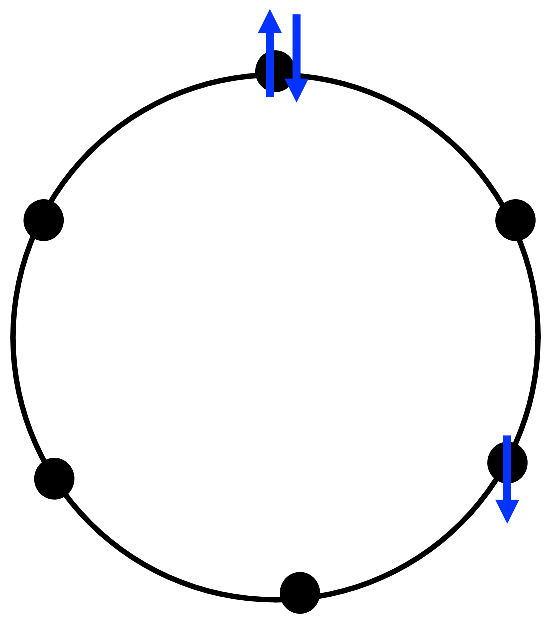
# 6-site Hubbard model

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

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)

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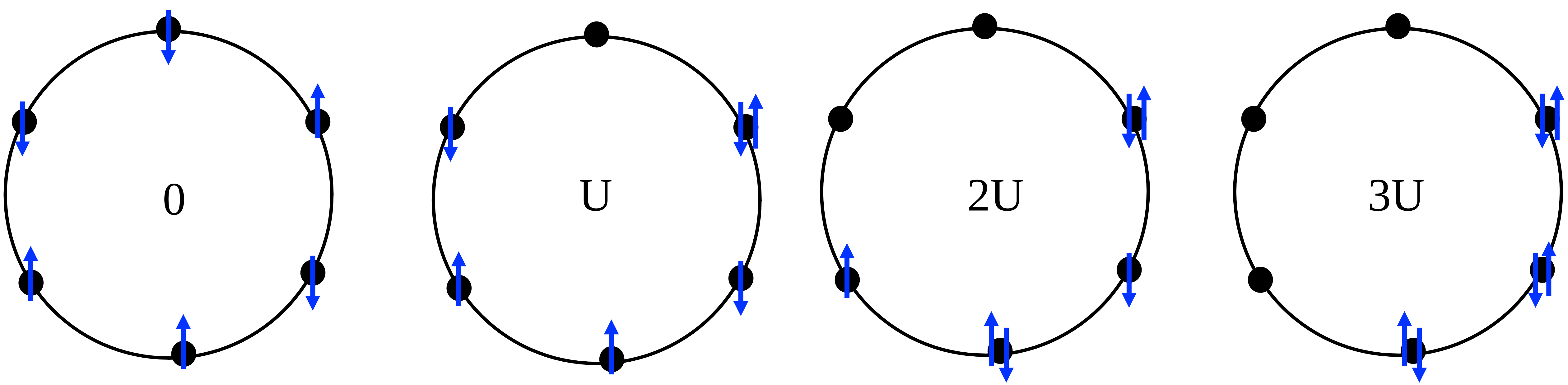
$$H = t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

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




implementation of $\sum_i n_{i\uparrow} n_{i\downarrow}$

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

implementation of $S_{iz}$

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

i=2

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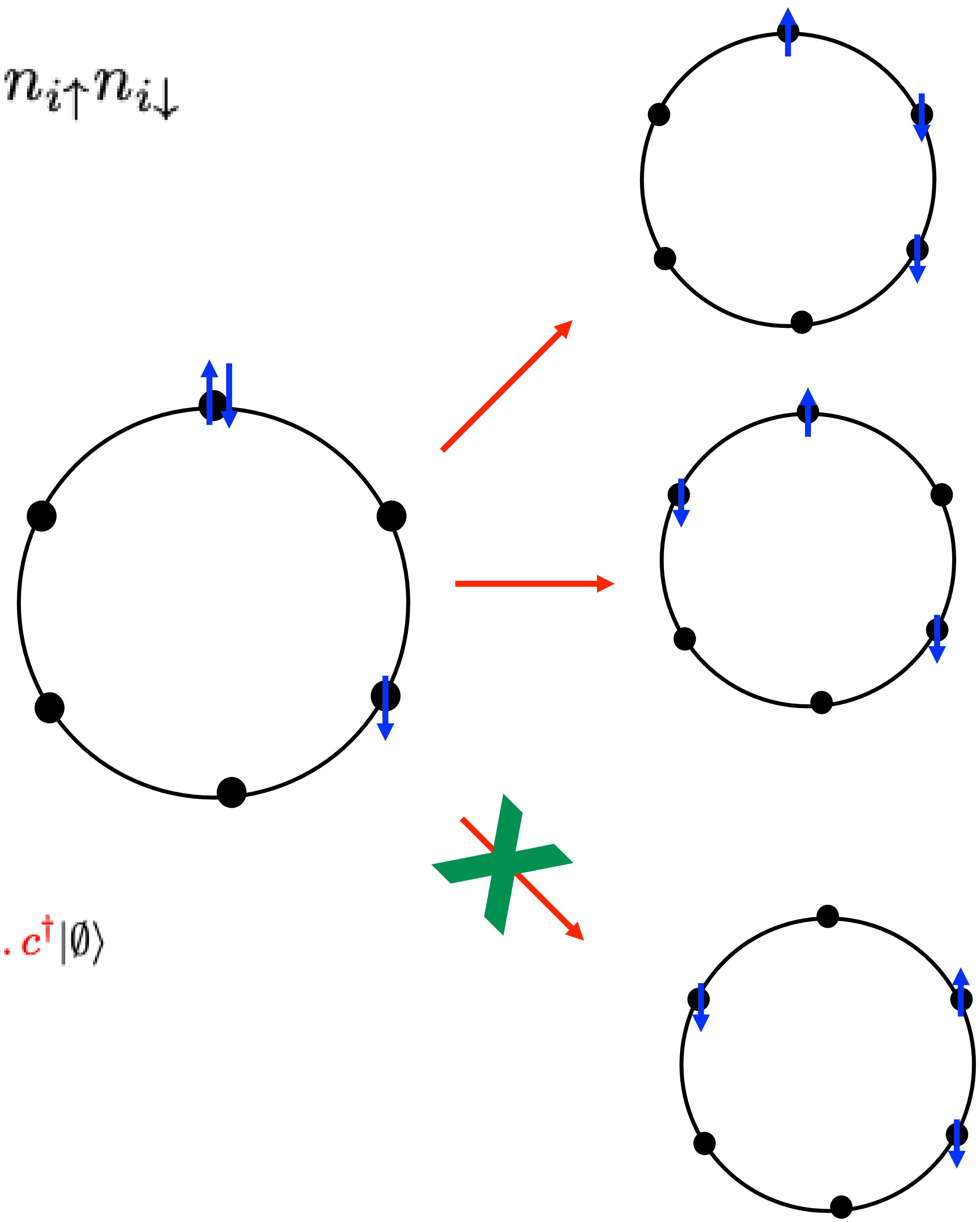
$$H = t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

