Symmetries I: Abelian

NRG: [Wilson1975], [Toth2008], [Weichselbaum2012b]. DMRG: [McCulloch2001], [McCulloch2002]

General tensor network: Singh, Pfeiffer, Vidal [Singh2010]

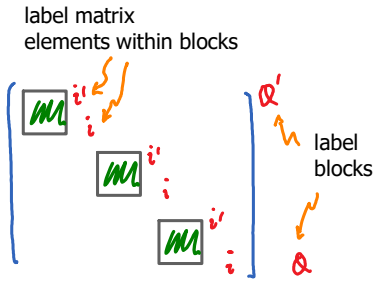
Goal: exploit symmetries of Hamiltonian!

If Hamiltonian has a symmetry, $[\hat{H}, \hat{Q}] = 0$, (generator of symmetry group)

then $\hat{H}$ is block-diagonal in $\hat{Q}$ eigenbasis:

$$\hat{Q}|q,i\rangle = q|q,i\rangle \Rightarrow \hat{H}|q,i\rangle = |q,i'\rangle H_{[q]}{}^{i'}{}_{i} \quad (1)$$

'multiplicity index' i enumerates different states with same q

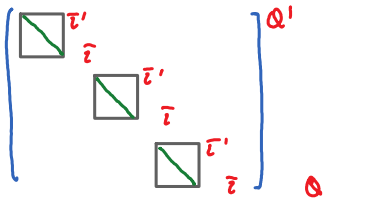


$$\langle q',i'|\hat{H}|q,i\rangle = \mathbb{1}^{q'}{}_{q} H_{[q]}{}^{i'}{}_{i}$$

Separate diagonalization of each block yields simultaneous eigenbasis of $\hat{H}$ and $\hat{Q}$.

$$\hat{Q}|q,\bar{\imath}\rangle = q|q,\bar{\imath}\rangle, \qquad \hat{H}|q,\bar{\imath}\rangle = E_{q,\bar{\imath}}|q,\bar{\imath}\rangle \quad (2)$$

(overbar will indicate energy eigenbasis)



$$\langle q',\bar{\imath}'|\hat{H}|q,\bar{\imath}\rangle = \mathbb{1}^{q'}{}_{q}\,\mathbb{1}^{\bar{\imath}'}{}_{\bar{\imath}}\,E_{q,\bar{\imath}}$$

(For non-Abelian symmetries, degenerate multiplets arise -- next lecture.)

Exploiting this structures reduces numerical costs!

1. Example, Abelian symmetry: XXZ-chain (spin ½) symmetry group: U(1)

$$\hat{H} = \sum_{\ell} J_z \hat{S}^z_{\ell}\hat{S}^z_{\ell+1} + \sum_{\ell}\frac{J}{2}\left(\hat{S}^+_{\ell}\hat{S}^-_{\ell+1} + \hat{S}^-_{\ell}\hat{S}^+_{\ell+1}\right) = \hat{H}^{zz} + \hat{H}^{sf} \quad (3)$$

(spin-flip)

Total spin, $\hat{S}^z_{tot} = \sum_{\ell}\hat{S}^z_{\ell}$, is conserved: $[\hat{H}, \hat{S}^z_{tot}] = 0$ 'Abelian U(1) symmetry' (4)

For Abelian symmetry, conserved quantum number is often called 'charge': $\hat{Q} \equiv 2\hat{S}^z_{tot}$.

(to avoid proliferation of ½ factors)

Conservation of $\hat{Q}_{tot}$ is obvious by inspection. But let us check explicitly:

One site: $\hat{S}^+_{\ell} = \begin{array}{c} \\ \uparrow \\ \downarrow \end{array}\begin{array}{c}\begin{array}{cc}\uparrow & \downarrow\end{array}\\ \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\end{array}$. $\hat{S}^-_{\ell} = \begin{array}{c} \\ \uparrow \\ \downarrow \end{array}\begin{array}{c}\begin{array}{cc}\uparrow & \downarrow\end{array}\\ \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\end{array}$ $\hat{Q}_{\ell} = 2\hat{S}^z_{\ell} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ (5)

