6-site Hubbard model

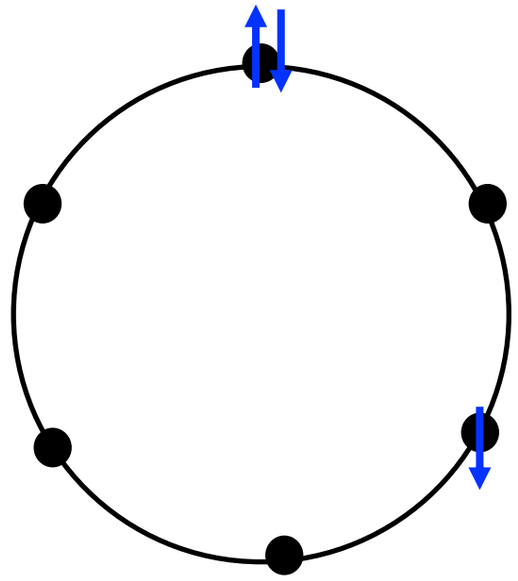
$$H = t \sum_{(ij),\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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:

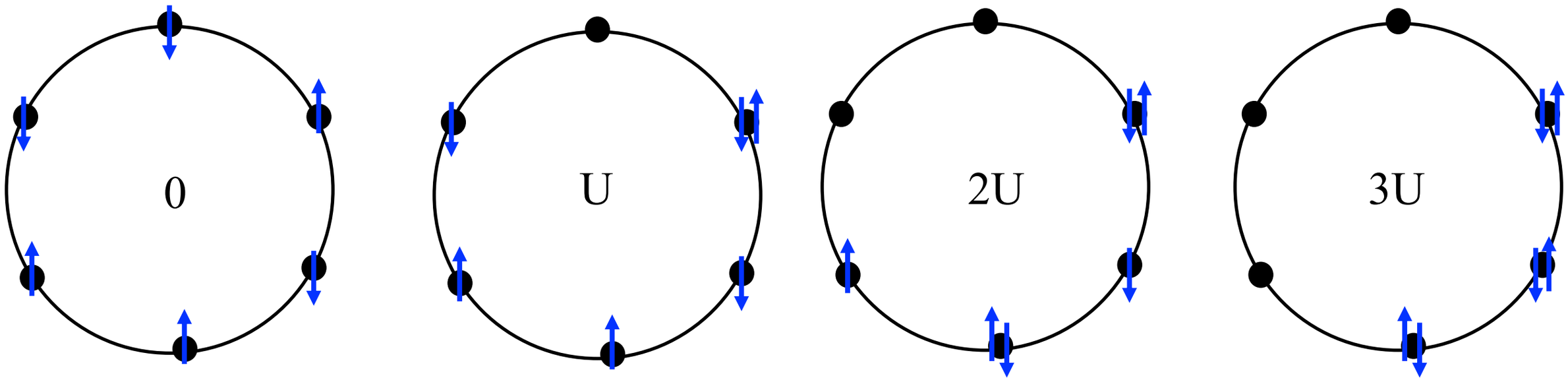
in binary code (10000|101000)



6-site Hubbard model

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

Matrix elements of the interaction part (diagonal in present basis):
Sector (3,3)



implementation of ■

(101000|100000) -> (101000).(100000) = 1

implementation of ■

(101000|100000) -> (101000)-(100000) = (001000)

i=2

6-site Hubbard model

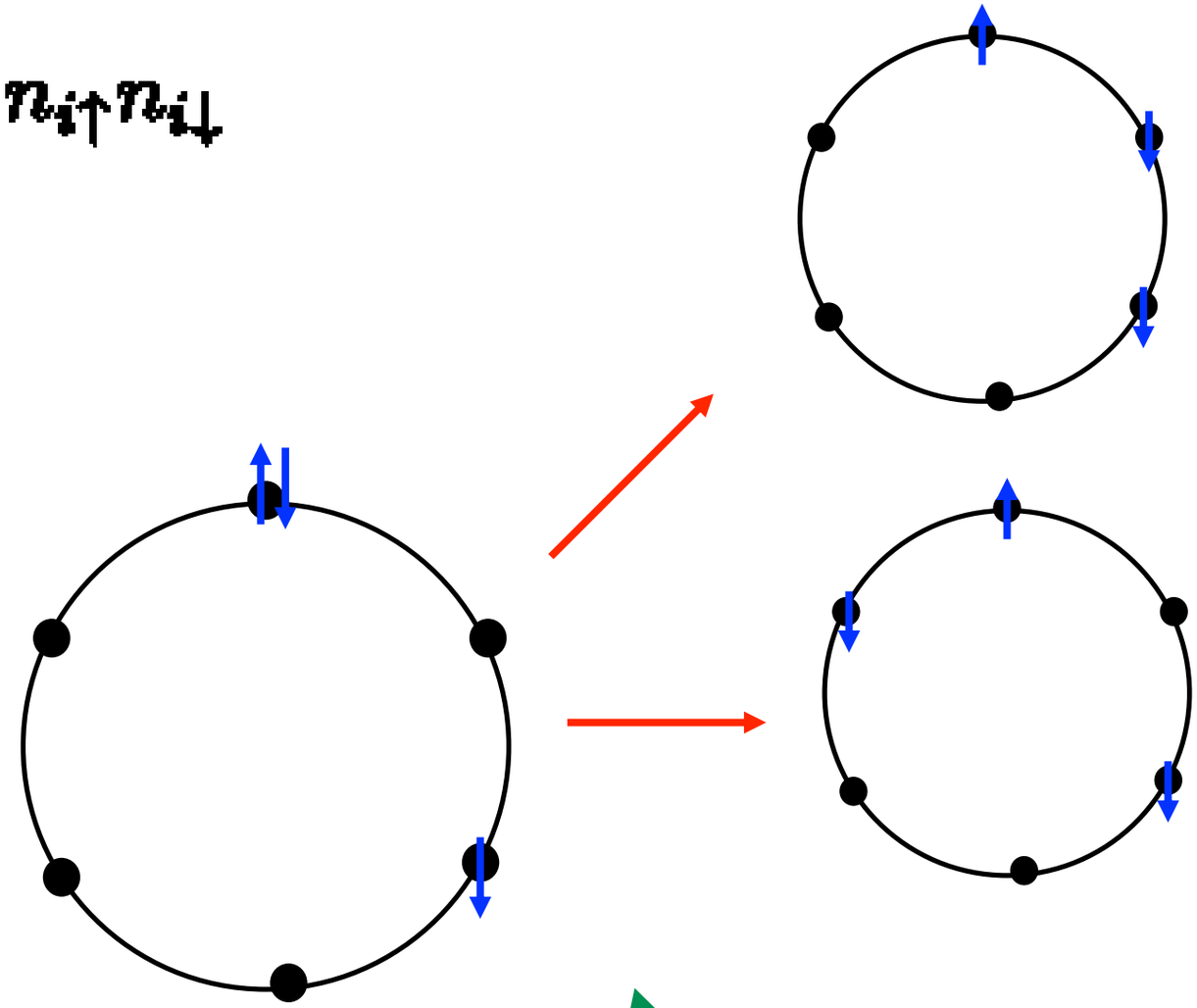
$$H = t \sum_{(ij),\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Matrix elements of the hopping part:

in binary code (10100|100000)