**Matrix elements** of the hopping part:

in binary code (10100|100000)

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

✓ (11000|000000)



**Signs**:

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

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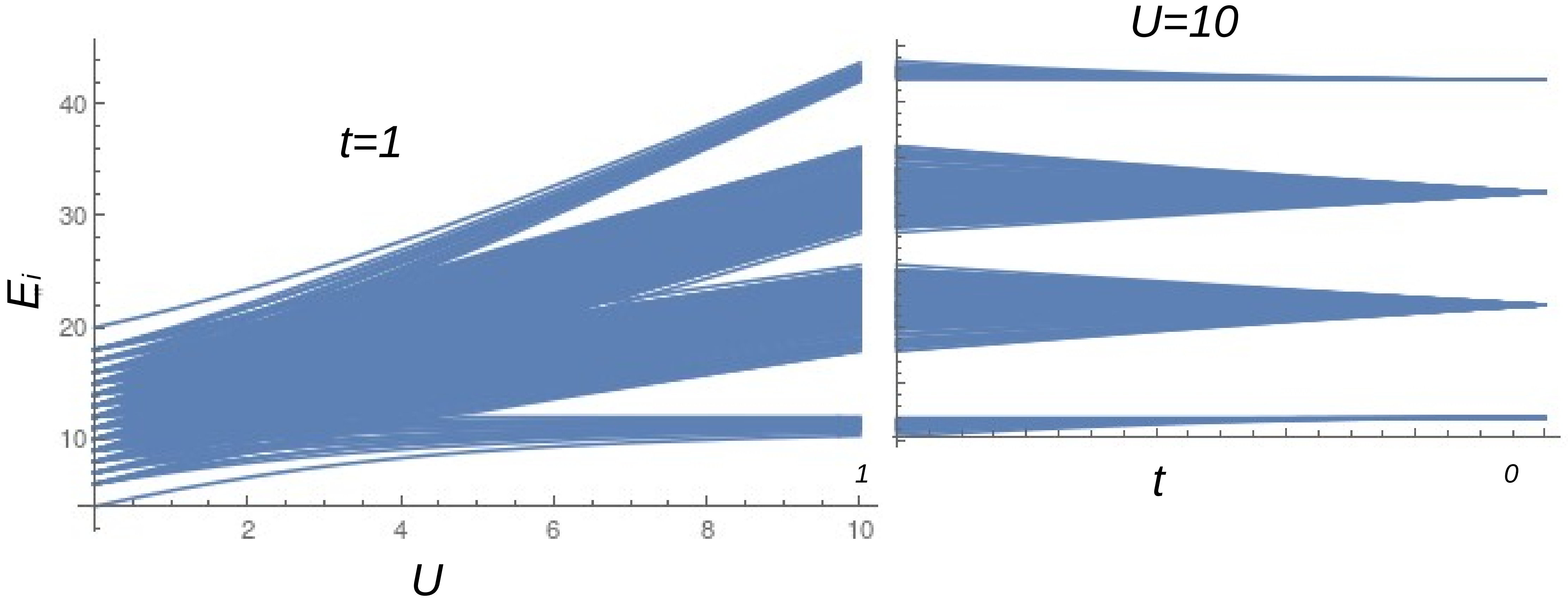
$$H = t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

**Spectrum** of eigenenergies:

Sector (3,3)



