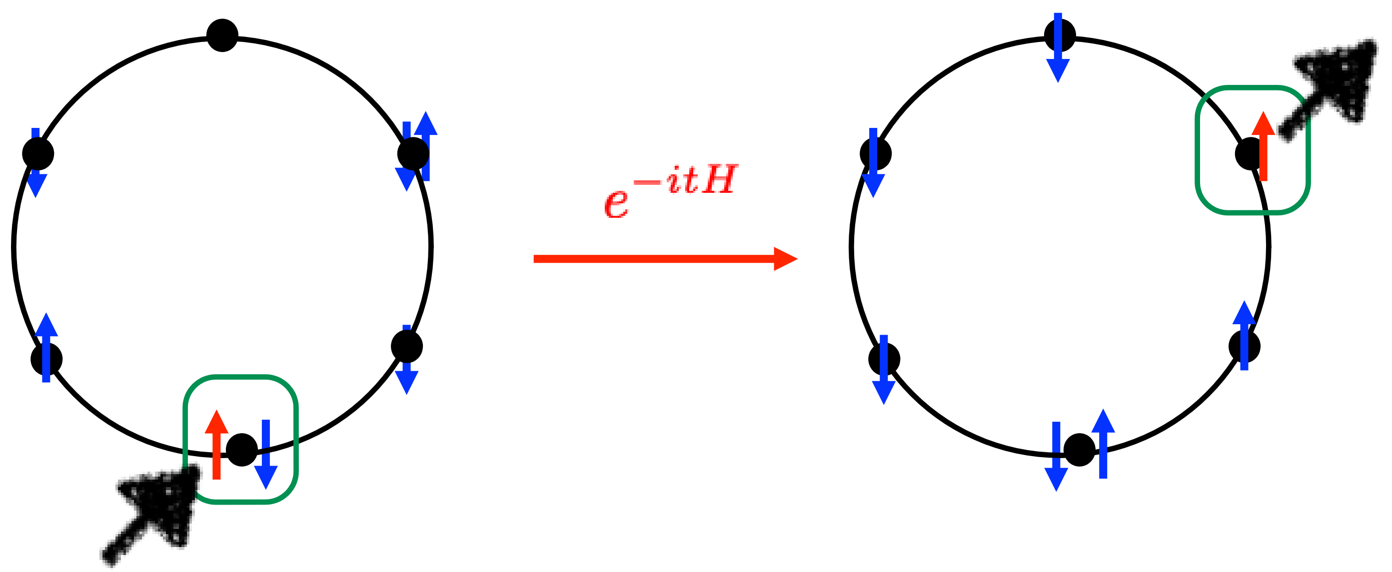
Note that operators taken at equal time fulfil the canonical commutation relations, but not at different times.

Time-dependent (dynamical) correlations

Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations

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



Spectral representation

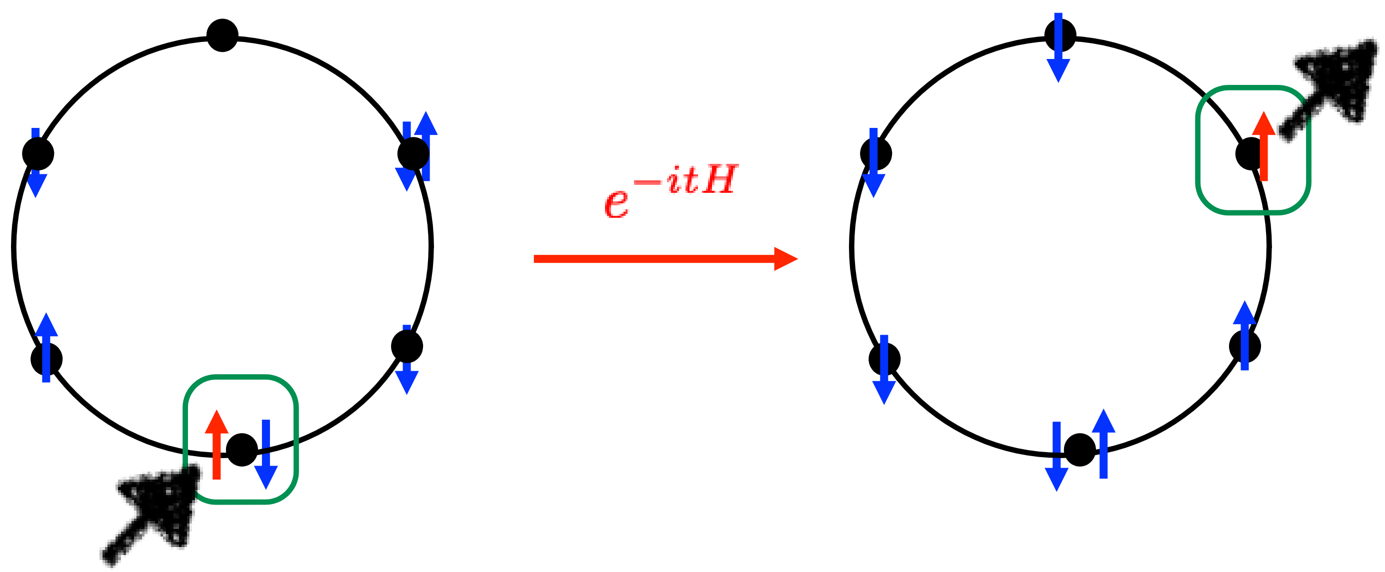
$$\begin{aligned}\langle \psi_g | e^{itH} A e^{-itH} B | \psi_g \rangle &= \sum_n \langle \psi_g | e^{itH} A | n \rangle \langle n | e^{-itH} B | \psi_g \rangle \\ &= \sum_n e^{-it(E_n - E_g)} \langle \psi_g | A | n \rangle \langle n | B | \psi_g \rangle\end{aligned}$$

Time-dependent (dynamical) correlations

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

Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations



Spectral representation

$$G_{AB}(t) = \langle \psi_g | e^{itH} A e^{-itH} B | \psi_g \rangle = \sum_n \langle \psi_g | e^{itH} A | n \rangle \langle n | e^{-itH} B | \psi_g \rangle$$
$$= \sum_n e^{-it(E_n - E_g)} \langle \psi_g | A | n \rangle \langle n | B | \psi_g \rangle$$

Fourier transform:

$$G_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G_{AB}(t) = \sum_n \langle \psi_g | A | n \rangle \langle n | B | \psi_g \rangle \int_{-\infty}^{\infty} dt e^{-it(\omega - \tilde{E}_n)}$$

Time-dependent (dynamical) correlations

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

Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations

Spectral representation

$$G_{AB}(t) = \langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle = \sum_n \langle\psi_g|e^{itH}A|n\rangle\langle n|e^{-itH}B|\psi_g\rangle$$
$$= \sum_n e^{-it(E_n-E_g)}\langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle$$

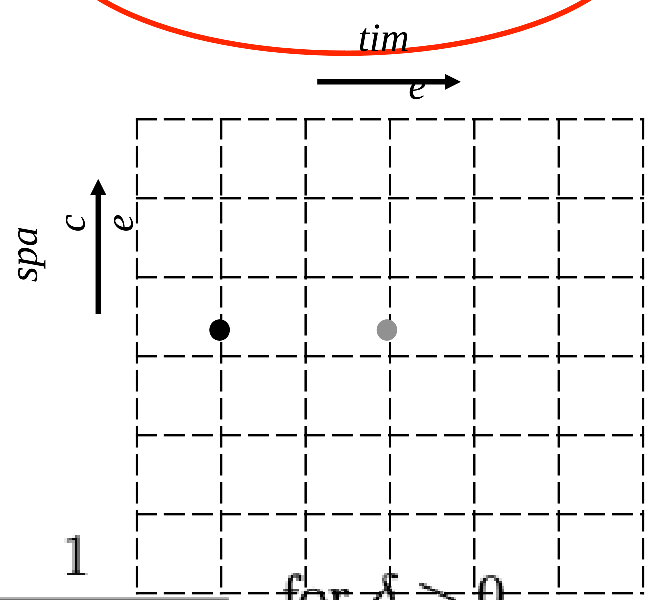
Fourier transform:

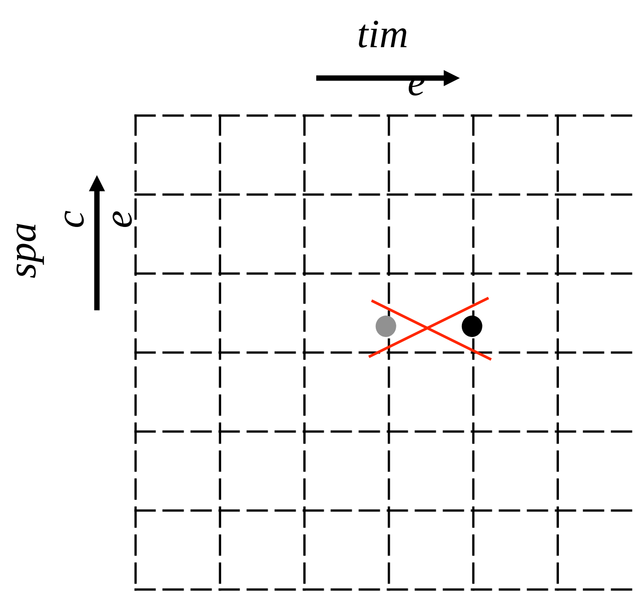
Problem

$$G_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}G_{AB}(t) = \sum_n \langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle \int_{-\infty}^{\infty} dt e^{-it(\omega-\tilde{E}_n)}$$