Consider matrix representation of operators in the direct-product basis of sites 1 and 2: $\{|q_1\rangle \otimes |q_2\rangle\}$

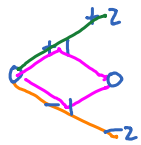
$$\hat{Q}_1 + \hat{Q}_2 = \hat{Q}_1 \otimes \hat{\mathbb{1}}_2 + \hat{\mathbb{1}}_1 \otimes \hat{Q}_2$$

$$\doteq \begin{pmatrix} +1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix} & \\ & -1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix} \end{pmatrix} + \begin{pmatrix} 1\cdot\begin{pmatrix}+1 & \\ & -1\end{pmatrix} & \\ & 1\cdot\begin{pmatrix}+1 & \\ & -1\end{pmatrix} \end{pmatrix} =$$

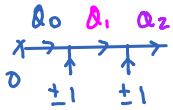
$$\begin{array}{c|c} Q' \backslash Q & \begin{array}{cccc} 2 & 0 & 0 & -2 \\ \uparrow\uparrow & \uparrow\downarrow & \downarrow\uparrow & \downarrow\downarrow \end{array} \\ \hline \begin{array}{c} 2 \\ 0 \\ 0 \\ -2 \end{array} & \begin{array}{c} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{array} \begin{pmatrix} \boxed{2} & & & \\ & \boxed{0} & & \\ & & \boxed{0} & \\ & & & \boxed{-2} \end{pmatrix} \end{array} \quad (6)$$

Total charge has 3 eigenvalues, $Q \in \{2, 0, -2\}$ degeneracies match number of ways to arrive at specified total charge:

with degeneracies: $1 \quad 2 \quad 1$



(7)



$$\frac{\hat{H}^{zz}}{\frac{1}{4}J_z} = \underbrace{4\hat{J}_1^z \hat{J}_2^z}_{\hat{Q}_1 \cdot \hat{Q}_2} \doteq \begin{pmatrix} +1\cdot(+1) & & & \\ & -1\cdot(+1) & & \\ & & -1\cdot(+1) & \\ & & & +1\cdot(+1) \end{pmatrix} = \begin{array}{c} Q' \backslash Q \quad 2 \quad 0 \quad 0 \quad -2 \\ 2 \quad \uparrow\uparrow \quad [1] \\ 0 \quad \uparrow\downarrow \quad [-1 \quad -1] \\ 0 \quad \downarrow\uparrow \\ -2 \quad \downarrow\downarrow \quad [1] \end{array} \qquad (8)$$

$$\frac{\hat{H}^{sf}}{\frac{1}{2}J} = \hat{S}_1^+ \hat{S}_2^- + \hat{S}_1^- \hat{S}_2^+ \doteq \begin{pmatrix} 1\cdot\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & & \\ & \ddots & \\ & & 0 \end{pmatrix} + \begin{pmatrix} \ddots & & \\ & 0 & \\ & & 1\cdot\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{pmatrix} = \begin{array}{c} \uparrow\uparrow \quad \uparrow\downarrow \quad \downarrow\uparrow \quad \downarrow\downarrow \\ \uparrow\uparrow \quad [0] \\ \uparrow\downarrow \quad [1 \quad 1] \\ \downarrow\uparrow \\ \downarrow\downarrow \quad [0] \end{array} \qquad (9)$$

Both (8) and (9) are block-diagonal $\Rightarrow [\hat{Q}_{tot}, \hat{H}_{12}] = 0$ (10)

Eigenstates of $\hat{H}_{12}$ will carry Q -eigenvalue as one of their quantum numbers.

<u>Bookkeeping for 2 sites</u> (using Q = z (Eigenvalue of $\hat{S}^z_{tot}$ as label) (11)

Label states as $|Q, i\rangle$, where the 'multiplicity label' i enumerate states having the same Q.