# 6-site Hubbard model

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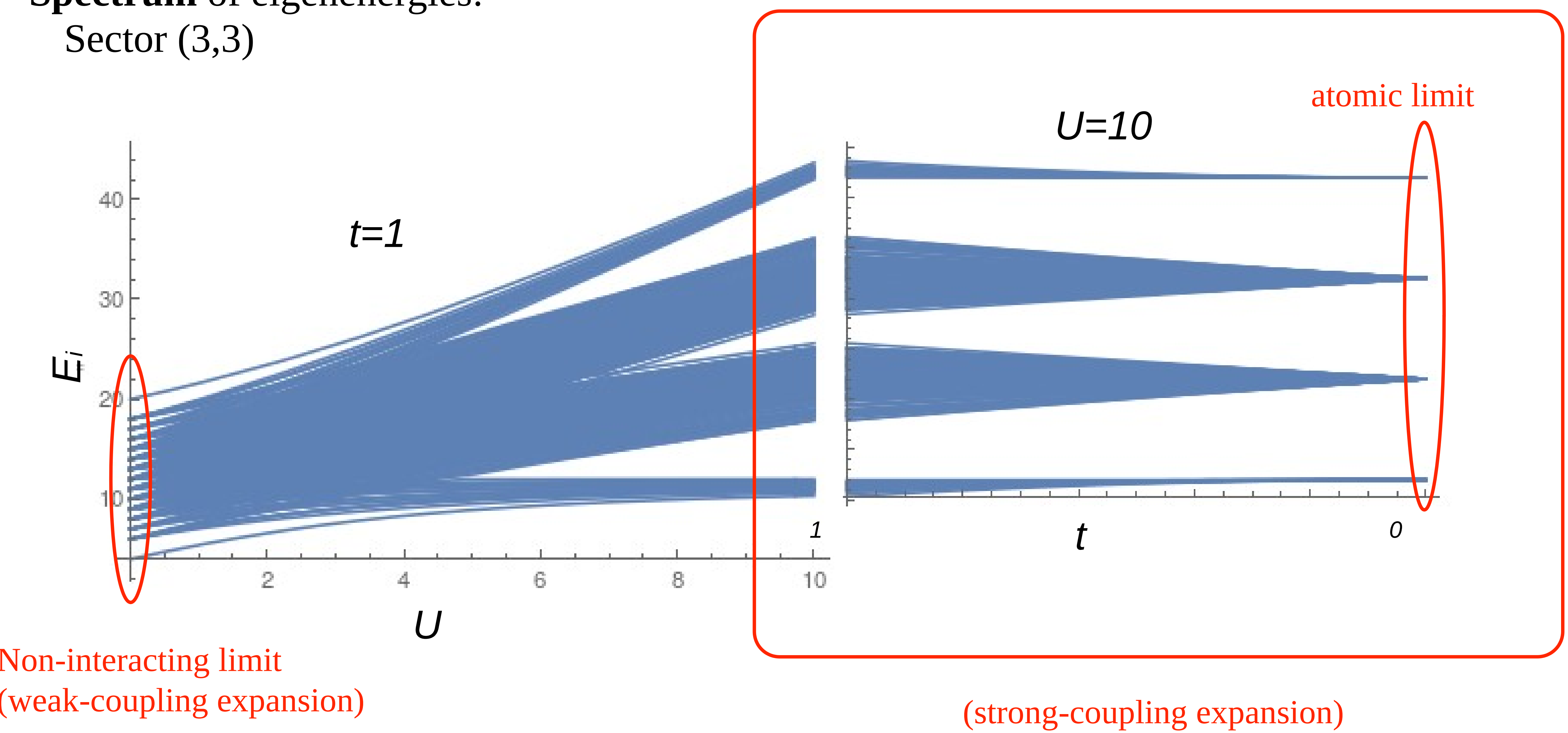


# 6-site Hubbard model

**Non-interacting** (canonical) bosons or fermions

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

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

$$c_b = U_{bi} c_i \,, \quad (c_b^\dagger = U_{bi}^* c_i^\dagger = U_{ib}^\dagger c_i^\dagger)$$

$$\{c_i\,, c_j^\dagger\} = U_{ia}^\dagger \{c_a, c_b^\dagger\} U_{bj} = U_{ia}^\dagger \delta_{ab} U_{bj} = \delta_{ij}$$

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

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

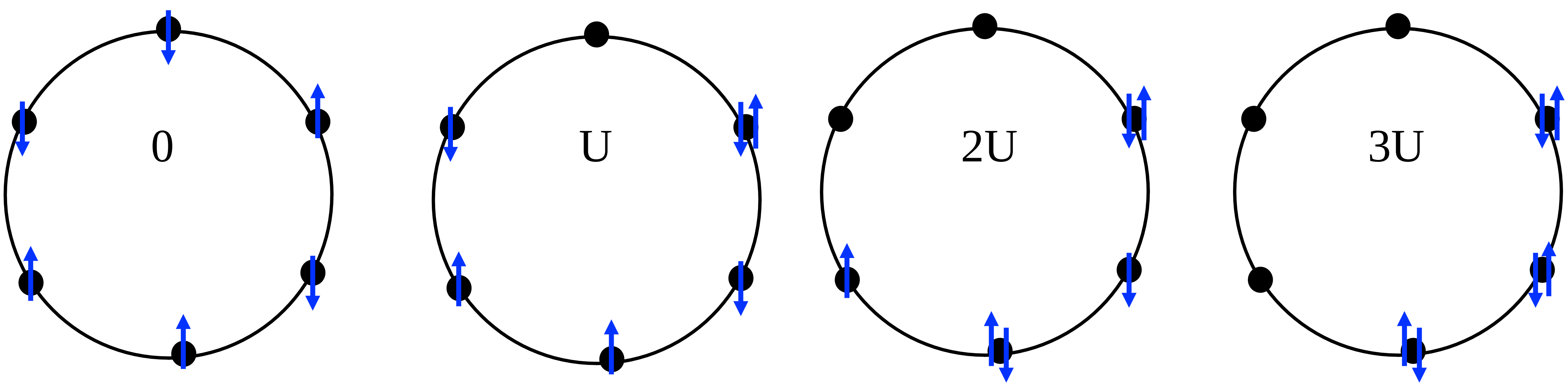
Canonical commutation relations!

