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

The sum can contain several copies of the same state

- if $T^R|a\rangle = |a\rangle \;\; \text{for some } R < N$
- 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) 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

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

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: $H_j|a\rangle = h^j_a T^{-l_j}|b_j\rangle$

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

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

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

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

Reflection symmetry (parity)

Define a reflection (parity) operator

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

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

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

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

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**

Semi-momentum states

Mix momenta +k and −k for k≠0,π

$$|a^\sigma(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} C_k^\sigma(r) T^r |a\rangle \qquad C_k^\sigma(r) = \begin{cases} \cos(kr), & \sigma = +1 \\ \sin(kr), & \sigma = -1. \end{cases}$$

$$k = m\frac{2\pi}{N}, \quad m = 1,\ldots,N/2-1, \quad \sigma = \pm 1$$

States with same k, different σ are orthogonal

Semi-momentum states with parity

This state has definite parity with p=+1 or p=−1 for any k

$$|a^\sigma(k,p)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r)(1+pP)T^r |a\rangle.$$

- (k,−1) and (k,+1) blocks
- the basis is of the same size as the original k-blocks
- but these states are real, not complex ⇒ computational advantage

- For k≠0,π, the p=-1 and p=+1 states are degenerate

Spin-inversion symmetry

Spin inversion operator: $Z|S_1^z, S_2^z, \ldots, S_N^z\rangle = |-S_1^z, -S_2^z, \ldots, -S_N^z\rangle$

In the magnetization block $m^z=0$ we can use eigenstates of Z

$$|a^\sigma(k,p,z)\rangle = \frac{1}{\sqrt{N_a^\sigma}} \sum_{r=0}^{N-1} C_k^\sigma(r)(1+pP)(1+zZ)T^r|a\rangle,$$

$$Z|a^\sigma(k,p,z)\rangle = z|a^\sigma(k,p,z)\rangle, \quad z=\pm 1$$

Example: block sizes

$m_z=0$, $k=0$ (largest momentum block)

$(p=\pm 1, z=\pm 1)$

N	$(+1,+1)$	$(+1,-1)$	$(-1,+1)$	$(-1,-1)$
8	7	1	0	2
12	35	15	9	21
16	257	183	158	212
20	2518	2234	2136	2364
24	28968	27854	27482	28416
28	361270	356876	355458	359256
32	4707969	4690551	4685150	4700500

Total spin S conservation

- difficult to exploit
- complicated basis states
- calculate S using **$S^2=S(S+1)$**

$$\begin{aligned}\mathbf{S}^2 &= \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_j \\ &= 2\sum_{i<j} \mathbf{S}_i \cdot \mathbf{S}_j + \frac{3}{4}N\end{aligned}$$