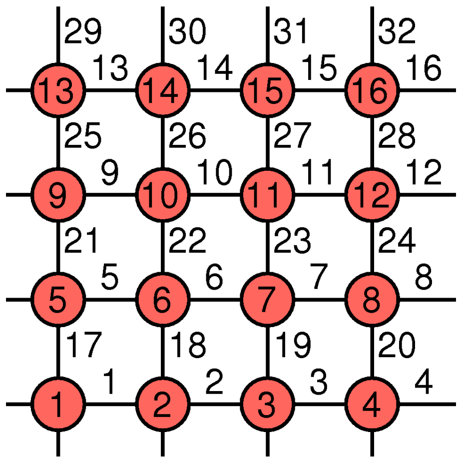
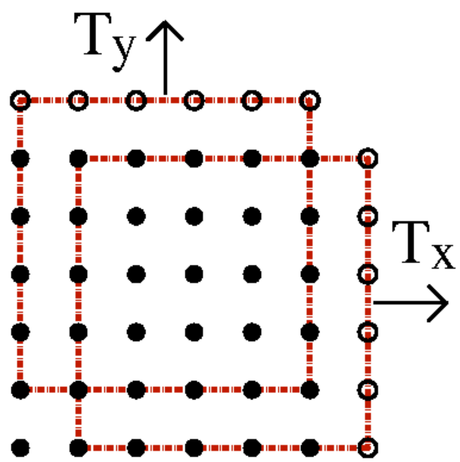
Exact diagonalization of 2D systems (simple square lattice)

Label lattice sites and bonds

- hamiltonian construction very similar to 1D chains using site and bond maps





2D momentum states ($L_x \times L_y$ lattice)

$$|a(\mathbf{k})\rangle = |a(k_x, k_y)\rangle = \frac{1}{\sqrt{N_a}} \sum_{x=1}^{L_x} \sum_{y=1}^{L_y} \mathrm{e}^{-i(k_x x + k_y y)} T_y^y T_x^x |a\rangle$$

$$k_\gamma = \frac{2\pi}{L_\gamma} m_\gamma, \quad m_\gamma = 0, 1, \ldots, L_\gamma - 1, \quad \gamma = x, y$$

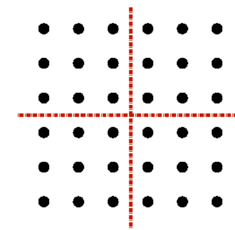
In this case it is very difficult to construct a real-valued basis

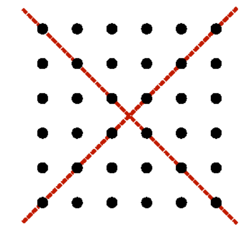
- use complex momentum states
- reflection (and/or rotation) symmetries can be used for special momenta

Using reflection symmetries (L×L lattice)

There are 8 different transformations of a square

- combination of reflections and rotations
- can choose the most convenient operations





$$\begin{pmatrix} 4 & 3 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 3 & 2 \\ 4 & 1 \end{pmatrix}\begin{pmatrix} 2 & 1 \\ 3 & 4 \end{pmatrix}\begin{pmatrix} 1 & 4 \\ 2 & 3 \end{pmatrix}$$

$$\begin{pmatrix} 3 & 4 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} 2 & 3 \\ 1 & 4 \end{pmatrix}\begin{pmatrix} 1 & 2 \\ 4 & 3 \end{pmatrix}\begin{pmatrix} 4 & 1 \\ 3 & 2 \end{pmatrix}$$

General form of the momentum state with other symmetries

$$|a^\sigma(\mathbf{k},\{q\})\rangle = \frac{1}{\sqrt{N_a}} \sum_{r_x=1}^{L_x} \sum_{r_x=1}^{L_x} \mathrm{e}^{-i(k_x x + k_y y)} T_y^{r_y} T_x^{r_x} Q |a\rangle$$