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

# 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 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

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

**Expectation values/correlation functions:**

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

Simple form for operator diagonal in a given basis

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

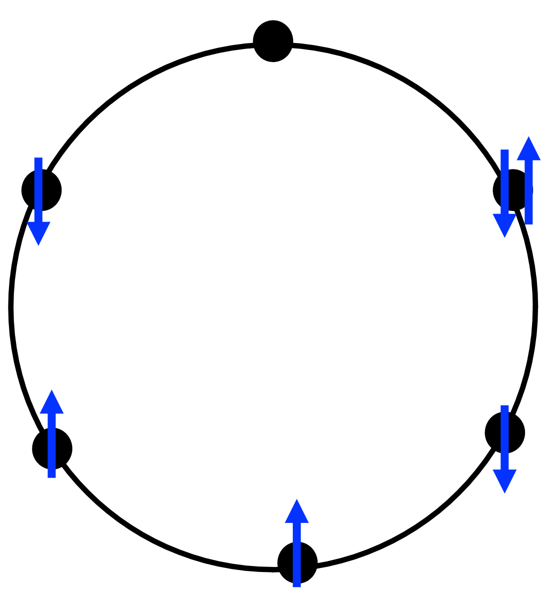
*The average value one gets when many measurement on site i are performed. Possible result of each individual measurement is 0, 1 and -1.*

*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):*

$$S_z \equiv \sum_i S_{iz}$$

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

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

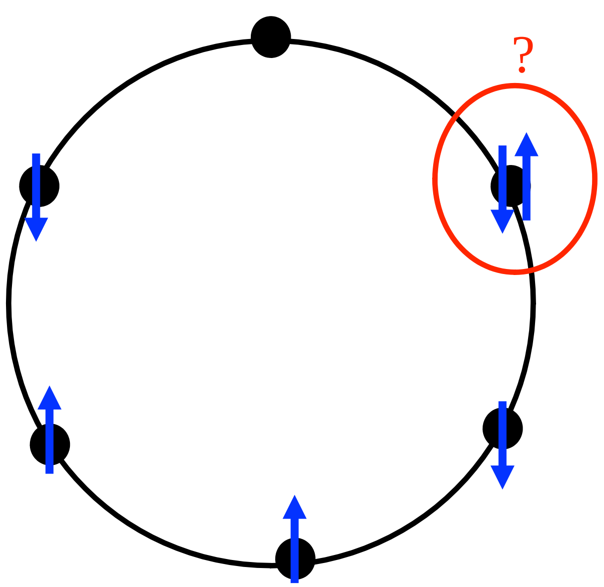
Conserved quantities (corresponding operators commute with Hamiltonian)