Retarded (causal) Green's function:

$$G_{AB}(t) = \Theta(t)\langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle$$





Treat omega as a complex variable:

$$\int_{-\infty}^{\infty} dt e^{it(\Omega-\tilde{E}_n)}\Theta(t) = \int_0^{\infty} dt e^{it(\omega-\tilde{E}_n)}e^{-\delta t} = \frac{1}{\omega+i\delta-\tilde{E}_n}, \text{ for } \delta > 0$$

Time-dependent (dynamical) correlations

Spectral representation

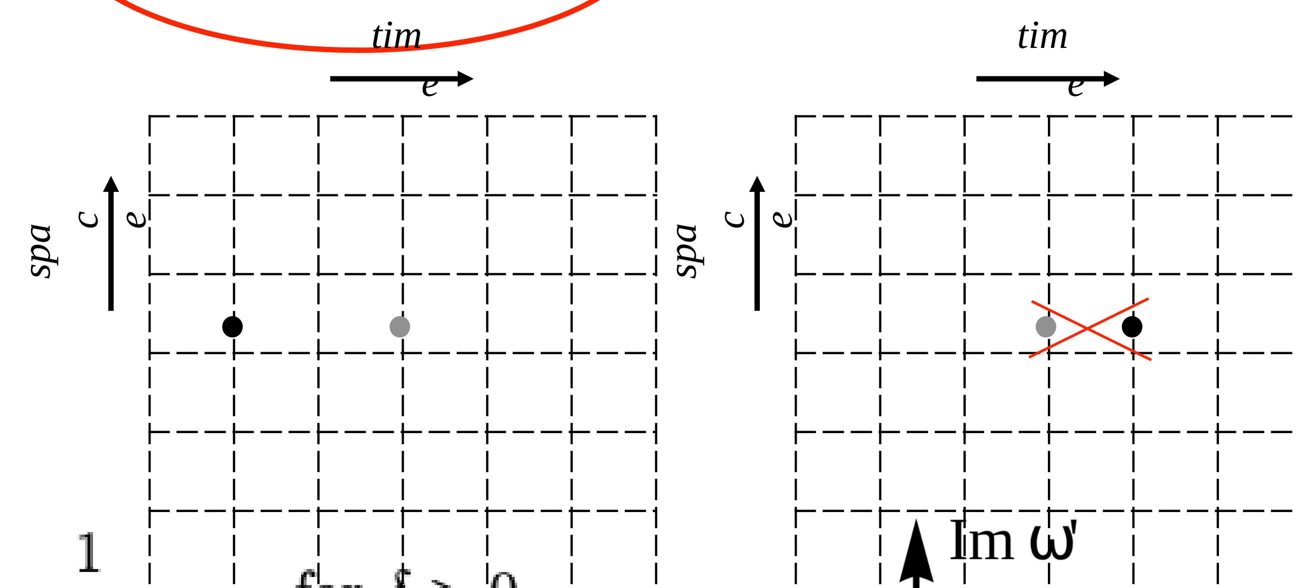
$$G_{AB}(t) = \langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle = \sum_n \langle\psi_g|e^{itH}A|n\rangle\langle n|e^{-itH}B|\psi_g\rangle$$

$$= \sum_n e^{-it(E_n-E_g)}\langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle$$

Fourier transform:

Problem

$$G_{AB}(\omega) = \int_{-\infty}^{\infty} dte^{i\omega t}G_{AB}(t) = \sum_n \langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle \int_{-\infty}^{\infty} dte^{-it(\omega-\tilde{E}_n)}$$

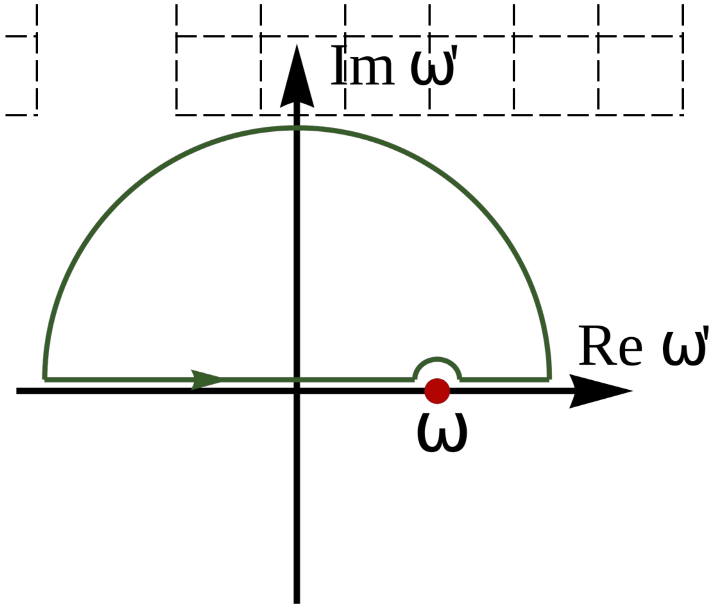


Retarded (causal) Green's function:

$$G_{AB}(t) = \Theta(t)\langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle$$

Treat omega as a complex variable:

$$\int_{-\infty}^{\infty} dte^{it(\Omega-\tilde{E}_n)}\Theta(t) = \int_0^{\infty} dte^{it(\omega-\tilde{E}_n)}e^{-\delta t} = \frac{1}{\omega+i\delta-\tilde{E}_n}, \text{ for } \delta > 0$$



Time-dependent (dynamical) correlations

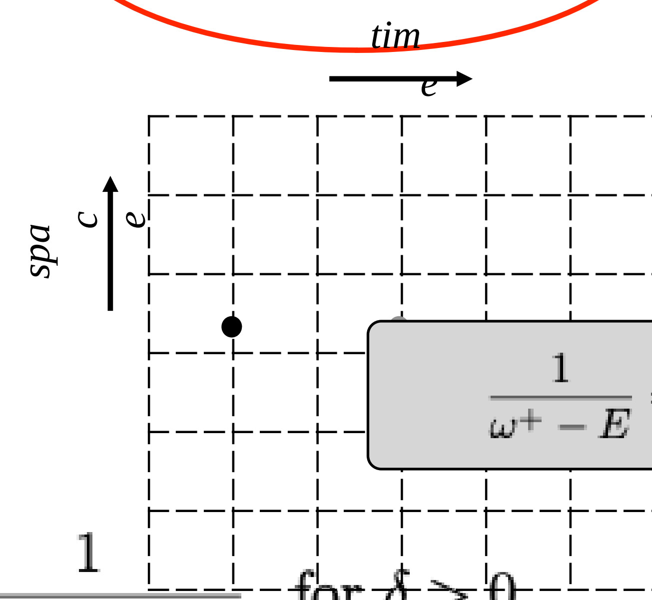
Spectral representation

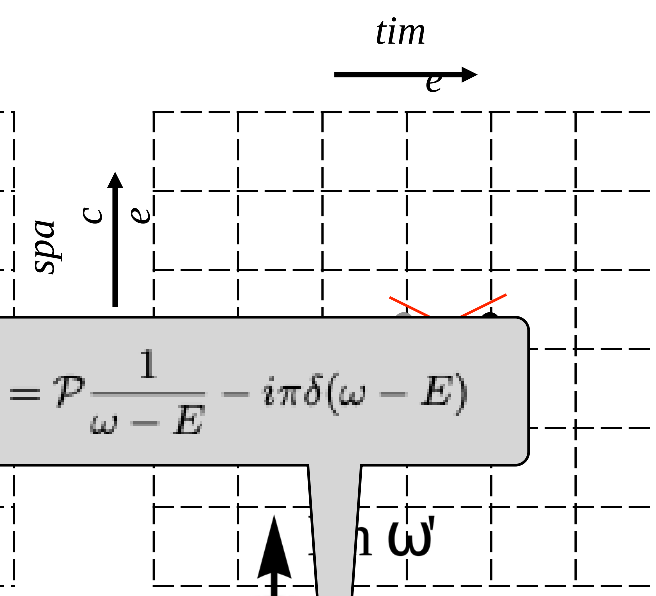
$$G_{AB}(t) = \langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle = \sum_n \langle\psi_g|e^{itH}A|n\rangle\langle n|e^{-itH}B|\psi_g\rangle$$
$$= \sum_n e^{-it(E_n-E_g)}\langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle$$

Fourier transform:

Problem

$$G_{AB}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G_{AB}(t) = \sum_n \langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle \int_{-\infty}^{\infty} dt e^{-it(\omega-\tilde{E}_n)}$$