List of states needed to describe 2 sites:

no sites	one site	two sites
Q	Q	Q
		2
	1	
0		0
	−1	
		−2

enumerates states with same charge

list index ν	charge Q	i	explicit representation	state
1	2	1	1	$\|\uparrow\uparrow\rangle$
2	0	1	$(1,0)^T := \begin{pmatrix}1\\0\end{pmatrix}$	$\|\uparrow,\downarrow\rangle$
		2	$(0,1)^T := \begin{pmatrix}0\\1\end{pmatrix}$	$\|\downarrow,\uparrow\rangle$
3	−2	1	1	$\|\downarrow\downarrow\rangle$

(12)

2-site Hamiltonian: $H_{12} \overset{(8,9)}{=} \frac{1}{4}J_z \begin{bmatrix} 1 & & \\ & -1 & -1 \\ & & 1 \end{bmatrix} + \frac{1}{2}J \begin{bmatrix} 0 & & \\ & 1 & 1 \\ & & 0 \end{bmatrix}$

List of sectors ('blocks') arising for 2-site Hamiltonian:

ν	Q'	Q	$\langle Q'\|H\|Q\rangle \sim \mathbb{1}^{Q'}_{Q}$
1	2	2	$\frac{1}{4}J_z$
2	0	0	$-\frac{1}{4}J_z\begin{pmatrix}1&\\&1\end{pmatrix} + \frac{1}{2}J\begin{pmatrix}&1\\1&\end{pmatrix}$
3	−2	−2	$\frac{1}{4}J_z$

The task of diagonalizing Hamiltonian splits into three separate tasks: diagonalizing three blocks (two of which are trivial).

(13)

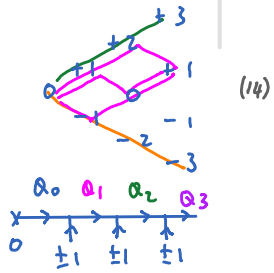
3. Sites

Next consider three sites 1, 2 and 3, with direct product basis $\{|Q_1\rangle \otimes |Q_2\rangle \otimes |Q_3\rangle\}$

$\hat{Q}_{tot} = \sum_{\ell=1}^{3} \hat{Q}_\ell$ has 4 eigenvalues, $Q \in \{3, 1, -1, -3\}$ degeneracies match number of ways to arrive specified at total charge:

total charge

with degeneracies: $\underline{1}$ $\underline{3}$ 3 $\underline{1}$



(14)

Matrix representation of Hamiltonian in direct product basis:

$$\frac{\hat{H}^{zz}}{\frac{1}{4}J^z} = \hat{Q}_1\hat{Q}_2\hat{1}_3 + \hat{1}_1\hat{Q}_2\hat{Q}_3$$

$$\doteq \begin{pmatrix} +1\cdot\begin{pmatrix} +1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix} & \\ & -1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix}\end{pmatrix} & \\ & -1\cdot\begin{pmatrix} +1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix} & \\ & -1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix}\end{pmatrix} \end{pmatrix} + \begin{pmatrix} +1\cdot\begin{pmatrix} +1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix} & \\ & -1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix}\end{pmatrix} & \\ & +1\cdot\begin{pmatrix} +1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix} & \\ & -1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix}\end{pmatrix} \end{pmatrix} =$$

Q' \ Q	+3	+1	+1	−1	+1	−1	−1	−3
	↑↑↑	↑↑↓	↑↓↑	↑↓↓	↓↑↑	↓↑↓	↓↓↑	↓↓↓
+3 ↑↑↑	2							
+1 ↑↑↓		0						
+1 ↑↓↑			−2					
−1 ↑↓↓				0				
+1 ↓↑↑					0			
−1 ↓↑↓						−2		
−1 ↓↓↑							0	
−3 ↓↓↓								2