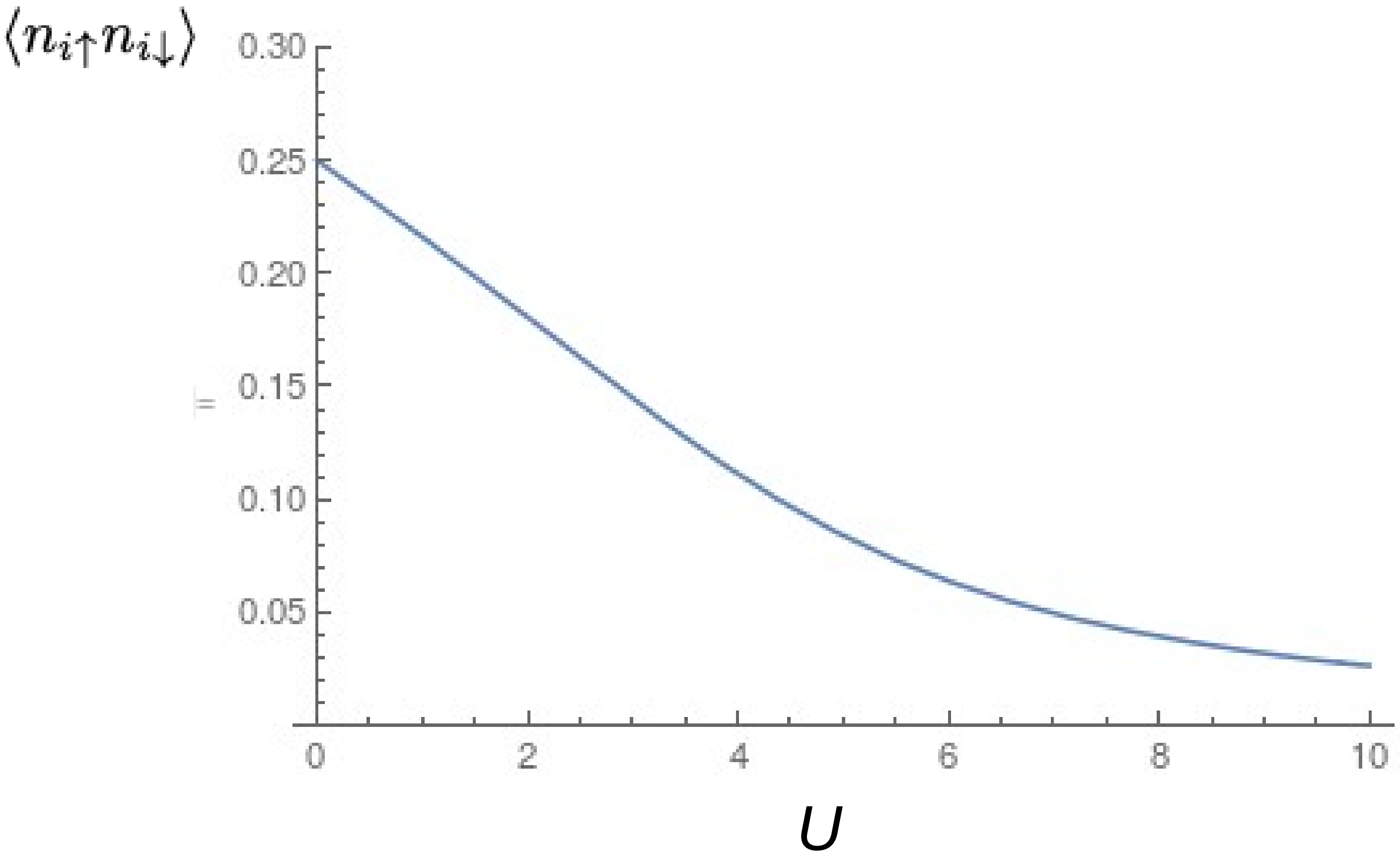
# 6-site Hubbard model

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

**Expectation values/correlation functions:**

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



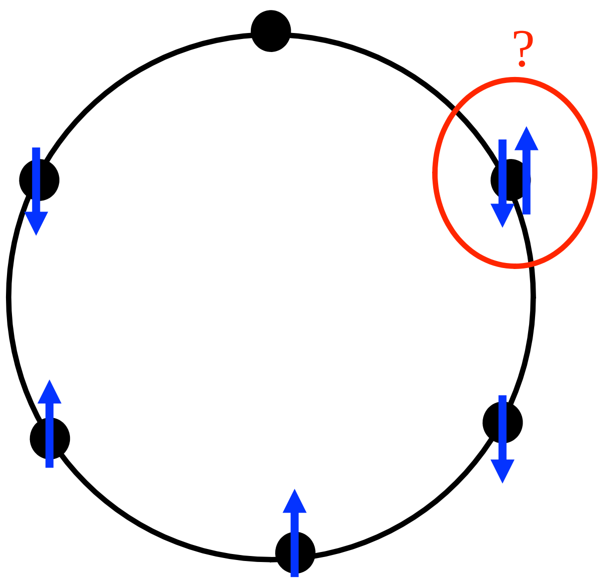



# 6-site Hubbard model

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

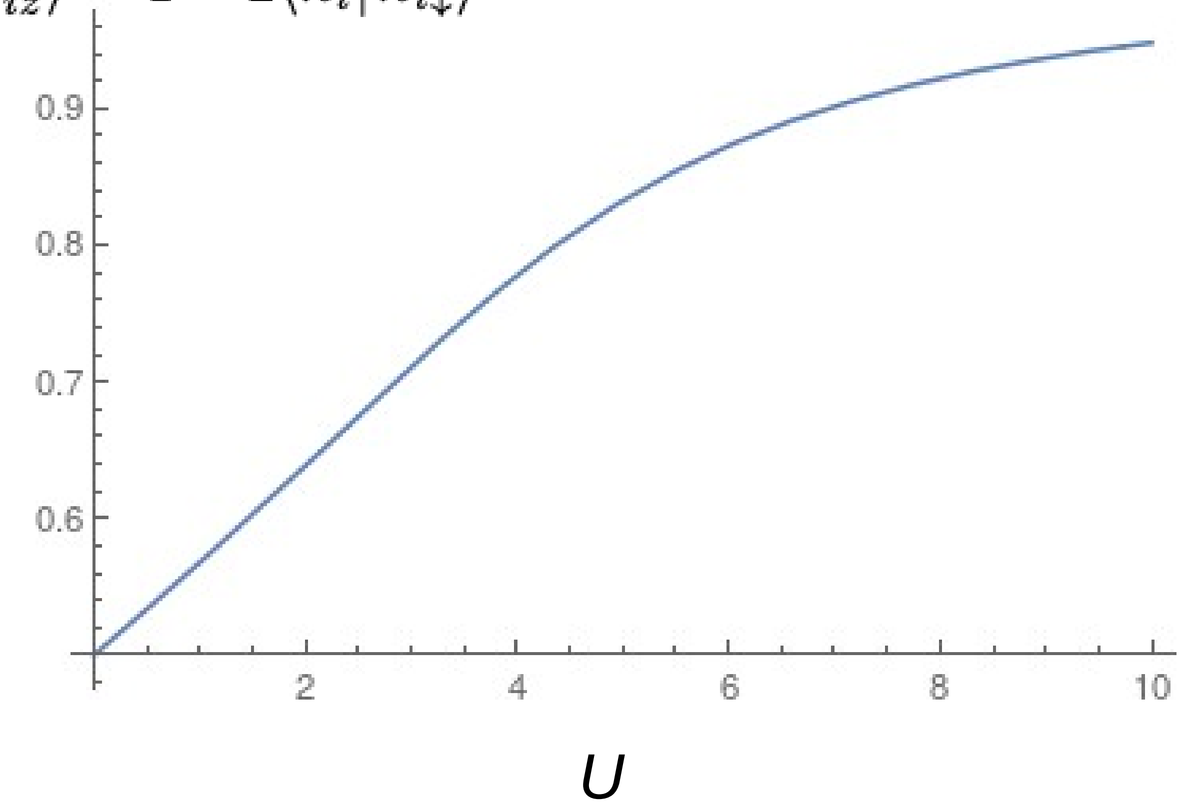
**Expectation values/correlation functions:**