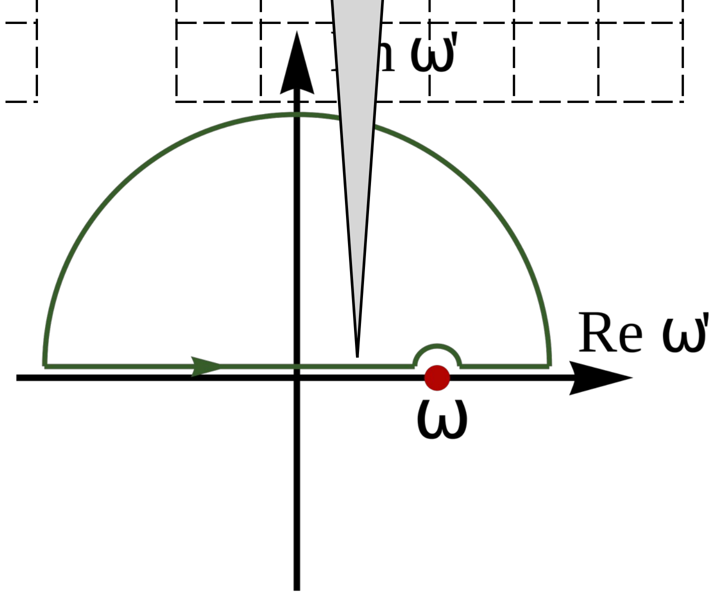
Retarded (causal) Green's function:

$$G_{AB}(t) = \Theta(t)\langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle$$

$$\frac{1}{\omega^+ - E} = \mathcal{P}\frac{1}{\omega - E} - i\pi\delta(\omega - E)$$

Treat omega as a complex variable:

$$\int_{-\infty}^{\infty} dt e^{it(\Omega-\tilde{E}_n)}\Theta(t) = \int_0^{\infty} dt e^{it(\omega-\tilde{E}_n)}e^{-\delta t} = \frac{1}{\omega + i\delta - \tilde{E}_n}, \text{ for } \delta > 0$$



Time-dependent (dynamical) correlations

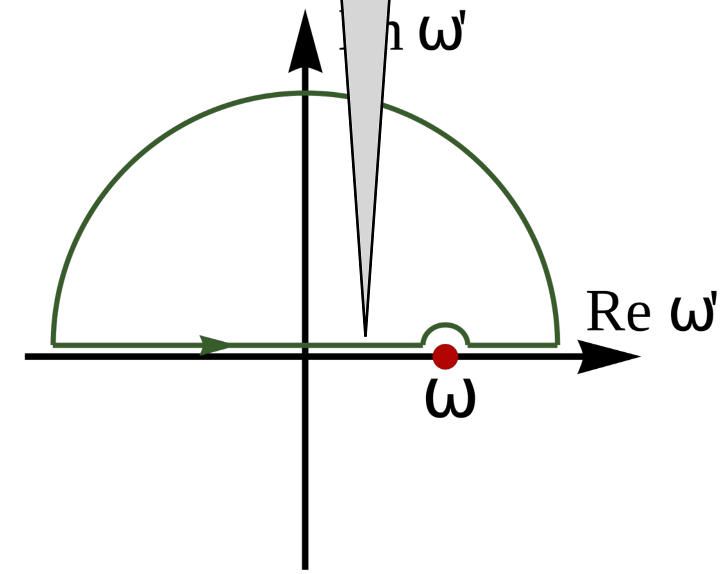
Spectral representation

Retarded (causal) Green's function:

$$G_{AB}(t) = \Theta(t)\langle\psi_g|e^{itH}Ae^{-itH}B|\psi_g\rangle$$

$$G_{AB}(\omega) \ = \sum_n \langle\psi_g|A|n\rangle\langle n|B|\psi_g\rangle \int_{-\infty}^{\infty} dt e^{-it(\omega-\tilde{E}_n)}$$

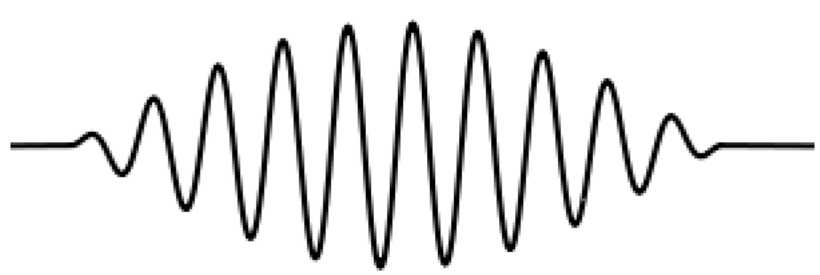
$$\frac{1}{\omega^+ - E} = \mathcal{P}\frac{1}{\omega - E} - i\pi\delta(\omega - E)$$

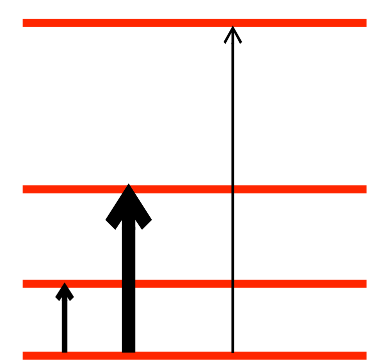


Physical meaning

$$\mathrm{Im}\, G_{AA}(\omega) = -i\pi \sum_n |\langle n|A|\psi_g\rangle|^2 \delta(\omega - \tilde{E}_n)$$

long ω-pulse





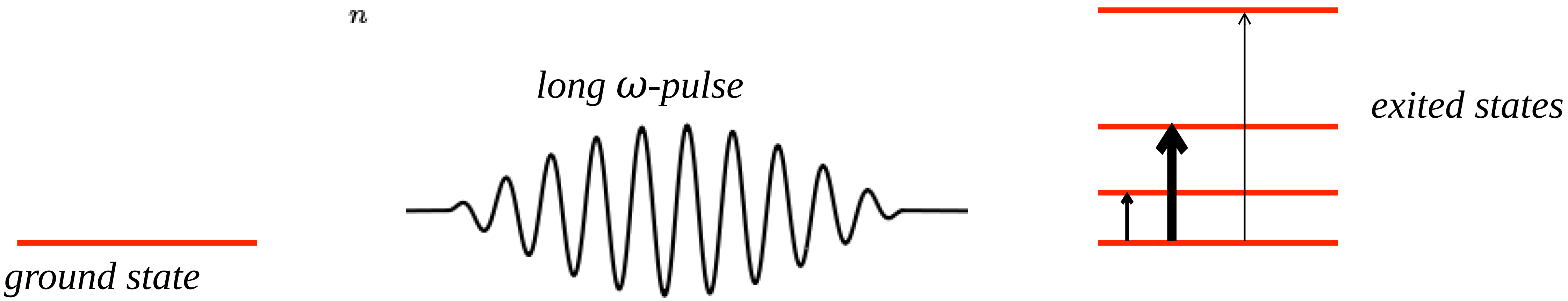
exited states

ground state

Time-dependent (dynamical) correlations

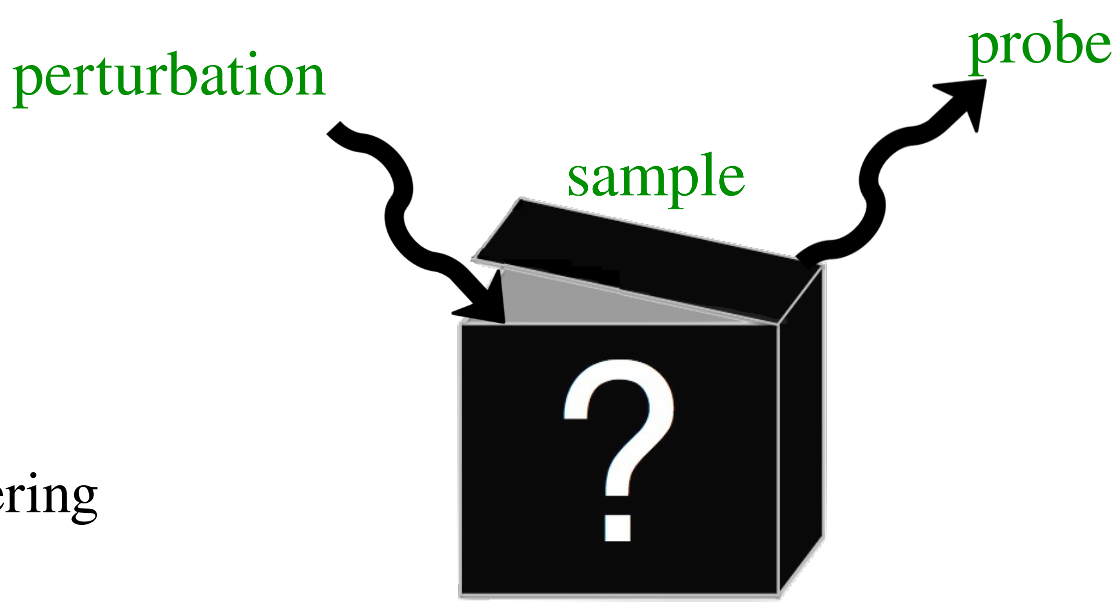
Physical meaning

$$\mathrm{Im}\, G_{AA}(\omega) = -i\pi \sum_n |\langle n|A|\psi_g\rangle|^2 \delta(\omega - \tilde{E}_n)$$



Examples:

$\langle c^\dagger(t) c(t')\rangle$	photoemission
$\langle \vec{j}(t) \vec{j}(t')\rangle$	transport, optics
$\langle \vec{S}(t) \vec{S}(t')\rangle$	magnetism, neutron scattering