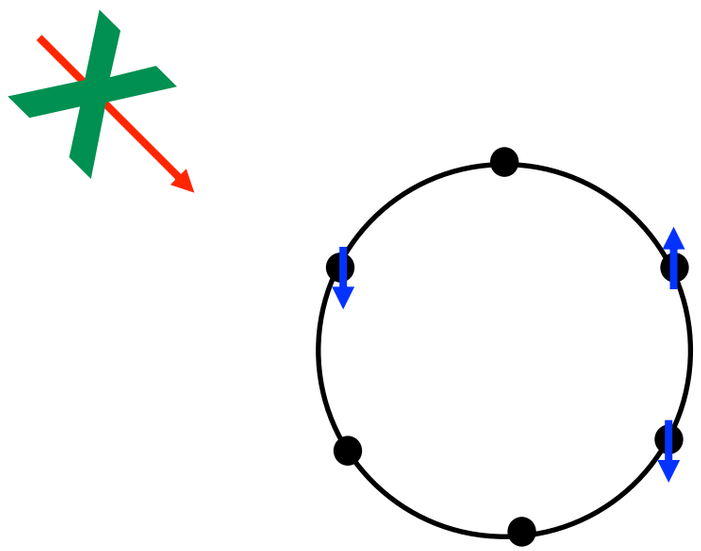
-> ~~-(01100|100000)~~

✓ (1$\underline{1}$000|000000)



Signs:

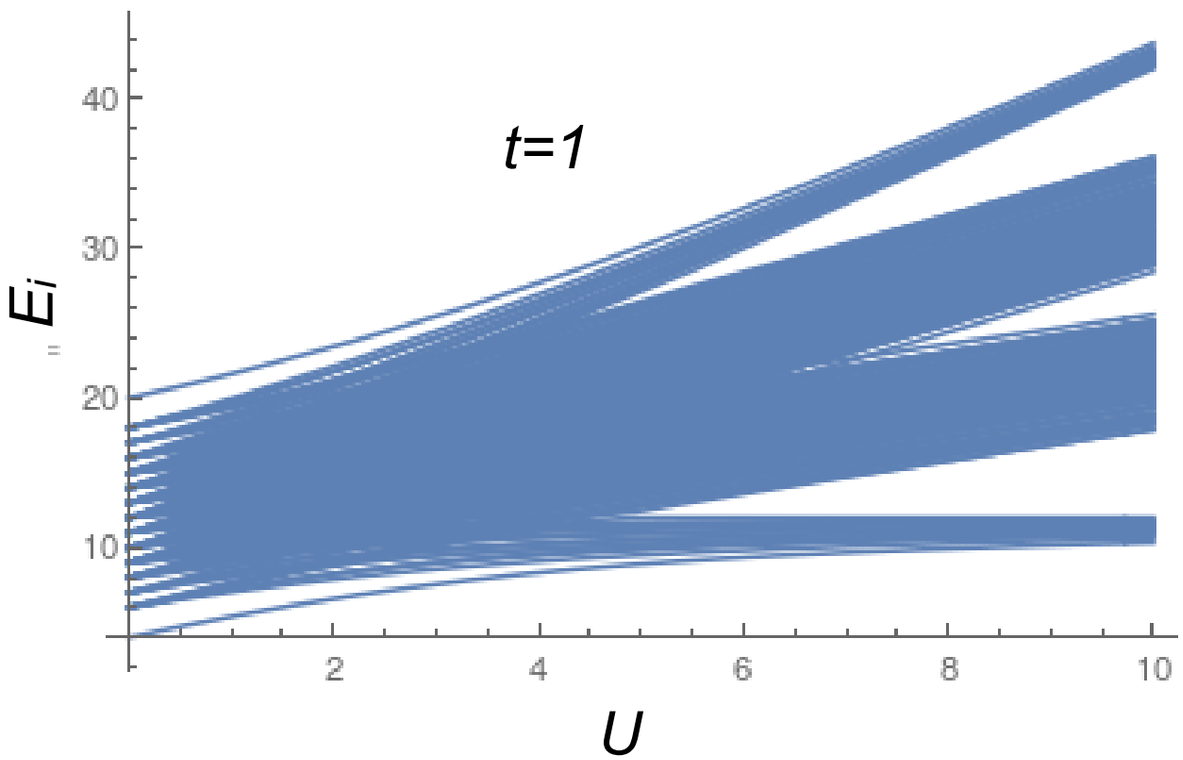
$$c_j |c^{\dagger} \ldots c^{\dagger} c^{\dagger}_j c^{\dagger} \ldots c^{\dagger} |\emptyset\rangle = (-1)^n c^{\dagger} \ldots c^{\dagger} c^{\dagger} \ldots c^{\dagger} |\emptyset\rangle$$

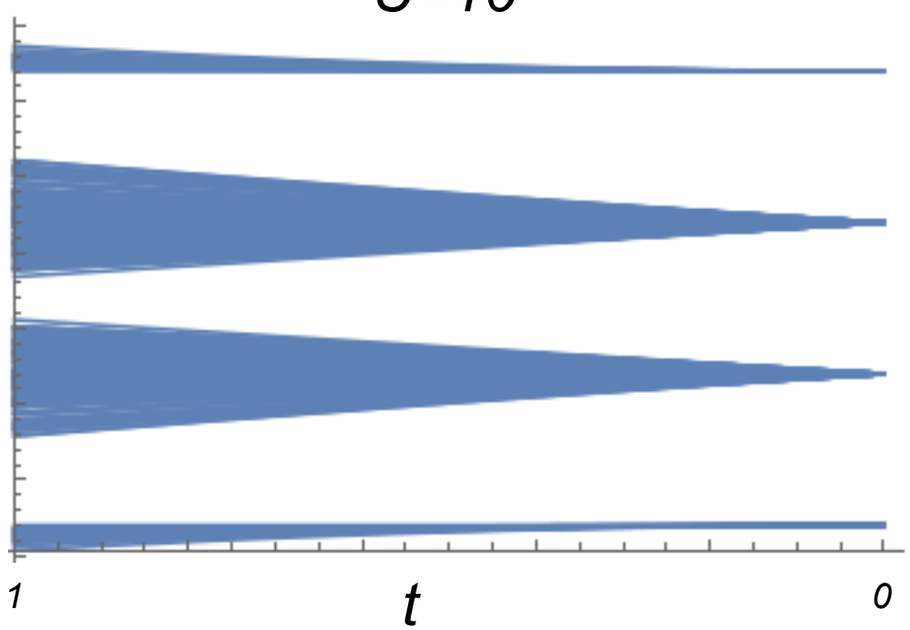


6-site Hubbard model

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

Spectrum of eigenenergies:
Sector (3,3)