Using three reflections; P_x, P_y, P_d

$$Q = \begin{cases} 1, & \text{general } \mathbf{k} \\ (1 + p_x P_x), & \mathbf{k} = (0, k_y), (\pi, k_y) \\ (1 + p_y P_y), & \mathbf{k} = (k_x, 0), (k_x, \pi) \\ (1 + p_e P_e)(1 + p_d P_d), & k_x = \pm k_y \\ (1 + p_d P_d)(1 + p_y P_y)(1 + p_x P_x), & \mathbf{k} = (0,0), (\pi,\pi), \ p_x = p_y \end{cases}$$

Lanczos results for the 2D Heisenberg model

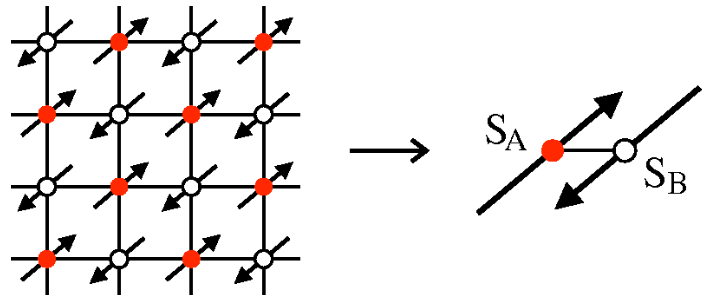
Ground state and lowest spin-S excitations on 4×4 and 6×6 lattices

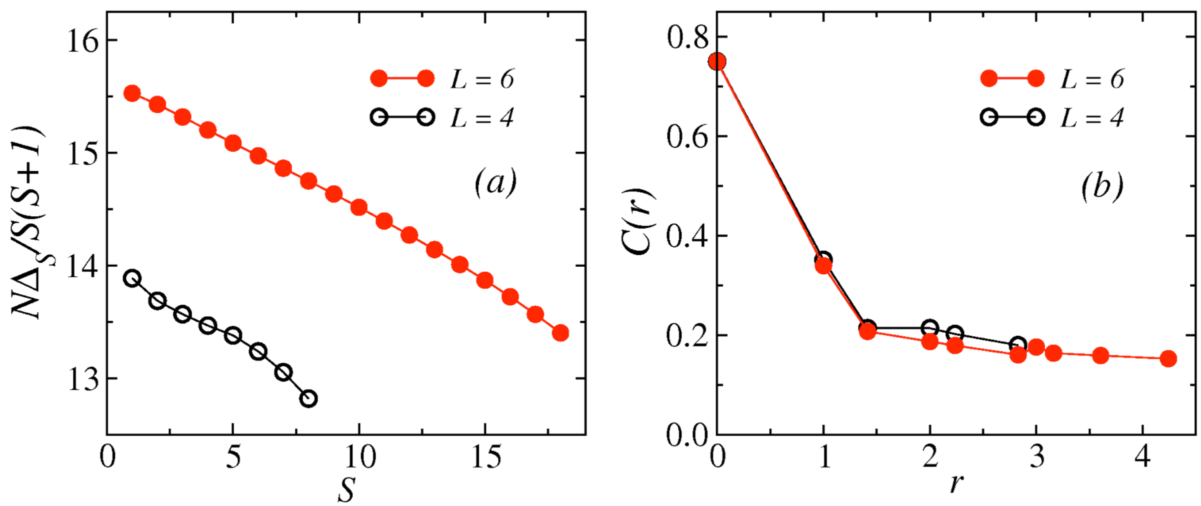
A fundamental aspect of the Néel state: **Quantum-rotor excitations**

- lowest-energy excitations of finite lattices
- not captured by spin-wave theory
- correspond to global rotations of the Neel order (frozen in spin-wave theory)

<u>Consider sublattices as two big spins</u>

- $S_A, S_B \sim N/2$
- effective interactions $\mathbf{J_{AB} \sim S_A \cdot S_B / N}$
- leads to $\boldsymbol{\Delta_S = E_S - E_0 \sim S(S+1)/N}$
- S = total spin of the excitation





staggered spin correlations show signs of order in the ground state

- but larger systems required to confirm (QMC)

Corrections to quantum-rotor energies seen for small systems

- quantum rotor energies should be good for S<<N