*(Fluctuating) local moment*




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

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



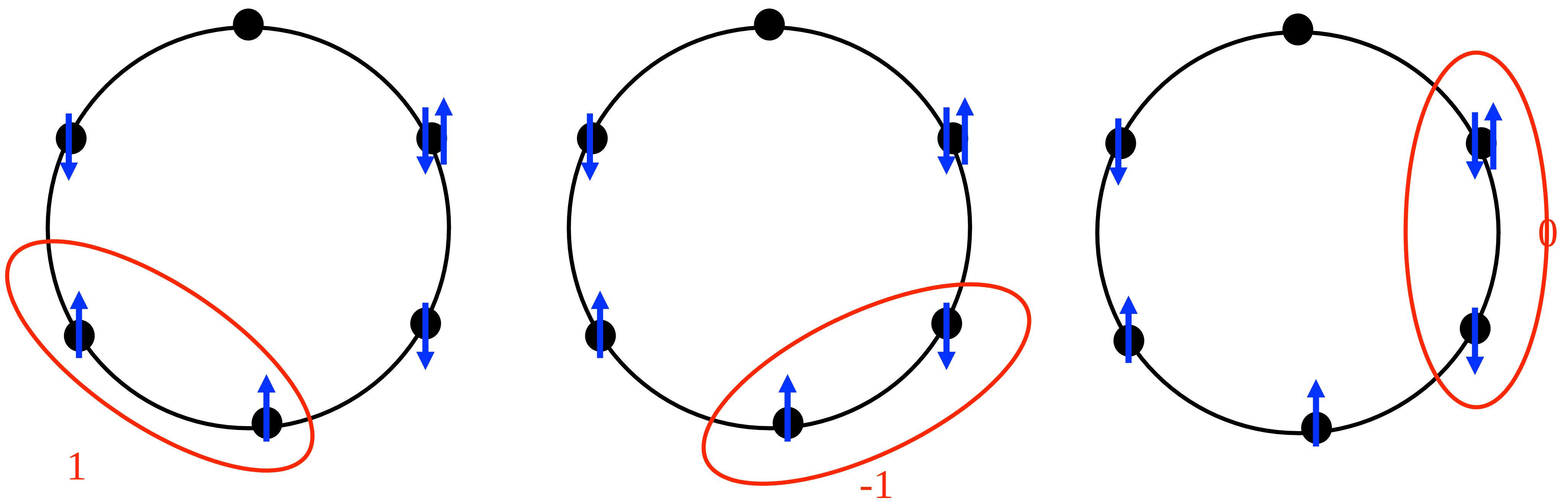
# 6-site Hubbard model

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

**Expectation values/correlation functions:**

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

*Weighted sum over configurations like*

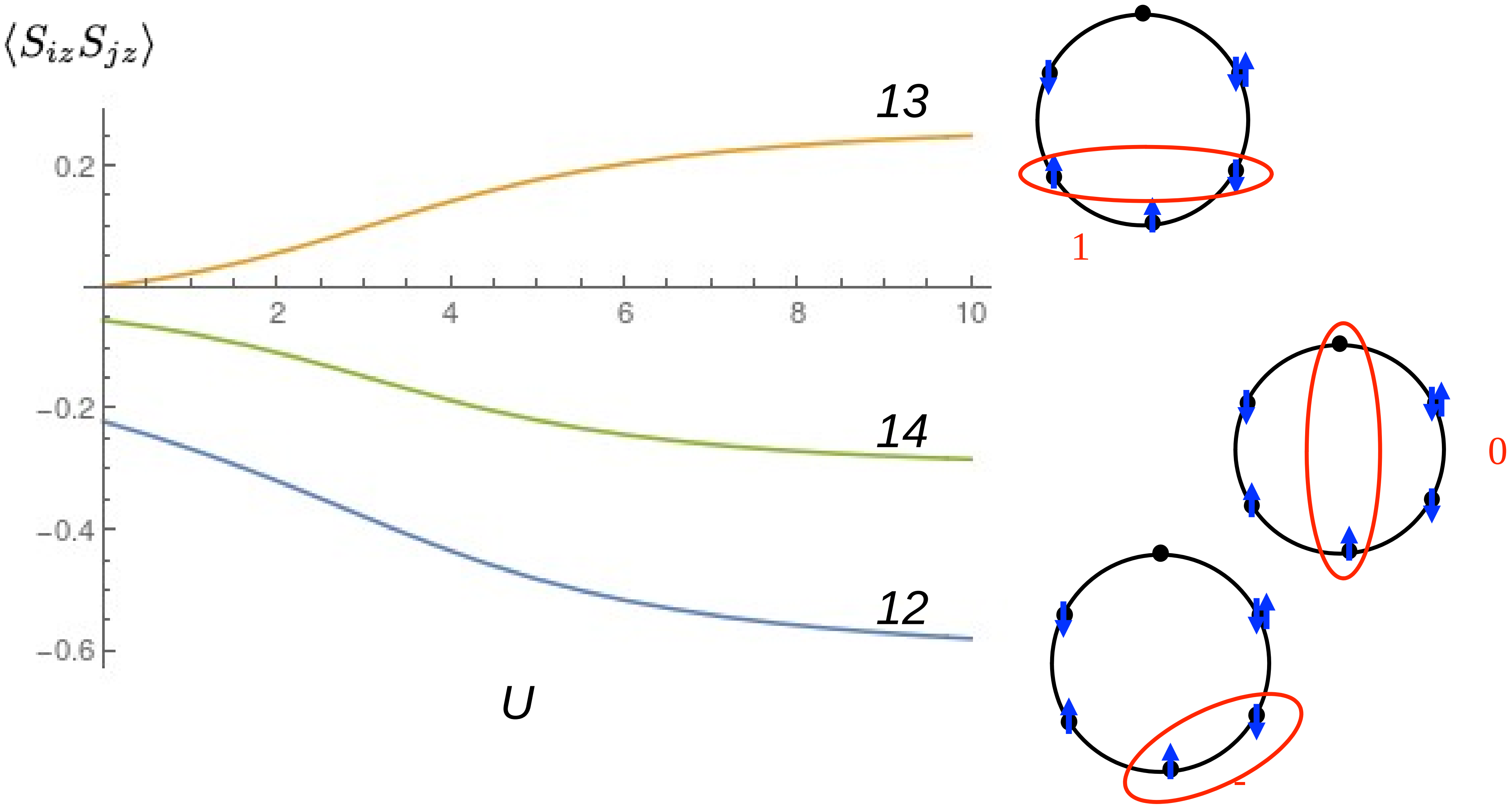



*Which one has the largest weight?*

# 6-site Hubbard model

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

**Expectation values/correlation functions:**

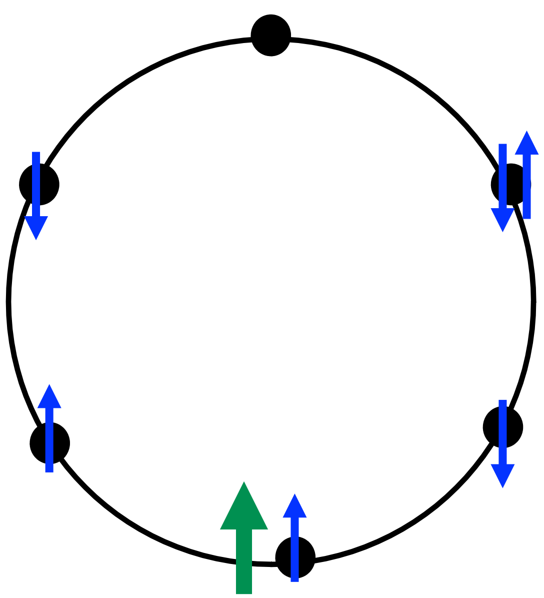


# 6-site Hubbard model

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

