The S=1/2 Heisenberg chain hamiltonian can be constructed according to:

$$
\begin{array}{l}
\textbf{do } a = 0, 2^N - 1 \\
\quad \textbf{do } i = 0, N-1 \\
\quad\quad j = \textbf{mod}(i+1, N) \\
\quad\quad \textbf{if } (a[i] = a[j]) \textbf{ then} \\
\quad\quad\quad H(a,a) = H(a,a) + \frac{1}{4} \\
\quad\quad \textbf{else} \\
\quad\quad\quad H(a,a) = H(a,a) - \frac{1}{4} \\
\quad\quad\quad b = \textbf{flip}(a,i,j);\ H(a,b) = \frac{1}{2} \\
\quad\quad \textbf{endif} \\
\quad \textbf{enddo} \\
\textbf{enddo}
\end{array}
$$

j is the “right” nearest-neighbor of i

- periodic boundary conditions

Diagonalizing the hamiltonian matrix

- on the computer
- gives the eigenvalues and eigenvectors

If U is the matrix whose columns are the eigenvectors of H, then

$$\langle n|A|n\rangle = [U^{T*}AU]_{nn}$$

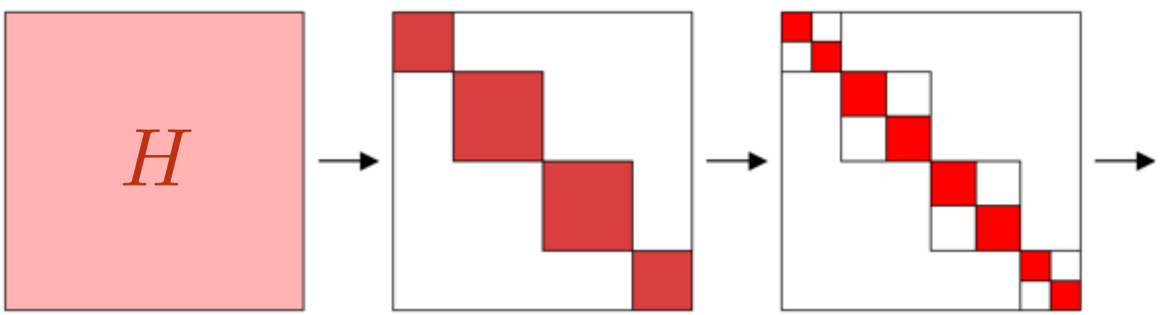
is the expectation value of some operator A in the n:th eigenstate

Problem: Matrix size $M=2^N$ becomes too large quickly

- maximum number of spins in practice; $N\approx 20$
- M^2 matrix elements to store, time to diagonalize $\propto M^3$

Using conservation laws (symmetries) for block-diagonalization

We can choose the basis in such a way that the H becomes block-diagonal



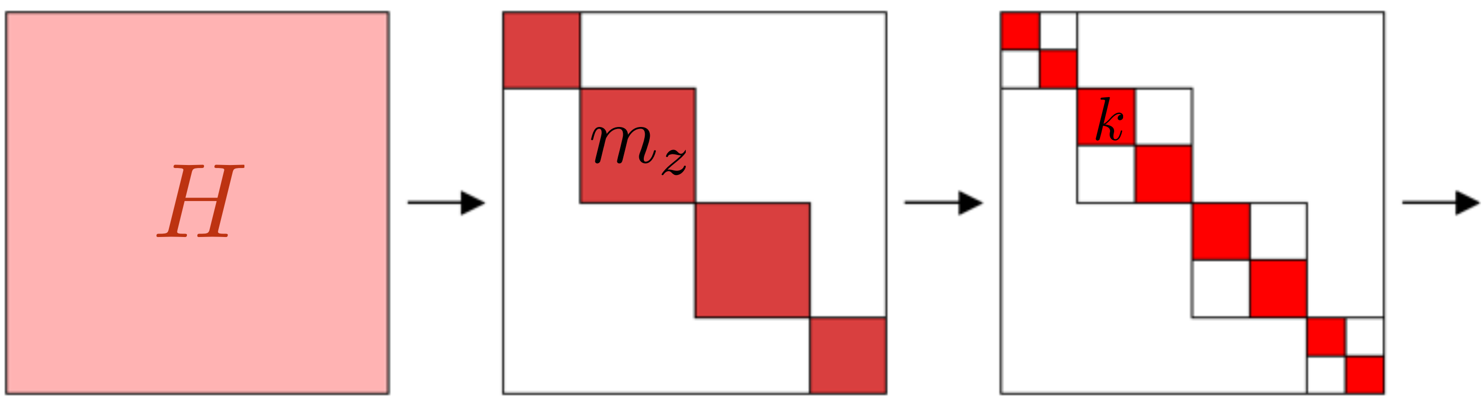
- the blocks can be diagonalized individually
- we can reach larger N (but not much larger, $N\approx 50$ is max)