(15)

$$\frac{\hat{H}^{sf}}{\frac{1}{2}J} = \left(\hat{S}_1^+\hat{S}_2^- + \hat{S}_1^-\hat{S}_2^+\right)\hat{1}_3 + \hat{1}_1\left(\hat{S}_2^+\hat{S}_3^- + \hat{S}_2^-\hat{S}_3^+\right)$$

$$\doteq \begin{pmatrix} & 1\cdot\begin{pmatrix}1 & 0\\ & 1\end{pmatrix} \\ 1\cdot\begin{pmatrix}1 & \\ 0 & 1\end{pmatrix} & \end{pmatrix} + \begin{pmatrix} 1\cdot\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} & \\ & 1\cdot\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\end{pmatrix} =$$

Q' \ Q	+3	+1	+1	−1	+1	−1	−1	−3
	↑↑↑	↑↑↓	↑↓↑	↑↓↓	↓↑↑	↓↑↓	↓↓↑	↓↓↓
+3 ↑↑↑								
+1 ↑↑↓			1					
+1 ↑↓↑		1						
−1 ↑↓↓					1			
+1 ↓↑↑				1				
−1 ↓↑↓							1	
−1 ↓↓↑						1		
−3 ↓↓↓								

(16)

The direct-product scheme does not automatically produce a block-diagonal structure for $\hat{H}^{sf}$, because it orders basis states in such a way that not all states with same Q appear in a contiguous block. To arrive at a block-diagonal structure, interchange 4th and 5th basis vectors (switch rows $4 \leftrightarrow 5$ & columns $4 \leftrightarrow 5$).

In rearranged basis with contiguous blocks of Q's, all terms of H are block-diagonal:

$$\frac{H^{zz}}{\frac{1}{4}J^z} =$$

Q' \ Q	+3	+1	+1	+1	−1	−1	−1	−3
	↑↑↑	↑↑↓	↑↓↑	↓↑↑	↑↓↓	↓↑↓	↓↓↑	↓↓↓
+3 ↑↑↑	+2							
+1 ↑↑↓		0			−2			
+1 ↑↓↑			0			−2		
+1 ↓↑↑		−2		0				
−1 ↑↓↓			−2		0			
−1 ↓↑↓				−2		0		
−1 ↓↓↑							0	
−3 ↓↓↓								0

,

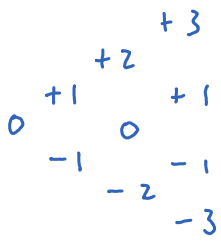
$$\frac{H^{sf}}{\frac{1}{2}J} =$$

Q' \ Q	+3	+1	+1	+1	−1	−1	−1	−3
	↑↑↑	↑↑↓	↑↓↑	↓↑↑	↑↓↓	↓↑↓	↓↓↑	↓↓↓
+3 ↑↑↑	0							
+1 ↑↑↓			1					
+1 ↑↓↑		1						
+1 ↓↑↑					1			
−1 ↑↓↓				1				
−1 ↓↑↓							1	
−1 ↓↓↑						1		
−3 ↓↓↓								0

(17)

Bookkeeping for 3 sites

List of states needed to describe 3 sites:



ν	charge Q	i (enumerates states with same charge)	explicit representation	state
1	3	1	1	$\|\uparrow\uparrow\uparrow\rangle$
2	1	1	$(1,0,0)^T$	$\|\uparrow\uparrow\downarrow\rangle$
		2	$(0,1,0)^T$	$\|\uparrow\downarrow\uparrow\rangle$
		3	$(0,0,1)^T$	$\|\downarrow\uparrow\uparrow\rangle$
3	-1	1	$(1,0,0)^T$	$\|\uparrow\downarrow\downarrow\rangle$
		2	$(0,1,0)^T$	$\|\downarrow\uparrow\downarrow\rangle$
		3	$(0,0,1)^T$	$\|\downarrow\downarrow\uparrow\rangle$
4	-3	1	1	$\|\downarrow\downarrow\downarrow\rangle$

(18)

3-site Hamiltonian:

$$H_{123} = \tfrac{1}{4} J_z \left[\begin{matrix} +2 & & & \\ & 0 & & \\ & & -2 & \\ & & & 0 \end{matrix} + \begin{matrix} 0 & & & \\ & -2 & & \\ & & 0 & \\ & & & 0 \end{matrix} \right] + \tfrac{1}{2} J \left[\begin{matrix} 0 & & & \\ & 1 & 1 & \\ & 1 & 1 & \\ & & & 0 \end{matrix} + \begin{matrix} 1 & & & \\ & 1 & 1 & \\ & 1 & 1 & \\ & & & 0 \end{matrix} \right]$$

(19)

List of sectors ('blocks') arising for 3-stite Hamiltonian:

The task of diagonalizing Hamiltonian can be split into four separate tasks (two of which are trivial).

