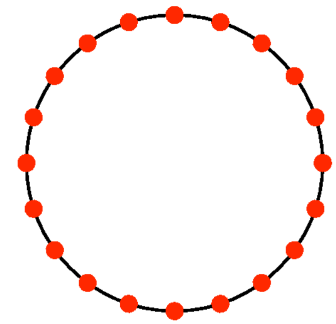
Momentum states (translationally invariant systems)



A periodic chain (ring), translationally invariant

- eigenstates with a fixed momentum (crystal momentum)
- quantum number 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

also [T,m_z]=0 → m_z blocks split into momentum blocks of H

- construct basis for given (m_z,k)

We have to construct a complete basis of eigenstates of k or (m_z,k)

A momentum state can be constructed from a **representative** state |a>

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

Convention: A representative |a> must be a state with the the lowest binary-integer representation among all its translations

- If |a> and |b> are representatives, then

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

|a> represents all its translations

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

The sum can contain several copies of the same state (periodicity R):

$$T^R|a\rangle = |a\rangle \quad \text{for some } R$$

- the total weight for the component |a> in |a(k)> is

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

- vanishes (state incompatible with k) unless kR=n2π
- the total weight of the representative is then N/R

Condition for periodicity compatible with momentum k=m2π/N:

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

Construct ordered list of representatives for given k

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

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

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

Pseudocode; basis construction

$$\begin{array}{l}
\textbf{do } s = 0, 2^N - 1 \\
\quad \textbf{call checkstate}(s, R) \\
\quad \textbf{if } R \geq 0 \textbf{ then } a = a + 1;\ s_a = s;\ R_a = R \textbf{ endif} \\
\textbf{enddo} \\
M = a
\end{array}$$

M = size of the H-block

Uses a subroutine **checkstate**(s,R)

- *R* = periodicity if state-integer s is a new representative
- store in list ***R_a*, *a*=1,...,*M***
- *R* = –1 if
  - the magnetization is not the one currently considered
  - some translation of |s> gives a state-integer smaller than s
  - |s> is not compatible with the momentum

Translations of the representative; cyclic permutation

Define function **cyclebits**(t,N)
- cyclic permutations of first N bits of integer t
- F90 function ishiftc(t,–1,N)

The representative has the lowest state-integer among all its translations

Pseudocode; checkstate() subroutine

$$
\begin{array}{l}
\textbf{subroutine checkstate}(s,R) \\
R=-1 \\
\textbf{if } (\sum_i s[i] \neq n_\uparrow) \textbf{ return} \\
t=s \\
\textbf{do } i=1,N \\
\quad t=\textbf{cyclebits}(t,N) \\
\quad \textbf{if } (t<s) \textbf{ then} \\
\quad\quad \textbf{return} \\
\quad \textbf{elseif } (t=s) \textbf{ then} \\
\quad\quad \textbf{if } (\textbf{mod}(k,N/i)\neq 0) \textbf{ return} \\
\quad\quad R=i;\ \textbf{return} \\
\quad \textbf{endif} \\
\textbf{enddo}
\end{array}
$$

check the magnetization

check if translated state has lower integer representation

check momentum compatibility
- k is the integer corresponding to the momentum; k=0,...,N-1
- momentum = k2π/N

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

$$H_0 = \sum_{j=1}^{N} S_j^z S_{j+1}^z, \quad H_j = \tfrac{1}{2}(S_j^+ S_{j+1}^- + S_j^+ S_{j+1}^-), \quad j = 1, \ldots, N$$

Act with H on a momentum state; use [H,T]=0

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

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

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

Shift summation index r and use definition of momentum state

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

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

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

Pseudocode; hamiltonian construction

First, some elements needed; recall

$$H_j|a\rangle = h_a^j T^{-l_j}|b_j\rangle$$

Finding the representative r of a state-integer s

- lowest integer among all translations

```
subroutine representative(s, r, l)
r = s; t = s; l = 0
do i = 1, N - 1
    t = cyclebits(t, N)
    if (t < r) then r = t; l = i endif
enddo
```

$$|r\rangle = T^l|s\rangle$$

Finding the location of the representative in the state list

- may not be there, if the new state is incompatible with k
- **b=–1** for not found in list

```
subroutine findstate(s, b)
b_min = 1; b_max = M
do
    b = b_min + (b_max - b_min)/2
    if (s < s_b) then
        b_max = b - 1
    elseif (s > s_b) then
        b_min = b + 1
    else
        exit
    endif
    if (b_min > b_max then
        b = -1; exit
    endif
enddo
```

Construct all the matrix elements

```
do a = 1, M
    do i = 0, N − 1
        j = mod(i + 1, N)
        if (s_a[i] = s_a[j]) then
            H(a, a) = H(a, a) + 1/4
        else
            H(a, a) = H(a, a) − 1/4
            s = flip(s_a, i, j)
            call representative(s, r, l)
            call findstate(r, b)
            if (b ≥ 0) then
                H(a, b) = H(a, b) + 1/2 sqrt(R_a/R_b) e^{i2πkl/N}
            endif
        endif
    enddo
enddo
```

Reflection symmetry (parity) Define a reflection (parity) operator

$$P|S_1^z, S_2^z, \ldots, S_N^z\rangle = |S_N^z, \ldots, S_2^z, S_1^z\rangle$$

Consider a hamiltonian for which [H,P]=0 and [H,T]=0; but note that [P,T]≠0

Can we still exploit both P and T at the same time? Consider the state

$$|a(k,p)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{-ikr} T^r (1 + pP)|a\rangle, \quad p = \pm 1$$

This state has momentum k, but does it have parity p? Act with P

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

$$= p \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} \mathrm{e}^{ikr} T^r (1 + pP)|a\rangle \;\; = p|a(k,p)\rangle \text{ if } k = 0 \text{ or } k = \pi$$

k=0,π momentum blocks are split into p=+1 and p=–1 sub-blocks

- [T,P]=0 in the k=0,π blocks
- physically clear because -k=k on the lattice for k=0,π
- we can exploit parity in a different way for other k →
- **semi-momentum states**