Simplest example; magnetization conservation

$$m_z = \sum_{i=1}^{N} S_i^z$$

• blocks correspond to fixed values of m_z
• no H matrix elements between states of different m_z
• A block is constructed by only including states with a given m_z
  • corresponds to ordering the states in a particular way

Number of states in the largest block (m_z =0): $N!/[(N/2)!]^2$



Other symmetries (conserved quantum numbers)
• can be used to further split the blocks
• but more complicated
  • basis states have to be constructed to obey symmetries
  • e.g., momentum states (using translational invariance)

Pseudocode: using magnetization conservation

Constructing the basis in the block of $n_\uparrow$ spins $\uparrow$

Store state-integers in ordered list $\mathbf{s_a}$, **a=1,....,M**

$$
\begin{array}{l}
\textbf{do } s = 0, 2^N - 1 \\
\quad\quad \textbf{if } (\sum_i s[i] = n_\uparrow) \textbf{ then } a = a + 1;\ s_a = s \textbf{ endif} \\
\textbf{enddo} \\
M = a
\end{array}
$$

Example; N=4, $n_\uparrow$=2

s_1=3	(0011)
s_2=5	(0101)
s_3=6	(0110)
s_4=9	(1001)
s_5=10	(1010)
s_6=12	(1100)

How to locate a state (given integer s) in the list?

- stored map s→a may be too big for s=0,...,2^N-1
- instead, we search the list s_a (here simplest way)

$$
\begin{array}{l}
\textbf{subroutine findstate}(s, b) \\
b_{\min} = 1;\ b_{\max} = M \\
\textbf{do} \\
\quad\quad b = b_{\min} + (b_{\max} - b_{\min})/2 \\
\quad\quad \textbf{if } (s < s_b) \textbf{ then} \\
\quad\quad\quad\quad b_{\max} = b - 1 \\
\quad\quad \textbf{elseif } (s > s_b) \textbf{ then} \\
\quad\quad\quad\quad b_{\min} = b + 1 \\
\quad\quad \textbf{else} \\
\quad\quad\quad\quad \textbf{exit} \\
\quad\quad \textbf{endif} \\
\textbf{enddo}
\end{array}
$$

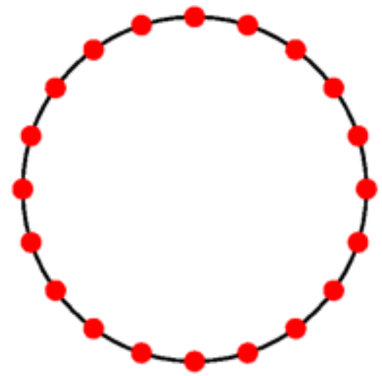
Finding the location ***b***
of a state-integer ***s*** in the list
- using bisection in the ordered list

Pseudocode; hamiltonian construction

- recall: states labeled a=1,...,M
- corresponding state-integers (bit representation) stored as s_a
- bit i, $s_a[i]$, corresponds to S^z_i

```
do a = 1, M                                  loop over states
    do i = 0, N-1                            loop over sites
        j = mod(i+1, N)
        if (s_a[i] = s_a[j]) then            check bits of state-integers
            H(a,a) = H(a,a) + 1/4
        else
            H(a,a) = H(a,a) - 1/4
            s = flip(s_a, i, j)              state with bits i and j flipped
            call findstate(s, b)
            H(a,b) = H(a,b) + 1/2
        endif
    enddo
enddo
```

Momentum states (translationally invariant systems)



A periodic chain (ring), translationally invariant

- the eigenstates have a momentum (crystal momentum) k

$$T|n\rangle = \mathrm{e}^{ik}|n\rangle \qquad k = m\frac{2\pi}{N}, \quad m = 0, \ldots, N-1,$$

The operator T translates the state by one lattice spacing

- for a spin basis state

$$T|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, S_1^z, \ldots, S_{N-1}^z\rangle$$

[T,H]=0 → momentum blocks of H

- can use eigenstates of T with given k as basis

A momentum state can be constructed from any **representative** state

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle$$

Construct ordered list of representatives
If |a> and |b> are representatives, then

$$T^r|a\rangle \neq |b\rangle \quad r \in \{1, \ldots, N-1\}$$

4-site examples
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

Convention: the representative is the one corresponding to the smallest integer