ν	Q'	Q	$\langle Q \vert H \vert Q' \rangle \sim \mathbb{1}^{Q'}_{Q}$
1	3	3	$\frac{1}{2} J_z$
2	1	1	$\frac{1}{2} J_z \begin{pmatrix} 0 & & \\ & -1 & \\ & & 0 \end{pmatrix} + \frac{1}{2} J \begin{pmatrix} 1 & 1 & \\ 1 & 1 & \\ & & 0 \end{pmatrix}$
3	-1	-1	$\frac{1}{2} J_z \begin{pmatrix} 0 & & \\ & -1 & \\ & & 0 \end{pmatrix} + \frac{1}{2} J \begin{pmatrix} 1 & 1 & \\ 1 & 1 & \\ & & 0 \end{pmatrix}$
4	-3	-3	$\frac{1}{2} J_z$

(20)

Summary of lessons learnt from example

For an Abelian symmetry, with $[\hat{H}, \hat{Q}] = 0$, the $\hat{Q}$-eigenstates can be labeled as $|Q, i\rangle$ (21)

- 'Q-label' or 'symmetry label': Q, eigenvalues of $\hat{Q}$
- 'i-label' or 'multiplicity label': i, enumerates <u>different</u> irreducible multiplets having same Q

  For an abelian symmetry each 'multiplet' contains just a single state, hence Q suffices for labeling states.

  (For nonabelian symmetry, it could contain several states, hence another internal label is needed: $|Q q, i\rangle$)

In group theory language: $|Q, i\rangle$ is a 'reducible multiplet' of $\hat{Q}$, the index i serves to 'reduce' it.

We need systematic, automatable way of generating all states $|Q, i\rangle$ and computing matrix elements

$$H_{[Q]}{}^{i'}_{i} = \langle Q, i' | \hat{H} | Q, i \rangle \quad (22)$$

Diagonalizing $H_{[Q]}$ yields symmetry- and energy eigenstates, $|Q, \bar{i}\rangle = |Q, i\rangle U_{[Q]}{}^{i}_{\bar{i}}$ (23)

with eigenenergies $E_{[Q]\bar{i}}$

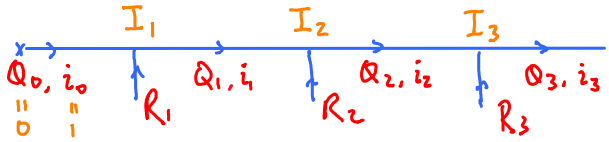
overbar will indicate energy eigenbasis

2. Iterative diagonalization with Abelian symmetry

Build chain iteratively, in $|Q, i\rangle$ basis:

Local basis for each site: $|\sigma\rangle =: |R\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$ for spin-1/2 chain

Ket:

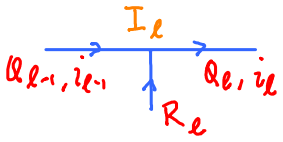


'sum rule' at each vertex:

$$\underbrace{Q_{\ell-1} + R_\ell}_{\text{in}} = \underbrace{Q_\ell}_{\text{out}} \qquad (1)$$

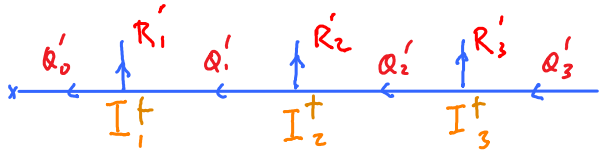
The 'identity matrix' I_ℓ transforms to 'symmetry eigenbasis':

$$|Q_\ell, i_\ell\rangle = |R_\ell\rangle\, |Q_{\ell-1}, i_{\ell-1}\rangle \left(I_\ell^{Q_{\ell-1}, R_\ell\, Q_\ell}\right)^{i_{\ell-1}, i_\ell} \qquad (2)$$



The i-index is often omitted in diagrams.