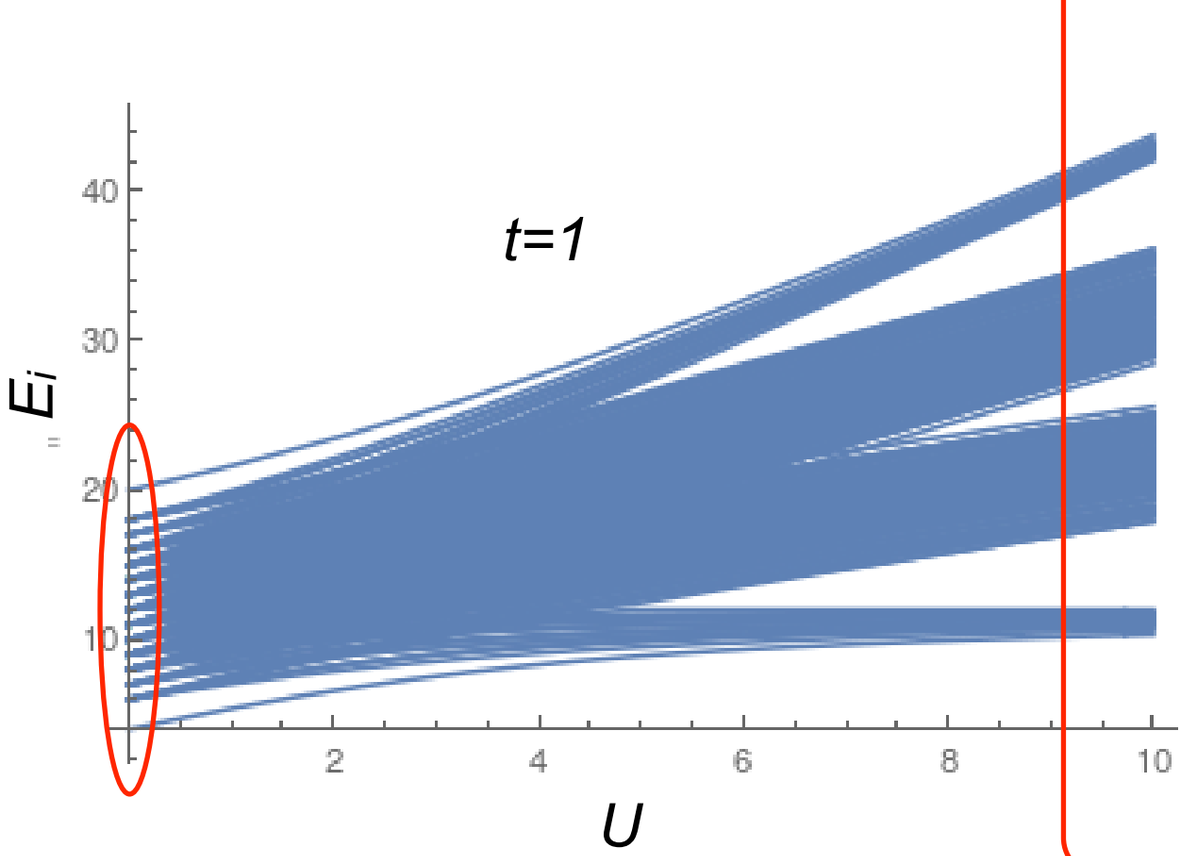




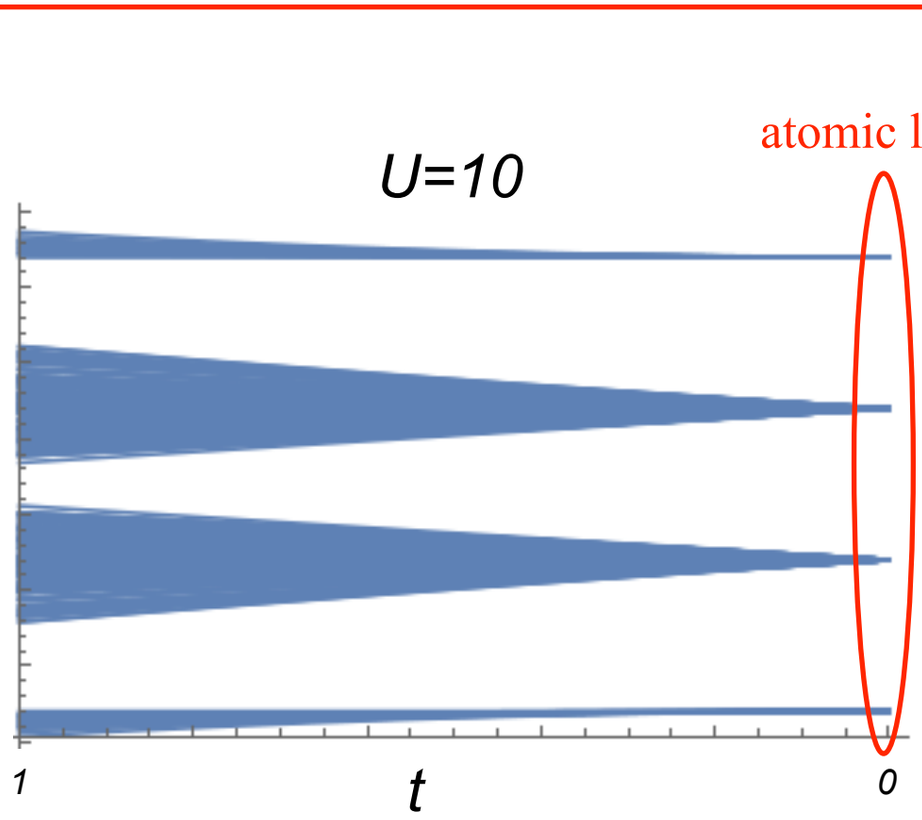
6-site Hubbard model

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

Spectrum of eigenenergies:
Sector (3,3)