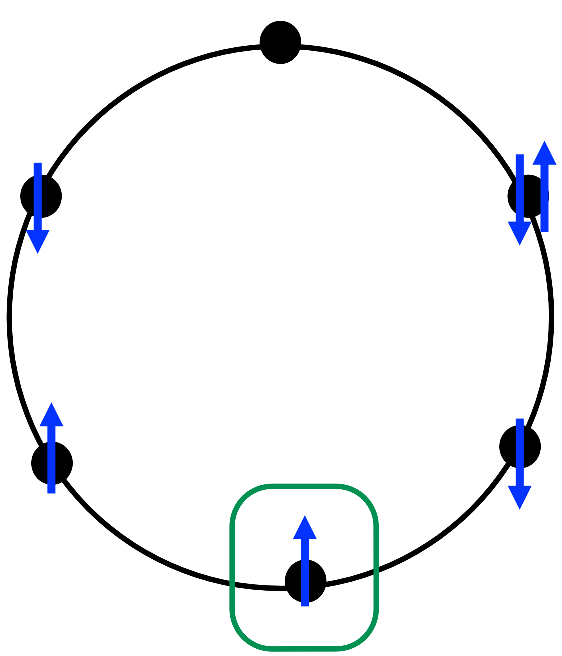


6-site Hubbard model

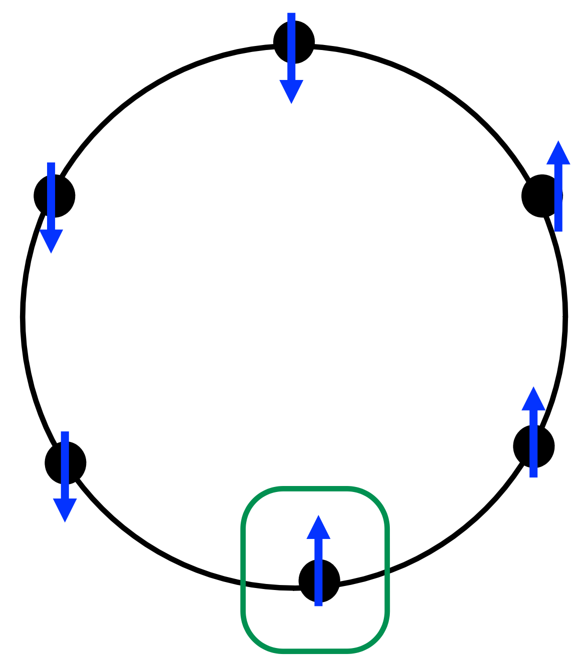
Why correlation functions?

- Contributions to interaction energy of the system
- Response to small perturbations

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

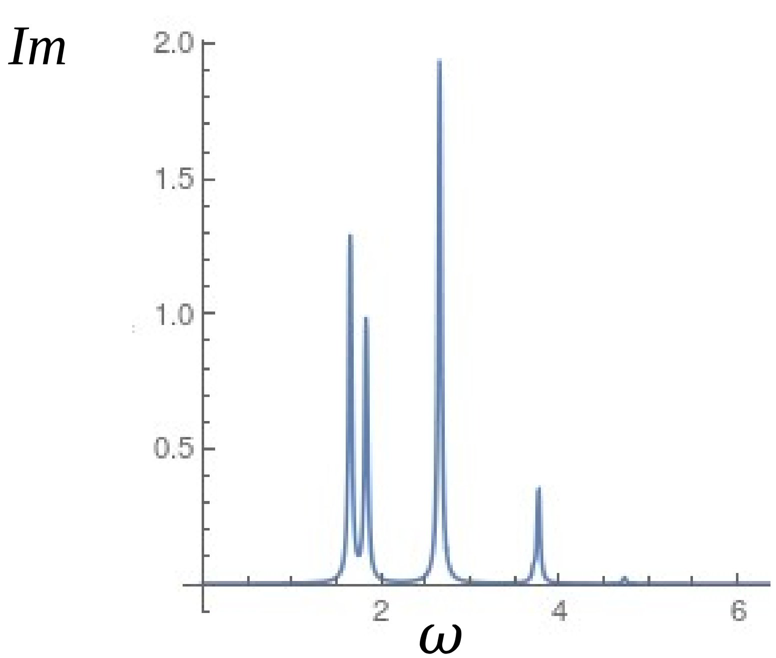


$$\xrightarrow{e^{-itH}}$$



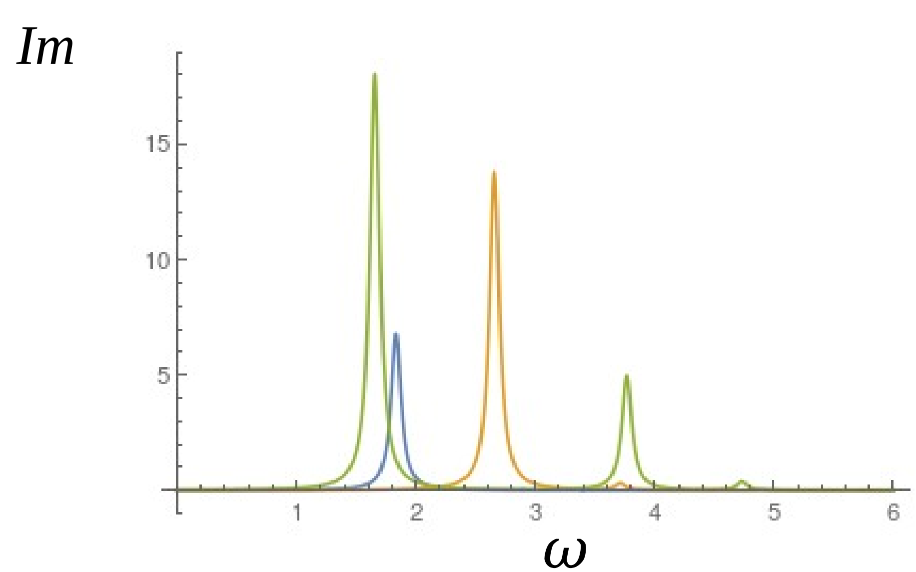
$\langle S_{iz} S_{iz} \rangle_{\omega}$