**Why correlation functions?**

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

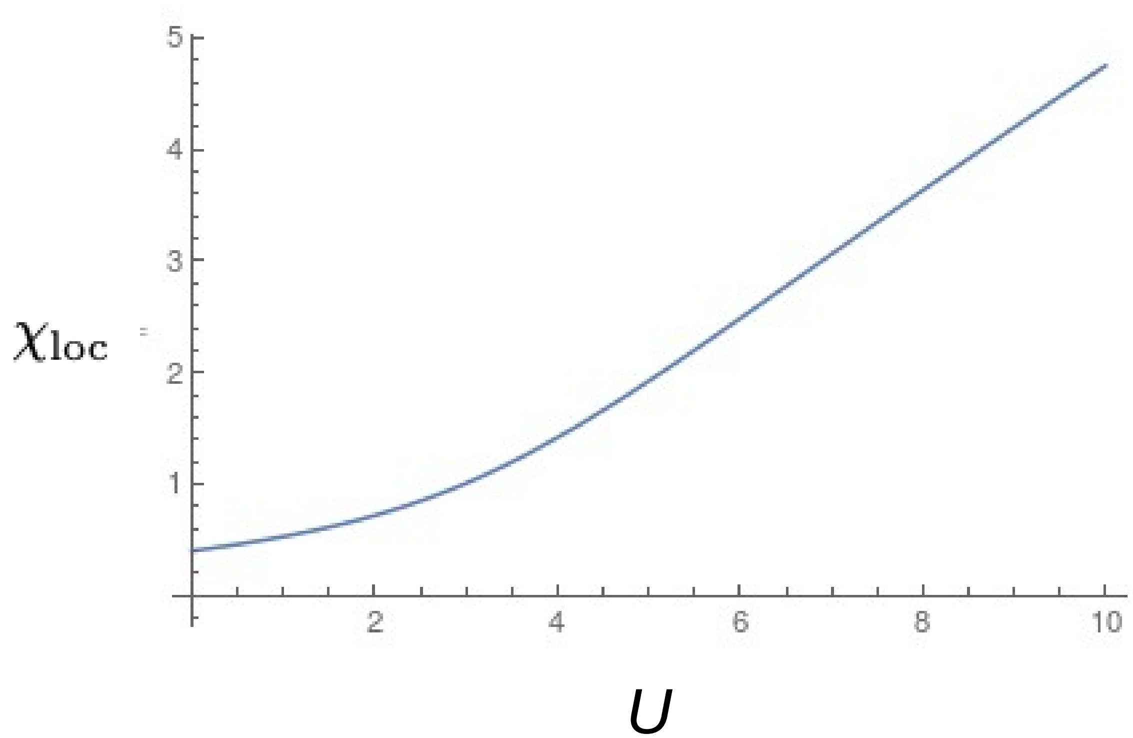


*external local field*

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

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

*Correction: Factor 2 missing in the recorded presentation*

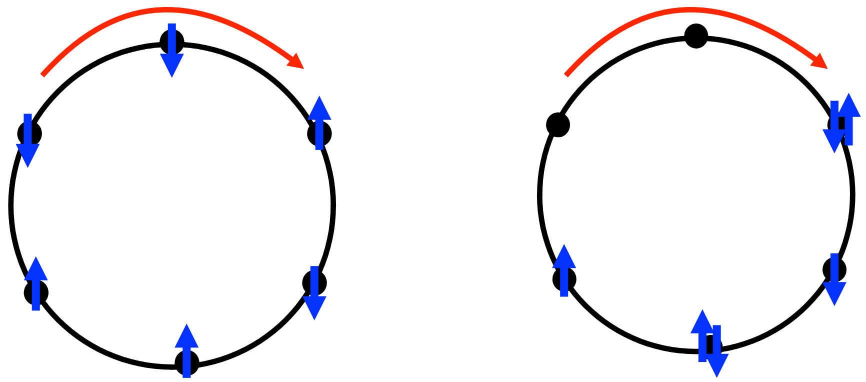


# 6-site Hubbard model

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

**What about symmetry?**

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



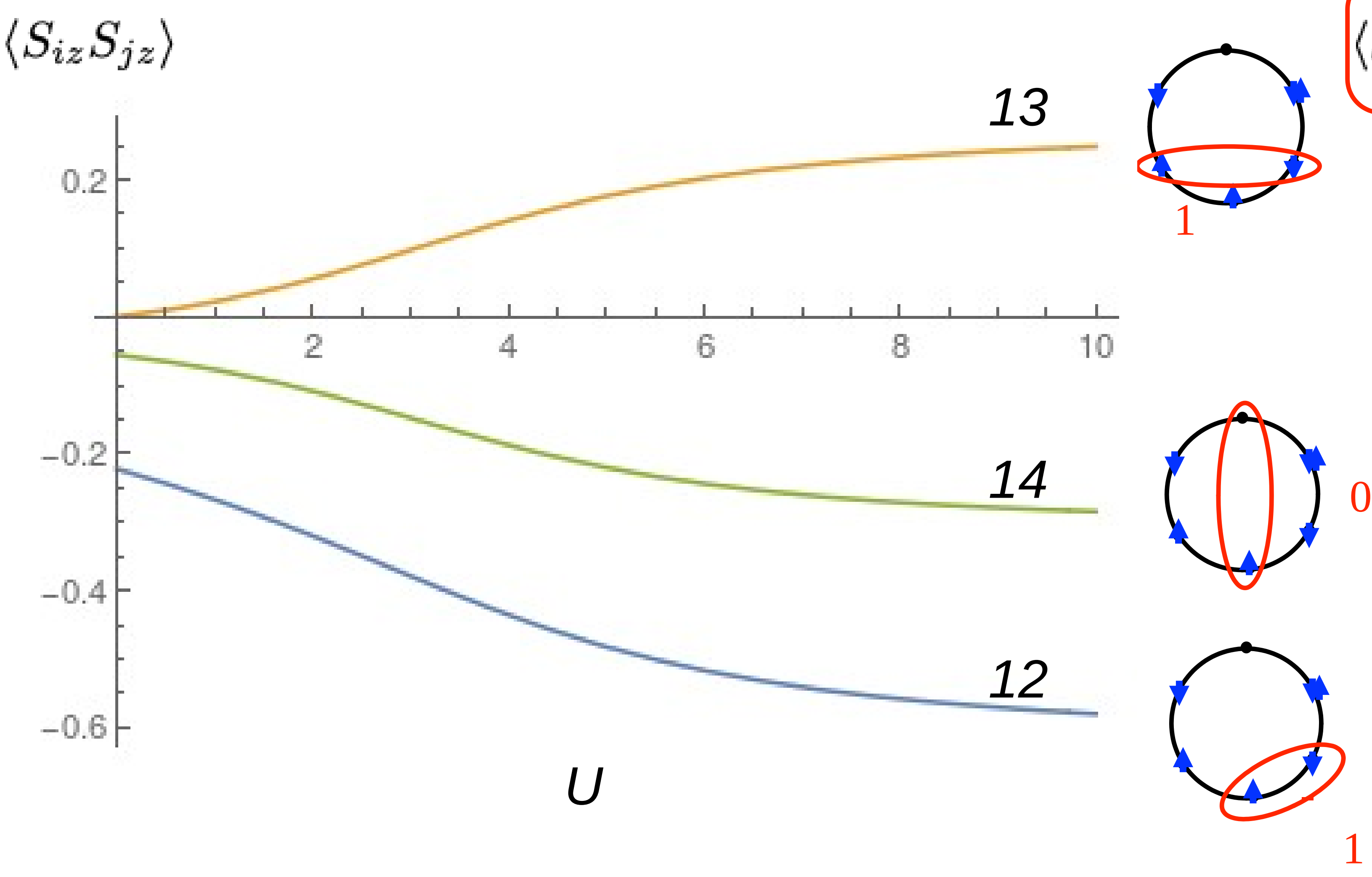
*This would require a bit more 'brain' input*

# 6-site Hubbard model

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

**Translation symmetry** is reflected in the correlation functions:

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




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

# 6-site Hubbard model

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$$\boxed{\langle S_z(\mathbf{k})S_z(\mathbf{k}')\rangle \equiv \langle\psi_g|\underbrace{S_z(\mathbf{k})S_z(\mathbf{k}')}_{\textit{invariant}}|\psi_g\rangle = ?}$$

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

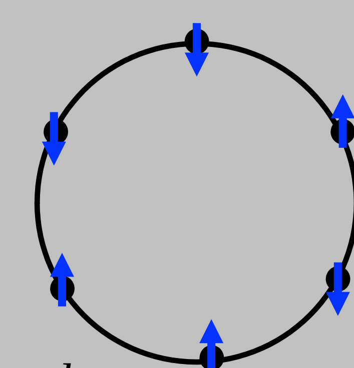
*k+k'+(k''-k'')=0 (mod 2*$\boldsymbol{\pi}$*)*

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

Correction:

*k''=*$\boldsymbol{\pi}$

*The ground state is dominated by the states of the type*



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

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