Non-interacting limit
(weak-coupling expansion)



(strong-coupling expansion)

6-site Hubbard model

Non-interacting (canonical) bosons or fermions

=> We can find all eigenstates by diagonalizing the 1-p Hamiltonian (= hopping matrix)

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

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

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

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

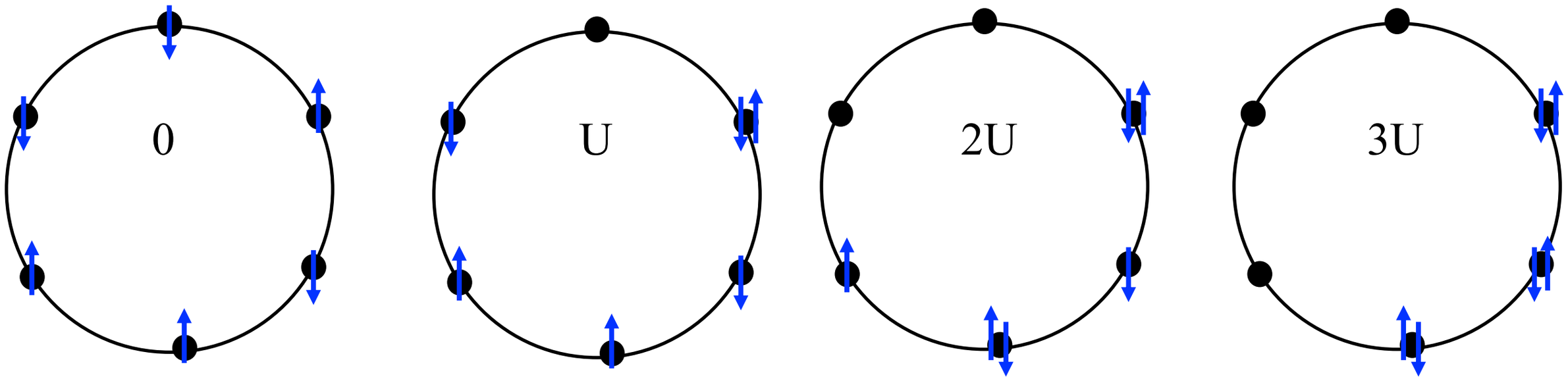
$$H|\phi\rangle = \left(\sum_{k=1}^{N} \epsilon_{i_k} \right) |\phi\rangle$$

Canonical commutation relations!

6-site Hubbard model

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

Large U >> t limit:
Sector (3,3)



Degeneracy:

$\binom{6}{3} = 20$

$6 \cdot 5 \cdot \binom{4}{2} = \cancel{120}$ 180

$\binom{6}{2} \cdot \binom{4}{2} \cdot 2 = \cancel{120}$ 180

$\binom{6}{3} = 20$

6-site Hubbard model

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

Expectation values/correlation functions:

$|\psi_g\rangle = \sum_l a_l |l\rangle$

Simple form for operator diagonal in a given basis

$$\langle S_{iz} \rangle = \langle \psi_g | S_{iz} | \psi_g \rangle = \sum_l \langle l | S_{iz} | l \rangle |a_l|^2$$

The average value one gets when many measurement on site i are performed. Possible result of each individual measurement is 0, 1 and -1.

At half filling (N=6)

$$\langle S_{iz} \rangle = 0 \qquad \langle n_{i\uparrow} \rangle = \frac{1}{2}$$

Fluctuations of S_z

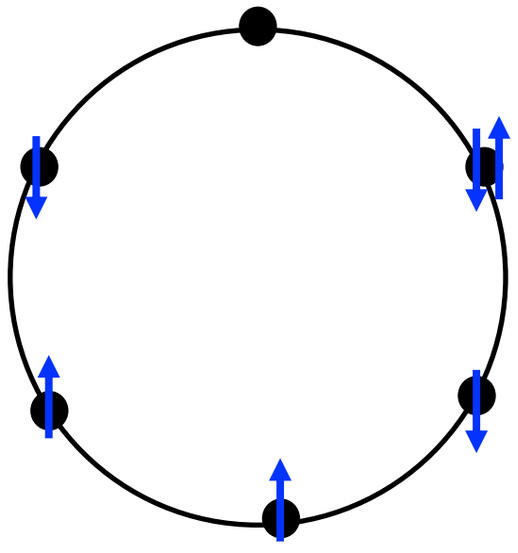
$$\langle S_{iz}^2 \rangle - \langle S_{iz} \rangle^2 \neq 0$$

Total moment (occupation number):

$S_z = \sum_i S_{iz}$

$$\langle S_z \rangle = 0 \qquad \langle (\delta S_z)^2 \rangle \equiv \langle (S_z - \langle S_z \rangle)^2 \rangle = 0$$

$$\langle N \rangle = 6 \qquad \langle (\delta N)^2 \rangle \equiv \langle (N - \langle N \rangle)^2 \rangle = 0$$



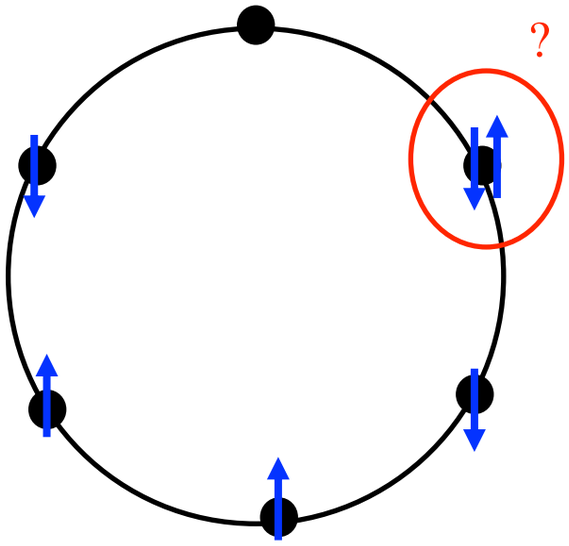
Conserved quantities (corresponding operators commute with Hamiltonian)