$\langle S_z(\mathbf{k}) S_z(-\mathbf{k}) \rangle_{\omega}$



$$S_z(\mathbf{k}) = \sum_{k} e^{i\mathbf{k}\cdot\mathbf{R}} S_{\mathbf{R}z}$$

$$\rightleftarrows$$

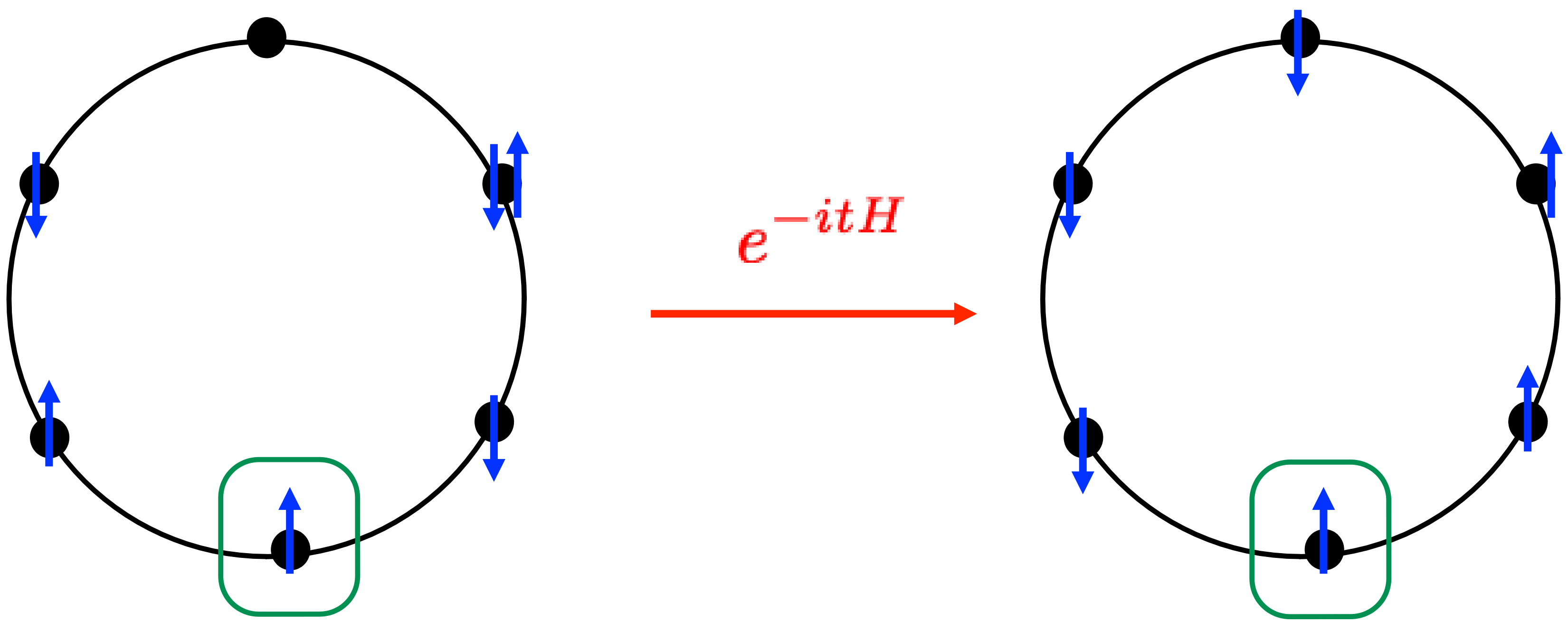


6-site Hubbard model

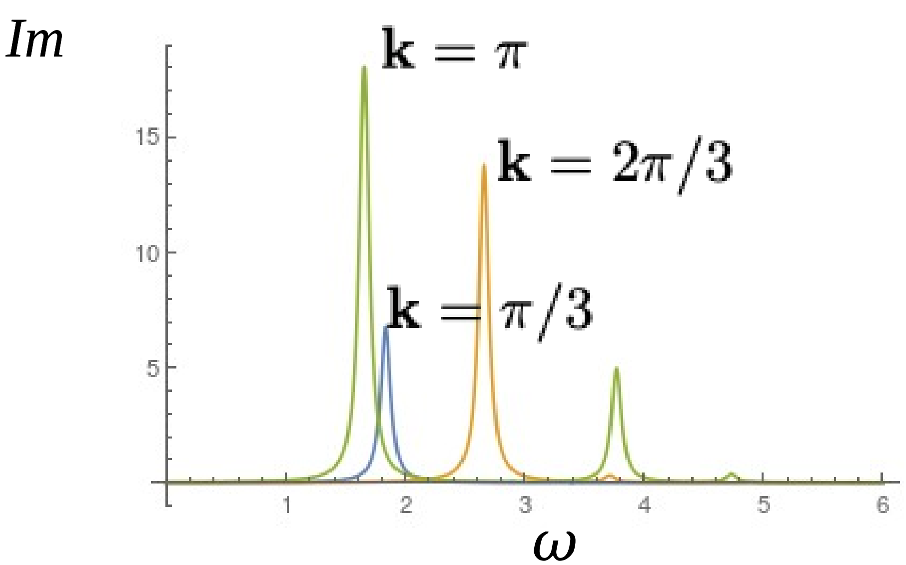
Why correlation functions?

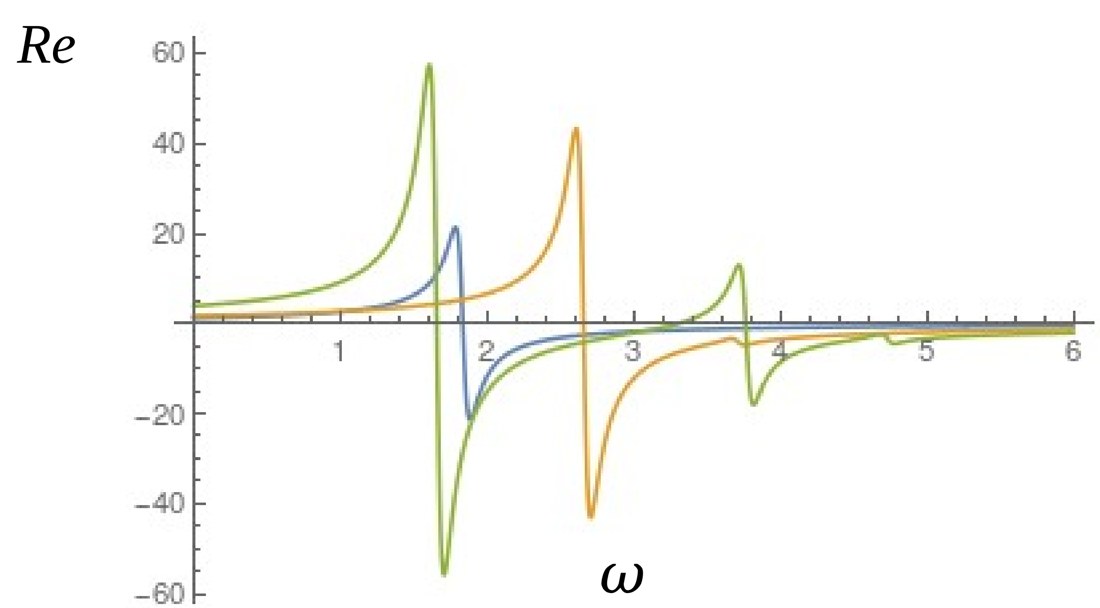
- Contributions to interaction energy of the system
- Response to small perturbations

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



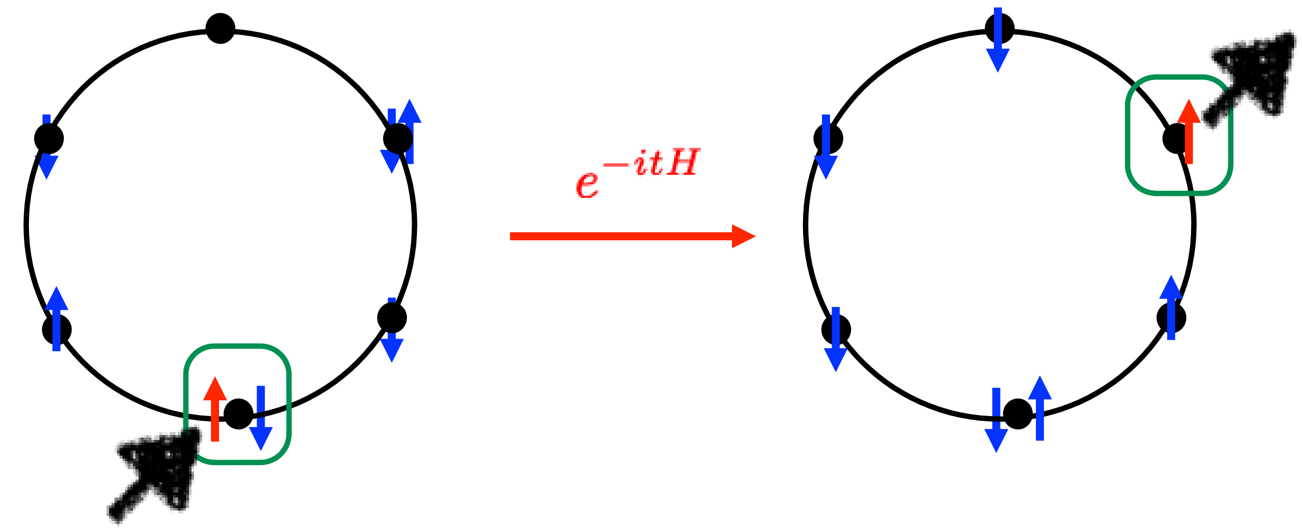
$\langle S_z(\mathbf{k}) S_z(-\mathbf{k}) \rangle_\omega$





6-site Hubbard model

1-particle propagator

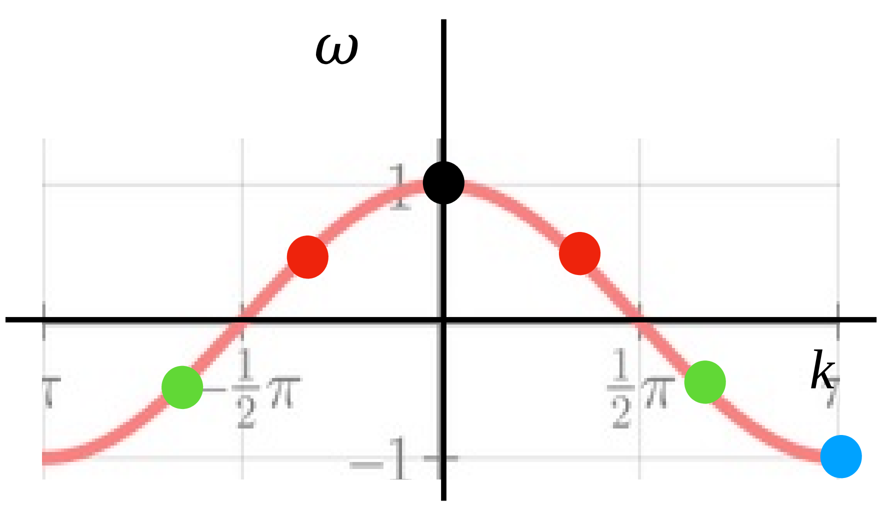


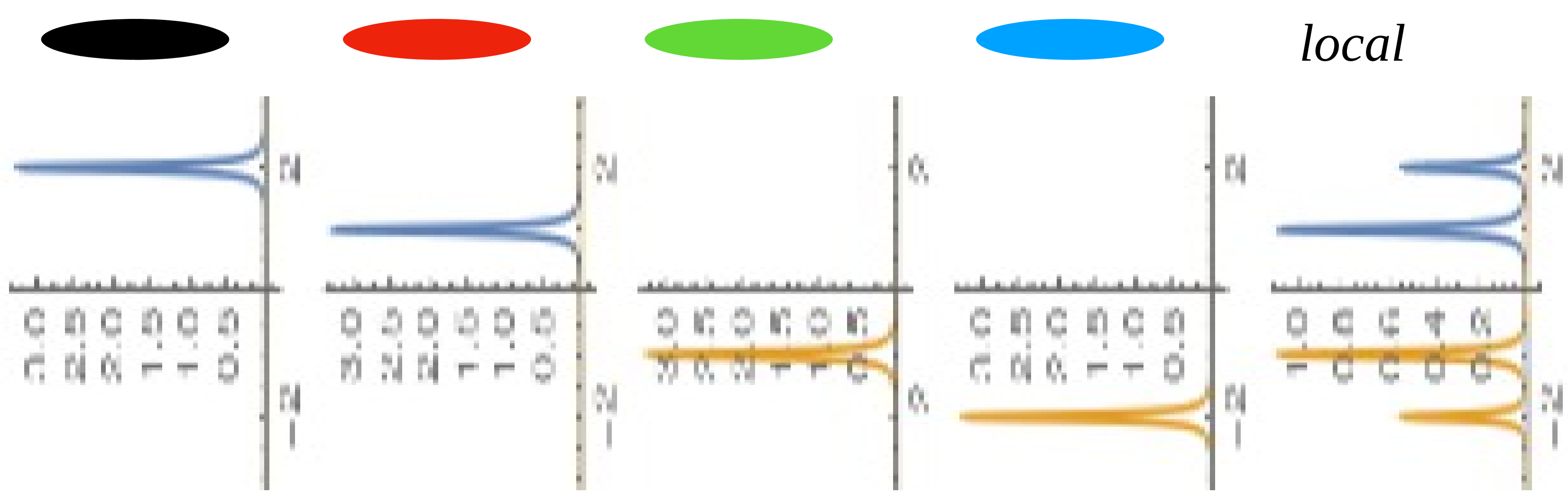
$$\langle c_{j\uparrow}(t)c^{\dagger}_{i\uparrow}(0)\rangle \equiv \langle\psi_g|e^{itH}c_{j\uparrow}e^{-itH}c^{\dagger}_{i\uparrow}|\psi_g\rangle$$

