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 contains 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): $N!/[(N/2)!]^2$

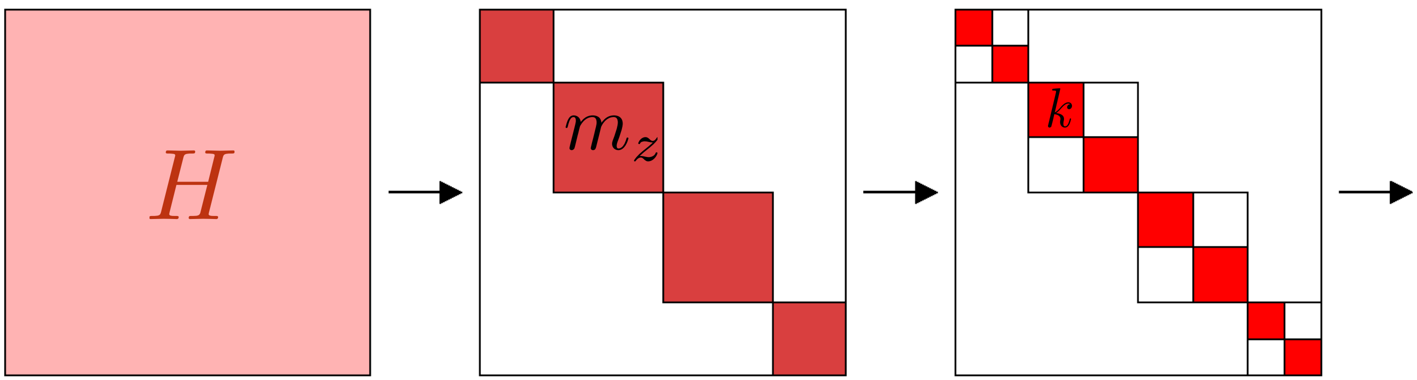
Example

N=4, m=0

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

this is now the state label

we have to store these numbers in a vector



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 ↑

Store state-integers in ordered list **s_a, a=1,....,M**

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

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)

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

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

- using bisection in the ordered list

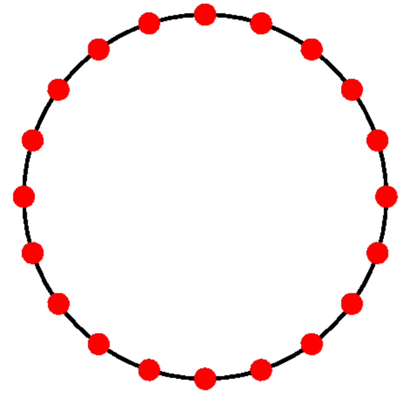
Pseudocode; hamiltonian construction

- 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 (H blocks labeled by k)

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

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

<u>4-site examples</u>
(**0011**)→(0110),(1100),(1001)
(**0101**)→(1010)

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

$$|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r |a\rangle, \qquad |a\rangle = |S_1^z, \ldots, S_N^z\rangle \qquad k = m\frac{2\pi}{N}$$

The sum can contain several copies of the same state

- if $T^R|a\rangle = |a\rangle$ for some $R < N$
- the total weight for this component is

$$1 + \mathrm{e}^{-ikR} + \mathrm{e}^{-i2kR} + \ldots + \mathrm{e}^{-ik(N-R)}$$

- vanishes (state incompatible with k and not in k block) unless kR=n2π
- the total weight of the representative is then N/R

$$kR = n2\pi \rightarrow \frac{mR}{N} = n \rightarrow m = n\frac{N}{R} \rightarrow \mathrm{mod}(m, N/R) = 0$$

Normalization of a state |*a*(k)> with periodicity R_a

$$\langle a(k)|a(k)\rangle = \frac{1}{N_a} \times R_a \times \left(\frac{N}{R_a}\right)^2 = 1 \rightarrow N_a = \frac{N^2}{R_a}$$

Basis construction: find all allowed representatives and their periodicities

(a_1, a_2, a_3, ..., a_M)
(R_1, R_2, R_3, ..., R_M)

The block size **M** is initially not known

- approximately 1/N of total size of fixed m_z block
- depends on the periodicity constraint for given k

The Hamiltonian matrix. Write $S = 1/2$ chain hamiltonian as

$$H_0 = \sum_{j=1}^{N} S^z_j S^z_{j+1}, \quad H_j = \tfrac{1}{2}(S^+_j S^-_{j+1} + S^+_j S^-_{j+1}), \quad j = 1, \dots, N$$

Act with H on a momentum state

$$H|a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H|a\rangle = \frac{1}{\sqrt{N_a}} \sum_{j=0}^{N} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r H_j|a\rangle,$$

$H_j|a\rangle$ is related to some representative: $H_j|a\rangle = h^j_a T^{-l_j}|b_j\rangle$

Here $h_a^j = 1/2$ for an off-diagonal operator if the spins are flippable

$$H|a(k)\rangle = \sum_{j=0}^{N} \frac{h^j_a}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^{(r-l_j)}|b_j\rangle$$

Shift summation index r and use definition of momentum state

$$H|a(k)\rangle = \sum_{j=0}^{N} h^j_a \mathrm{e}^{-ikl_j} \sqrt{\frac{N_{b_j}}{N_a}} |b_j(k)\rangle$$

➙ matrix elements

$$\langle a(k)|H_0|a(k)\rangle = \sum_{j=1}^{N} S^z_j S^z_j,$$

$$\langle b_j(k)|H_{j>0}|a(k)\rangle = \mathrm{e}^{-ikl_j} \frac{1}{2} \sqrt{\frac{R_a}{R_{b_j}}}, \qquad |b_j\rangle \propto T^{-l_j} H_j|a\rangle,$$