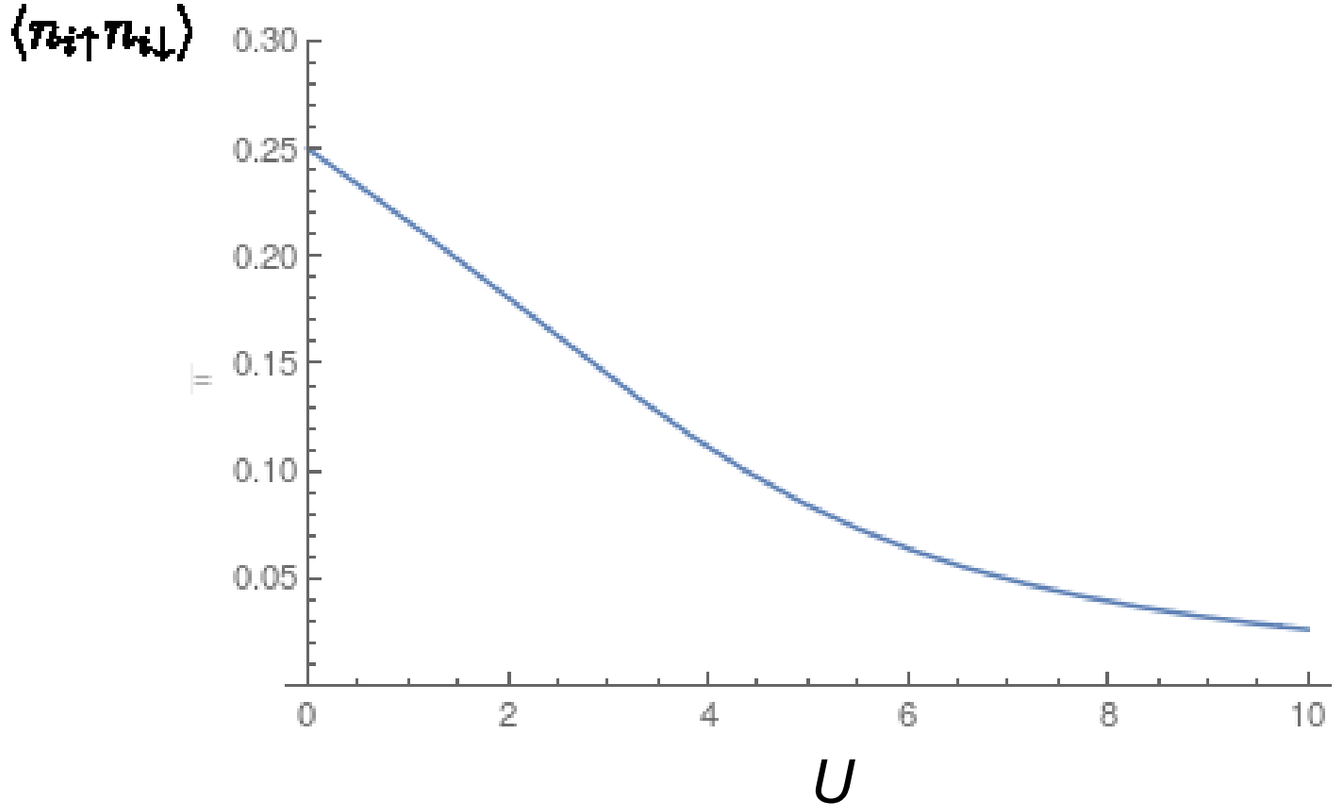
6-site Hubbard model

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

Expectation values/correlation functions:

Double occupancy: (probability to find two electrons in a given site) $\langle n_{i\uparrow} n_{i\downarrow} \rangle$



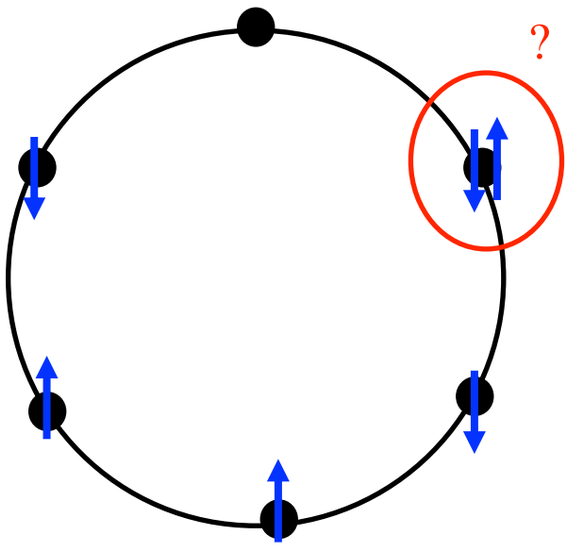


6-site Hubbard model

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

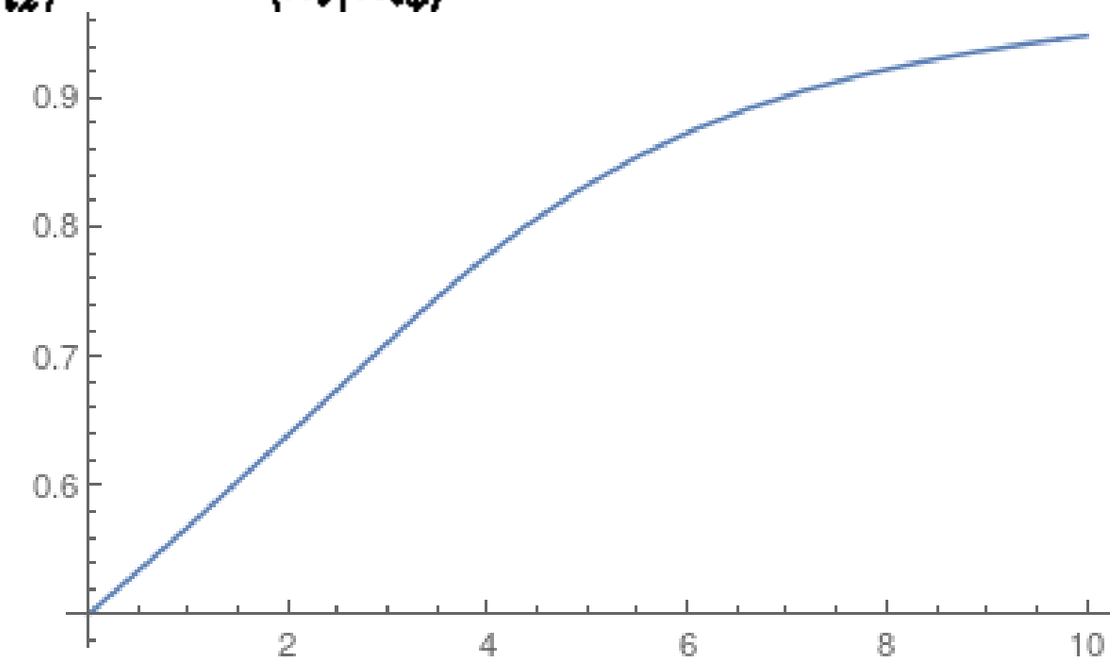
Expectation values/correlation functions:

(Fluctuating) local moment



$$\langle n_{i\uparrow} \rangle = \frac{1}{2}$$

$$\langle S^2_{iz} \rangle = 1 - 2\langle n_{i\uparrow} n_{i\downarrow} \rangle$$



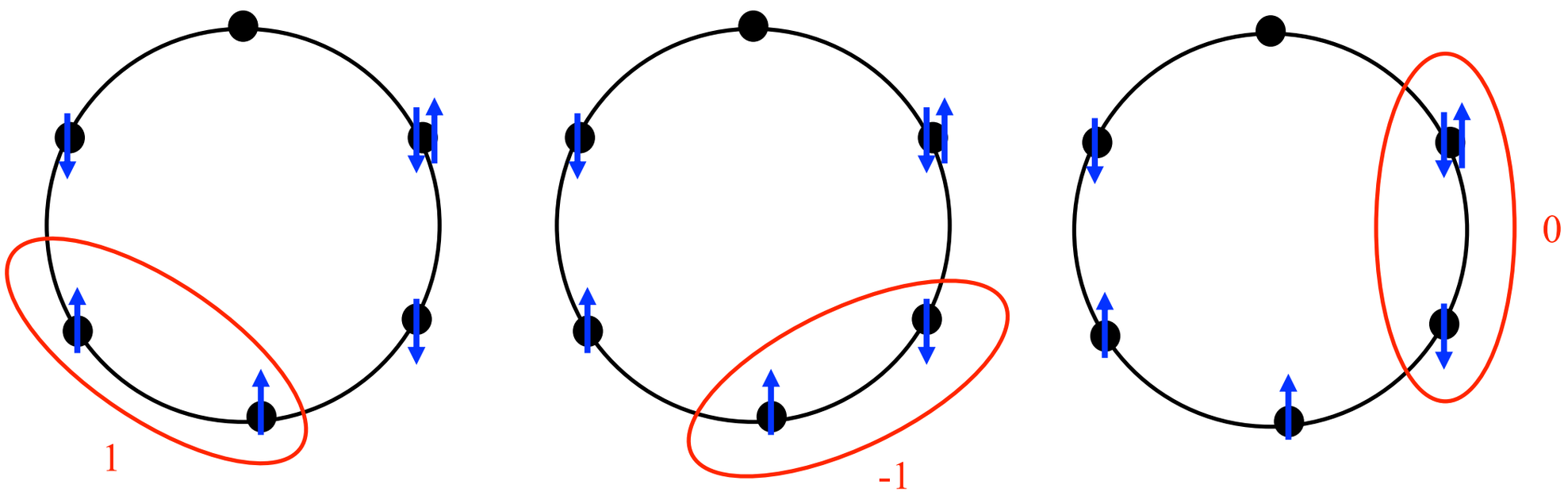
6-site Hubbard model

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

Expectation values/correlation functions:

Non-local spin-spin correlation function $\langle S_{iz} S_{jz} \rangle$

Weighted sum over configurations like

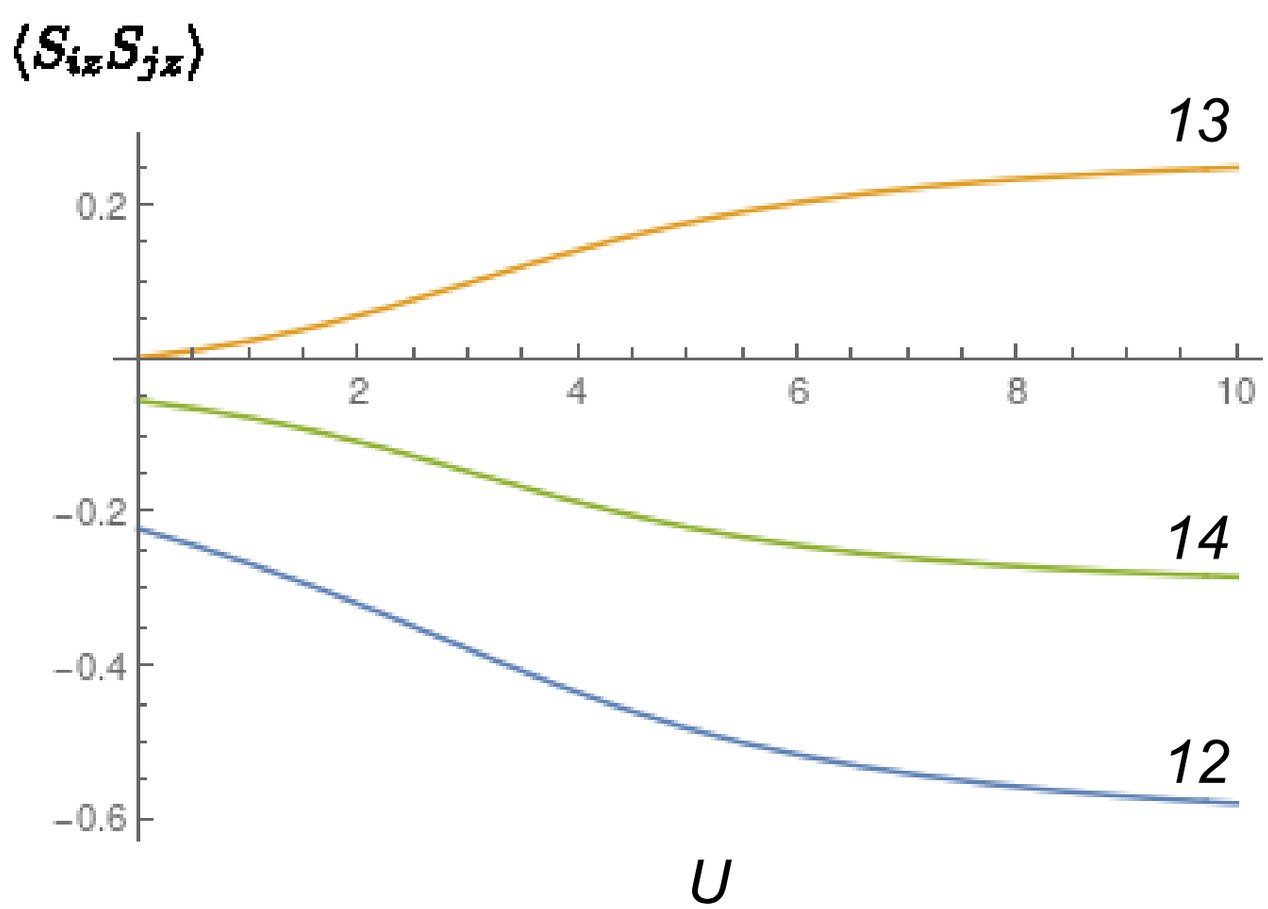


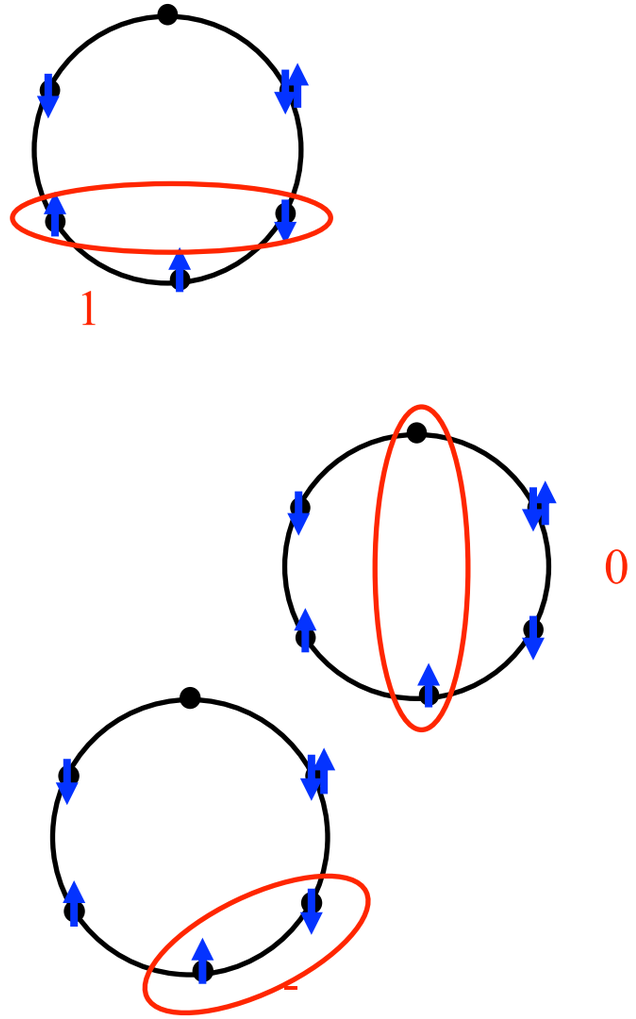
Which one has the largest weight?

6-site Hubbard model

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

Expectation values/correlation functions:



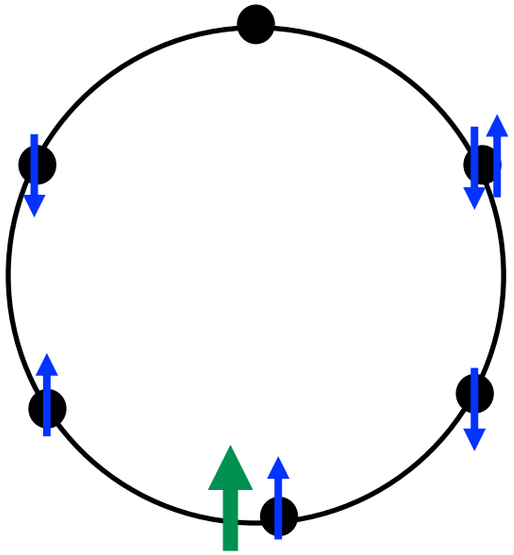


6-site Hubbard model

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

Why correlation functions?

- Contributions to interaction energy of the system $\langle n_{i\uparrow} n_{i\downarrow} \rangle$
- Response to small perturbations

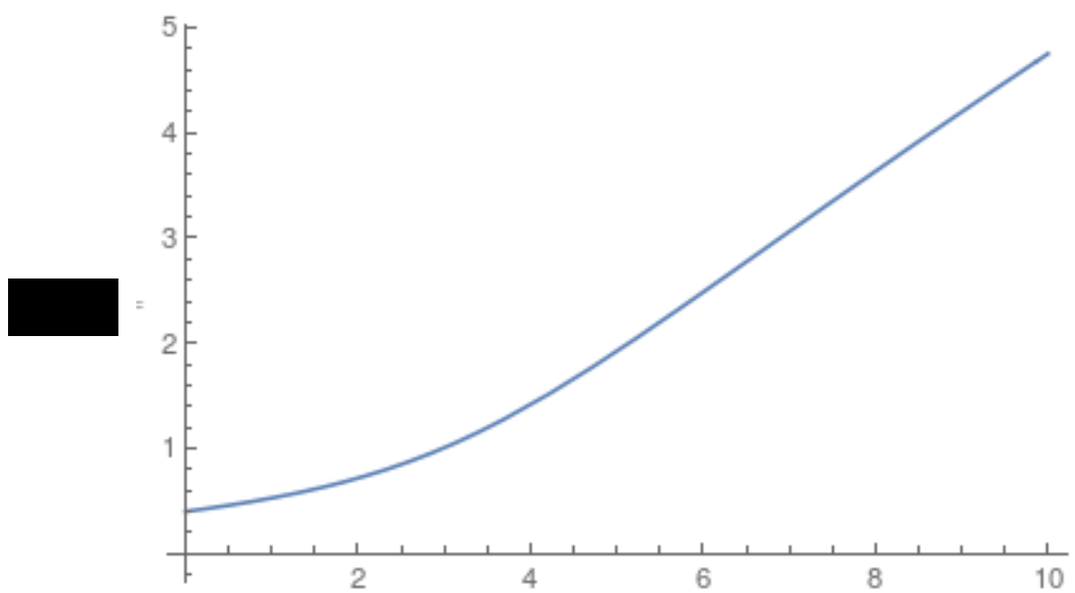


external local field

$$\delta\langle S_{iz} \rangle = \chi_{\mathrm{loc}} \cdot \delta h$$

$$\chi_{\mathrm{loc}} = 2 \sum_{n>g} \frac{|\langle \psi_n | S_{iz} | \psi_g \rangle|^2}{E_n - E_g}$$

Correction: Factor 2 missing in the recorded presentation

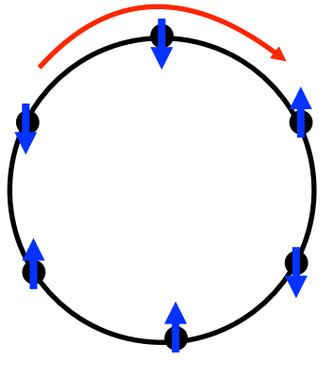


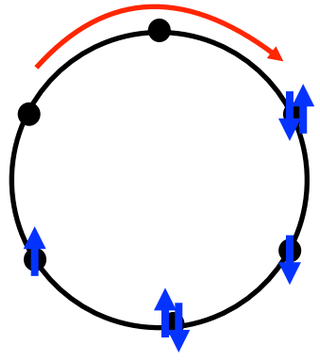
6-site Hubbard model

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

What about symmetry?