1-particle spectral function

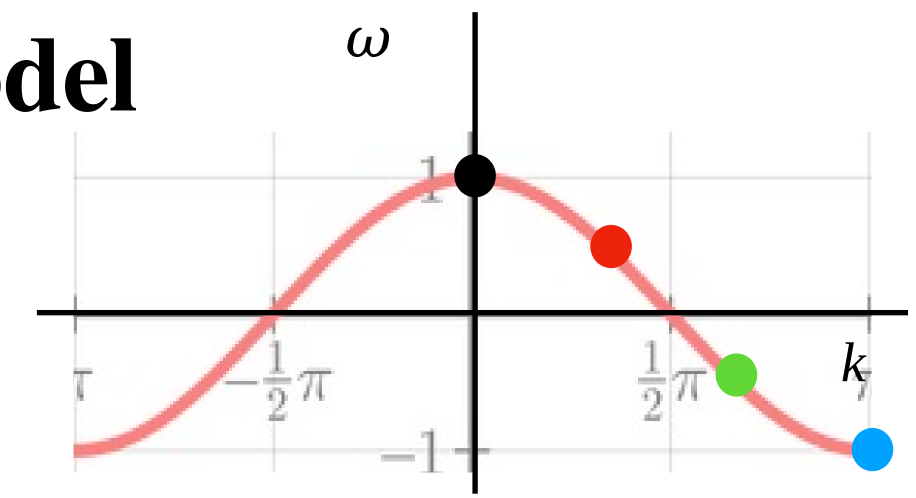
$$A(\omega) = \begin{cases} \sum_l |\langle n+1, l|c_i^{\dagger}|n,0\rangle|^2\delta(\omega - (E_l^{n+1} - E_0^n)), & \omega > 0 \\ \sum_l |\langle n-1, l|c_i|n,0\rangle|^2\delta(\omega + (E_l^{n-1} - E_0^n)), & \omega < 0 \end{cases}$$

Non-interacting case (U=0) - relationship to 1P eigenenergies



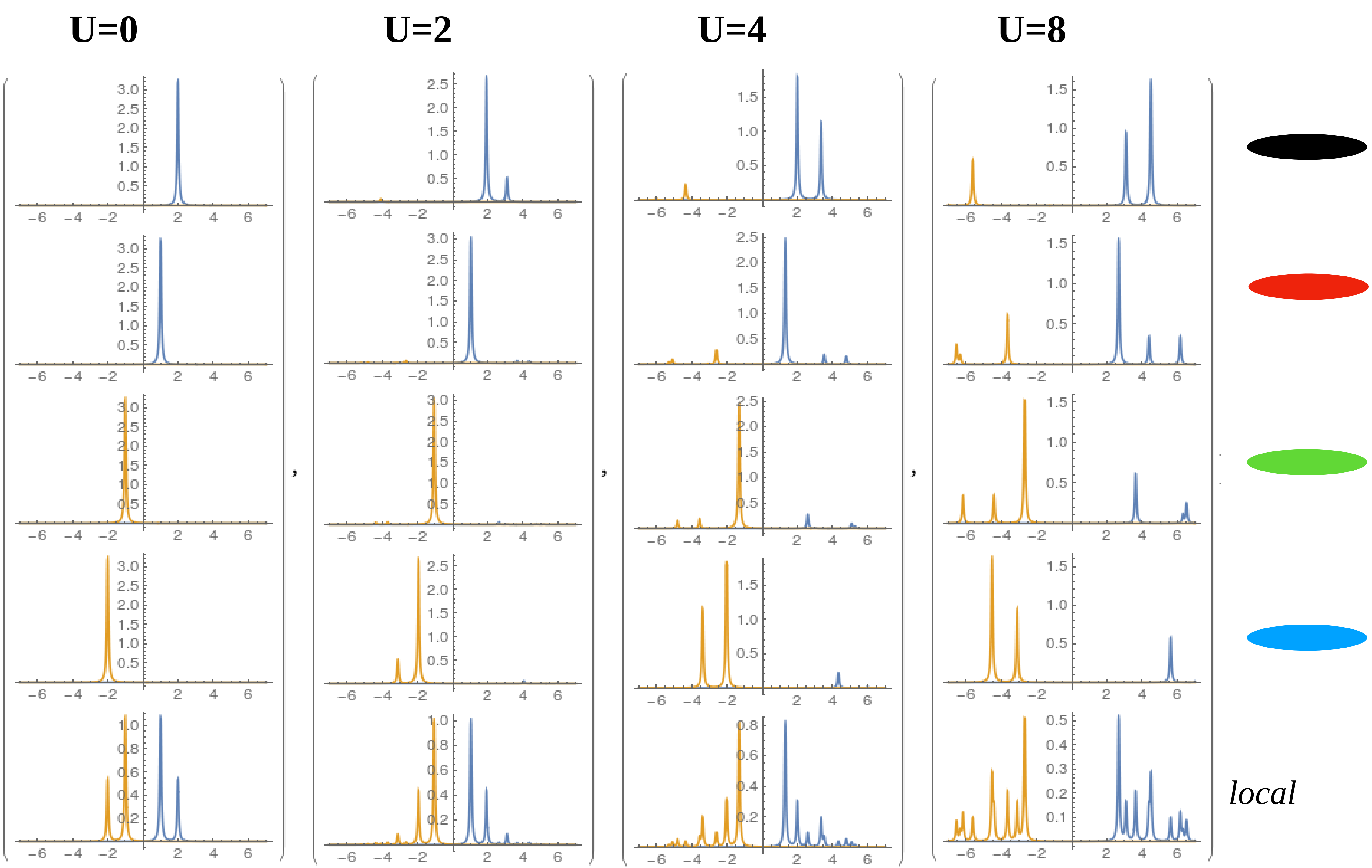


6-site Hubbard model

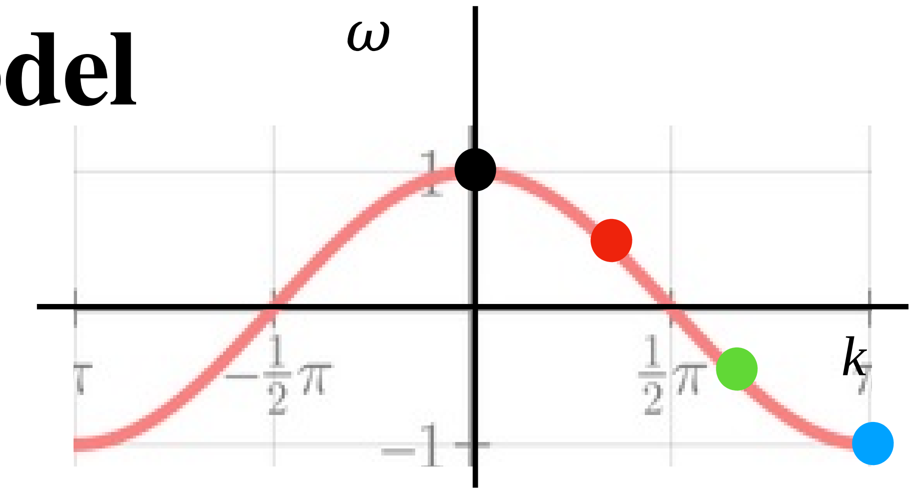


1-particle spectral function

$$A(\omega) = \begin{cases} \sum_l |\langle n+1, l|c_i^\dagger|n,0\rangle|^2 \delta(\omega - (E_l^{n+1} - E_0^n)), & \omega > 0 \\ \sum_l |\langle n-1, l|c_i|n,0\rangle|^2 \delta(\omega + (E_l^{n-1} - E_0^n)), & \omega < 0 \end{cases}$$



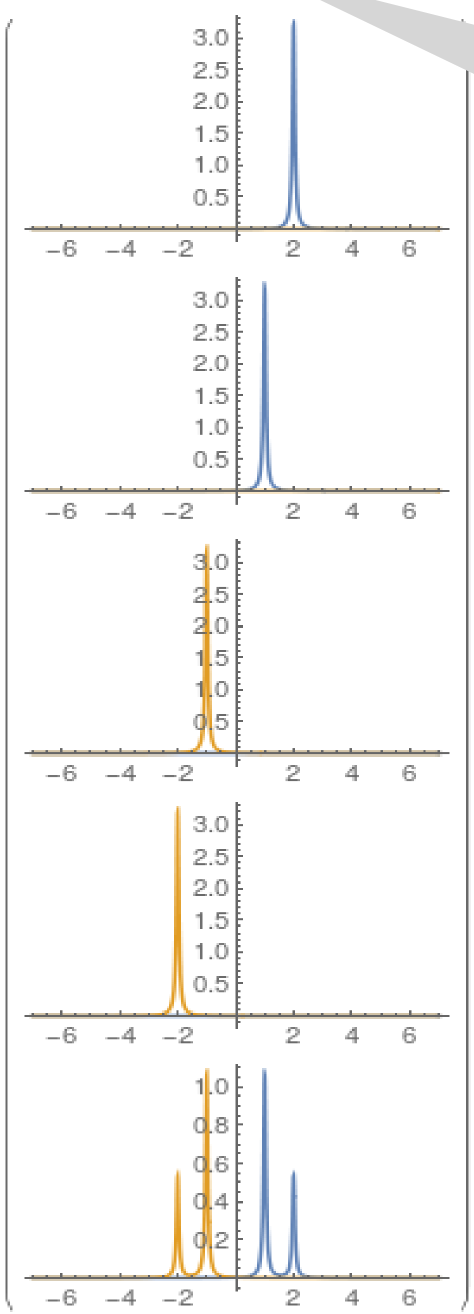
6-site Hubbard model



1-particle spectral function

$$A(\omega) = \begin{cases} \sum_l |\langle n+1, l | c_i^\dagger | n, 0\rangle|^2 \delta(\omega - (E_l^{n+1} - E_0^n)), & \omega > 0 \\ \sum_l |\langle n-1, l | c_i | n, 0\rangle|^2 \delta(\omega + (E_l^{n-1} - E_0^n)), & \omega < 0 \end{cases}$$

U=0 **U=2** **U=4** **U=8**



$$H = \sum_{a,b} h_{ab} c_a^\dagger c_b$$

$$c_b = U_{bi} c_i, \quad (c_b^\dagger = U_{bi}^* c_i^\dagger = U_{ib}^\dagger c_i^\dagger) \qquad \{c_i, c_j^\dagger\} = U_{ia}^\dagger \{c_a, c_b^\dagger\} U_{bj} = U_{ia}^\dagger \delta_{ab} U_{bj} = \delta_{ij}$$

$$H = \sum_i \epsilon_i c_i^\dagger c_i$$

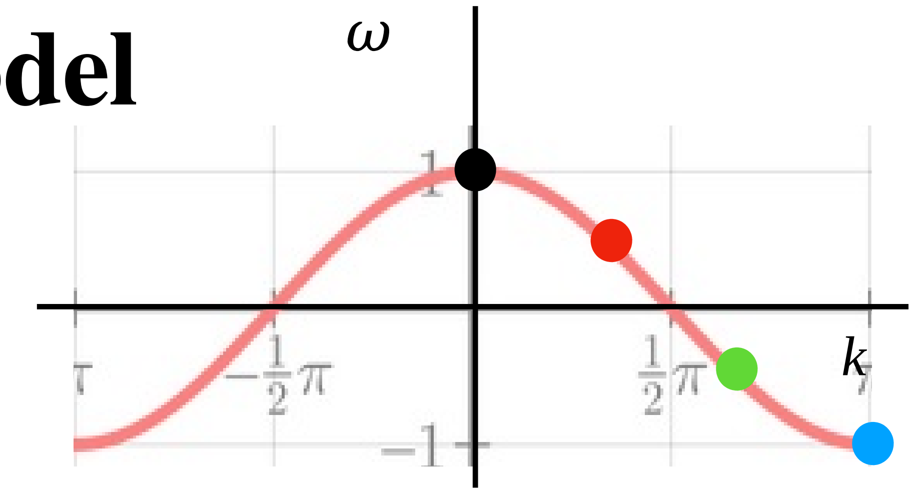
$$|\phi\rangle = c_{i_1}^\dagger \dots c_{i_N}^\dagger |\mathrm{vac}\rangle$$

Canonical commutation relations!

$$H|\phi\rangle = \left(\sum_{k=1}^{N} \epsilon_{i_k}\right) |\phi\rangle$$

$$A_j(\omega) = \delta(\omega - \epsilon_j)$$

6-site Hubbard model



1-particle spectral function

$$A(\omega) = \begin{cases} \sum_l |\langle n+1, l|c_i^\dagger|n,0\rangle|^2 \delta(\omega - (E_l^{n+1} - E_0^n)), & \omega > 0 \\ \sum_l |\langle n-1, l|c_i|n,0\rangle|^2 \delta(\omega + (E_l^{n-1} - E_0^n)), & \omega < 0 \end{cases}$$

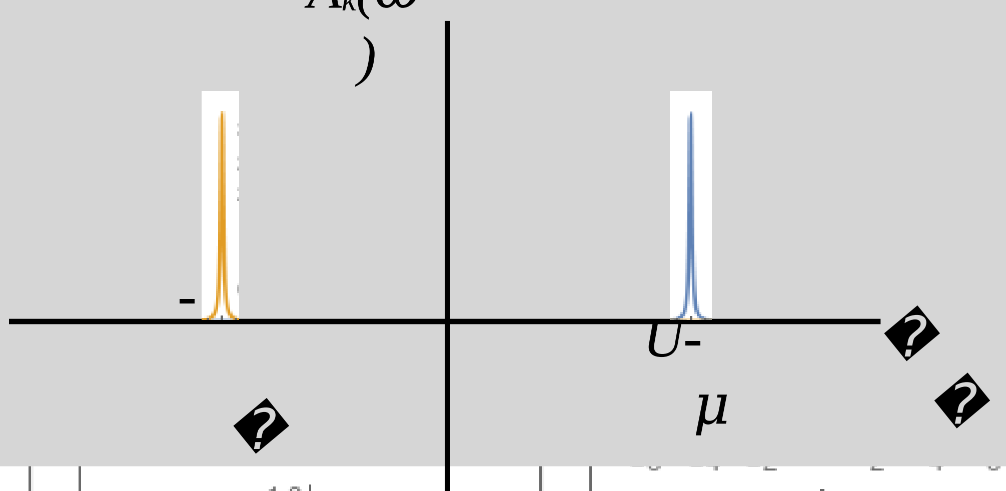
U=0 **U=2** **U=4** **U=8**

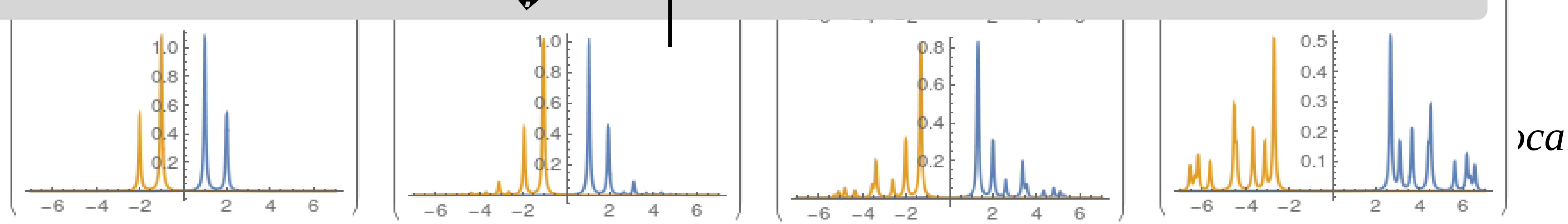
Large U (atomic problem, t=0)

$$H = -\mu(n_{i\uparrow} + n_{i\uparrow}) + U n_{i\uparrow} n_{i\downarrow}$$

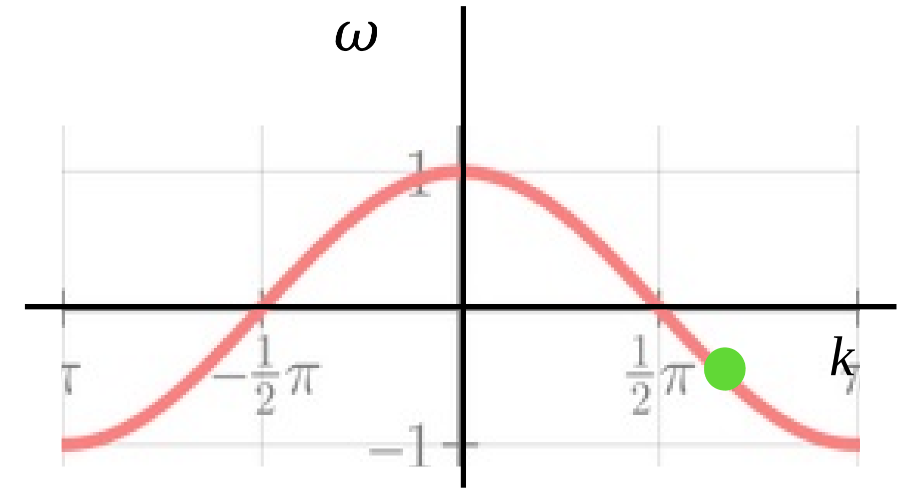
$\langle \uparrow\downarrow | c_{i\uparrow}^\dagger | \downarrow \rangle$ $\quad E^{n+1} - E^n = (-2\mu + U) - (-\mu) = -\mu + U$