- We have used conservation of N and S_z when constructing the basis
- We did not use translation symmetry





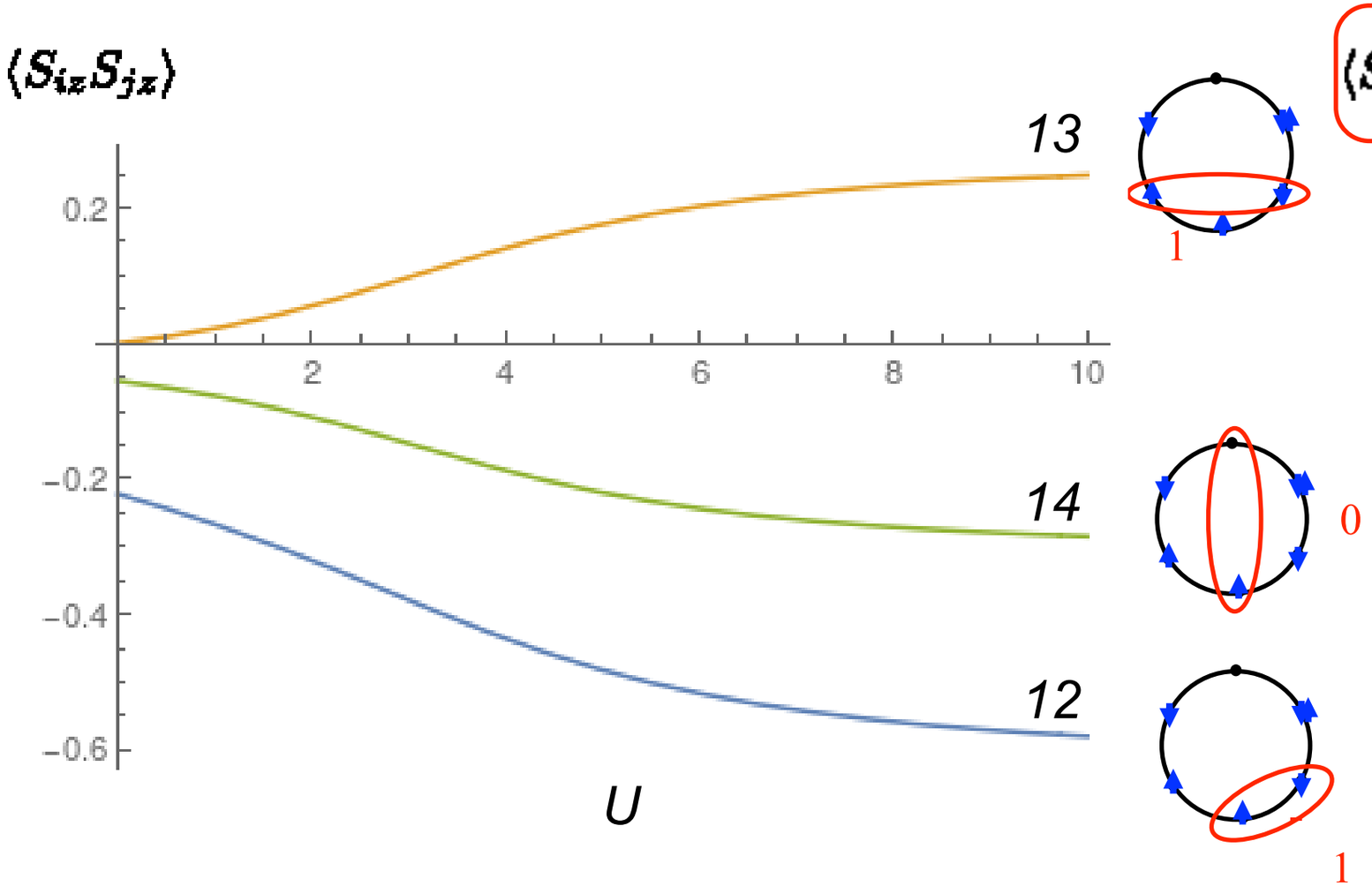
This would require a bit more 'brain' input

6-site Hubbard model

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

Translation symmetry is reflected in the correlation functions: $S_z(\mathbf{k}) = \sum_{k} e^{i\mathbf{k}\cdot\mathbf{R}} S_{\mathbf{R}z}$

$\langle S_z(\mathbf{k}) S_z(\mathbf{k}') \rangle \equiv \langle \psi_g | S_z(\mathbf{k}) S_z(\mathbf{k}') | \psi_g \rangle = ?$



1

0

1

6-site Hubbard model

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

Translation symmetry is reflected in the correlation functions:

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

$$\langle S_z(\mathbf{k}) S_z(\mathbf{k}') \rangle \equiv \langle \psi_g | S_z(\mathbf{k}) S_z(\mathbf{k}') | \psi_g \rangle = ?$$

invariant

~~*invariant: (k''=0)*~~

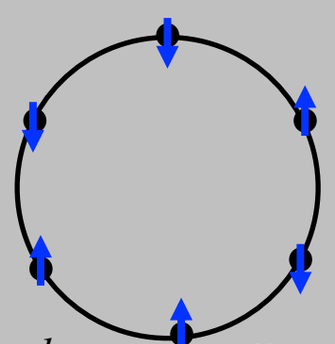
$k+k'+(k''-k'')=0 \ (\mathrm{mod}\ 2\ )$

=> $\langle S_z(\mathbf{k}) S_z(-\mathbf{k}') \rangle = \delta_{\mathbf{k}\mathbf{k}'}$

Correction:

k''=

The ground state is dominated by the states of the type



The ground state phase does not matter as pointed out correctly.

6-site Hubbard model

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Translation symmetry is reflected in the correlation functions: $S_z(\mathbf{k}) = \sum_{k} e^{i\mathbf{k}\cdot\mathbf{R}} S_{\mathbf{R}z}$