$\langle \emptyset | c_{i\downarrow} | \downarrow \rangle$ $\quad E^{n-1} - E^n = 0 - (-\mu) = \mu$





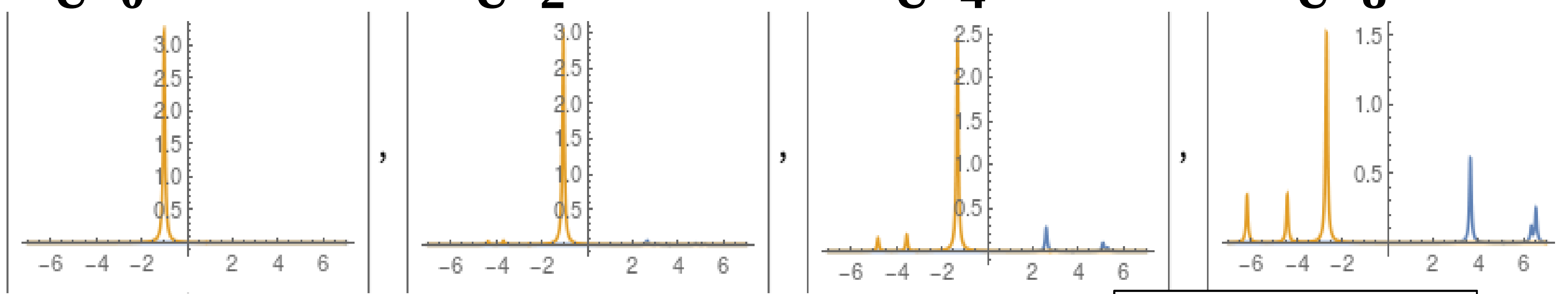
Infinite system

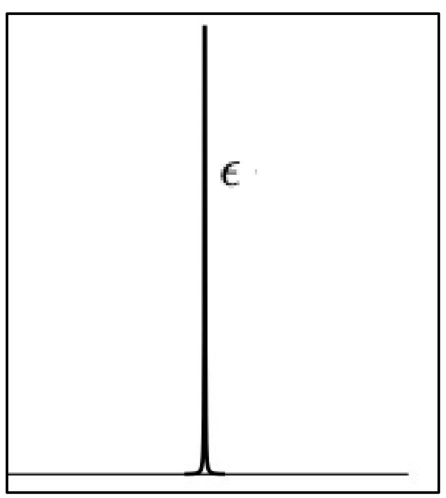


1-particle spectral function

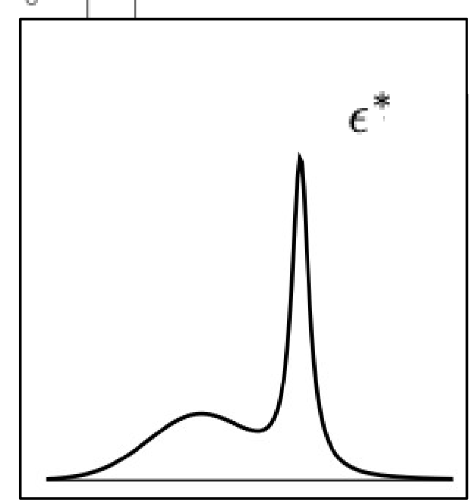
$$A(\omega) = \begin{cases} \sum_l |\langle n+1, l|c_i^\dagger|n,0\rangle|^2 \delta(\omega - (E_l^{n+1} - E_0^n)), & \omega > 0 \\ \sum_l |\langle n-1, l|c_i|n,0\rangle|^2 \delta(\omega + (E_l^{n-1} - E_0^n)), & \omega < 0 \end{cases}$$

U=0 **U=2** **U=4** **U=8**



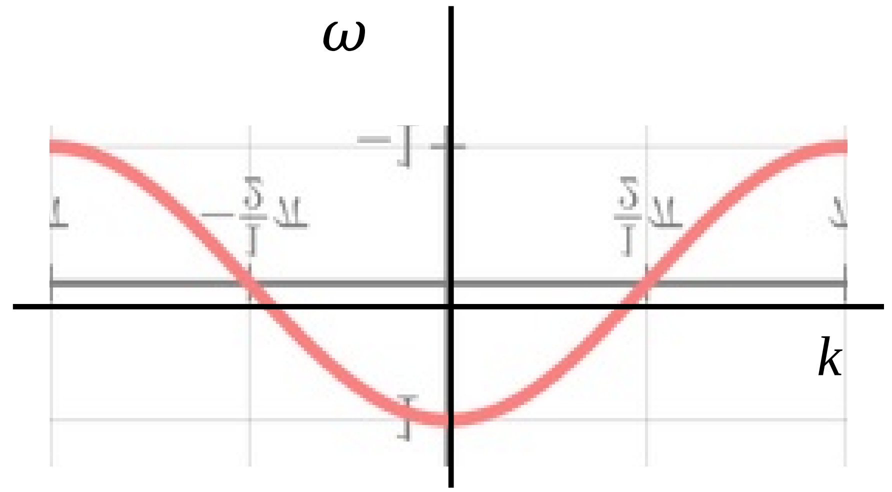


non-interacting (bare)



interacting (dressed)

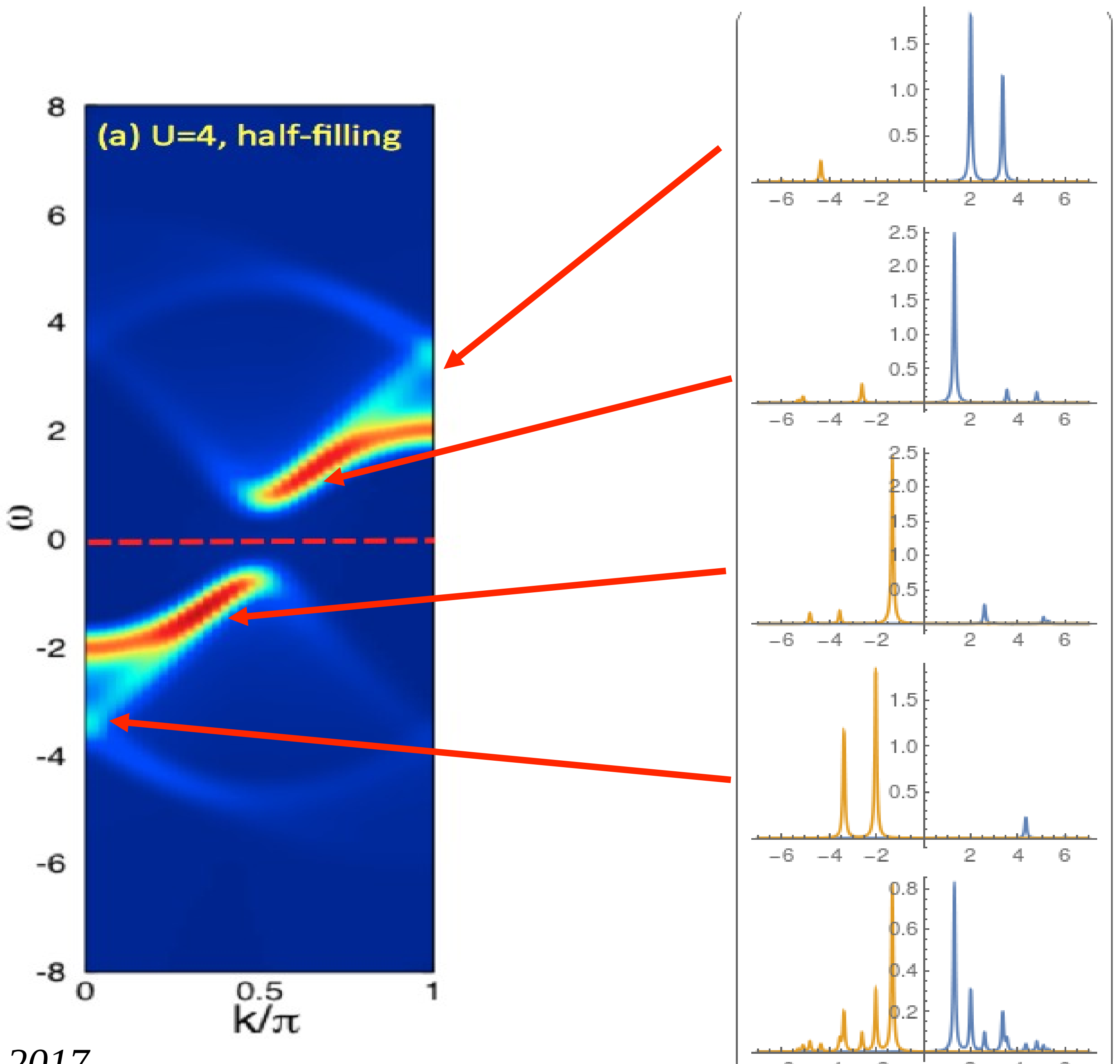
Infinite system



1-particle spectral function

$$A(\omega) = \begin{cases} \sum_l |\langle n+1, l|c_i^\dagger|n,0\rangle|^2 \delta(\omega - (E_l^{n+1} - E_0^n)), & \omega > 0 \\ \sum_l |\langle n-1, l|c_i|n,0\rangle|^2 \delta(\omega + (E_l^{n-1} - E_0^n)), & \omega < 0 \end{cases}$$

U=4



Nocera et al. 2017