Bra:

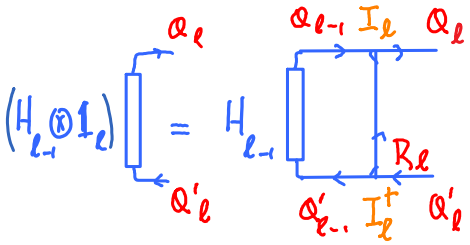


'sum rule' at each vertex:

$$\underbrace{Q'_{\ell-1} + R'_\ell}_{\text{out}} = \underbrace{Q'_\ell}_{\text{in}} \qquad (3)$$

I_ℓ -matrices encode the sum rules, thereby yielding a block-diagonal Hamiltonian.

Induction: if $H_{\ell-1}$ is block-diagonal, so is $H_\ell = H_{\ell-1} \otimes \mathbb{1}_\ell + S^+_{\ell-1} \otimes S^-_\ell + S^-_{\ell-1} \otimes S^+_\ell$:

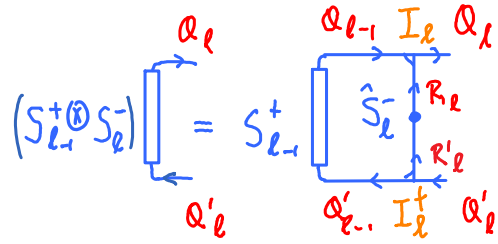


$$\langle Q'_{\ell-1}|\hat{H}_{\ell-1}|Q_{\ell-1}\rangle \neq 0 \Rightarrow Q'_{\ell-1} = Q_{\ell-1} \qquad (4)$$

$$\langle Q_{\ell-1}, R_\ell|\hat{I}_\ell|Q_\ell\rangle \neq 0 \Rightarrow Q_{\ell-1} + R_\ell = Q_\ell \qquad (5)$$

$$\langle Q'_\ell|\hat{I}_\ell|Q'_{\ell-1}, R_\ell\rangle \neq 0 \Rightarrow Q'_\ell = Q'_{\ell-1} + R_\ell \qquad (6)$$

These relations imply: $Q'_\ell \overset{(6)}{=} Q'_{\ell-1} + R_\ell \overset{(4)}{=} Q_{\ell-1} + R_\ell \overset{(5)}{=} Q_\ell \Rightarrow$ block-diagonal (7)



$$\langle Q'_{\ell-1}|\hat{S}^+_{\ell-1}|Q_{\ell-1}\rangle \neq 0 \Rightarrow Q'_{\ell-1} = Q_{\ell-1} + 1 \qquad (8)$$

$$\langle R'_\ell|\hat{S}^-_\ell|R_\ell\rangle \neq 0 \Rightarrow R'_\ell = R_\ell - 1 \qquad (9)$$

$$\langle Q_{\ell-1}, R_\ell|\hat{I}_\ell|Q_\ell\rangle \neq 0 \Rightarrow Q_{\ell-1} + R_\ell = Q_\ell \qquad (10)$$

$$\langle Q'_\ell|\hat{I}_\ell|Q'_{\ell-1}, R'_\ell\rangle \neq 0 \Rightarrow Q'_\ell = Q'_{\ell-1} + R'_\ell \qquad (11)$$

These relations imply: $Q'_\ell \overset{(11)}{=} Q'_{\ell-1} + R'_\ell \overset{(9)}{=} (Q_{\ell-1} + 1) + (R_\ell - 1) \overset{(5)}{=} Q_\ell \Rightarrow$ block-diagonal (12)

This is no surprise: if every vertex satisfies charge conservation, so does entire diagram!

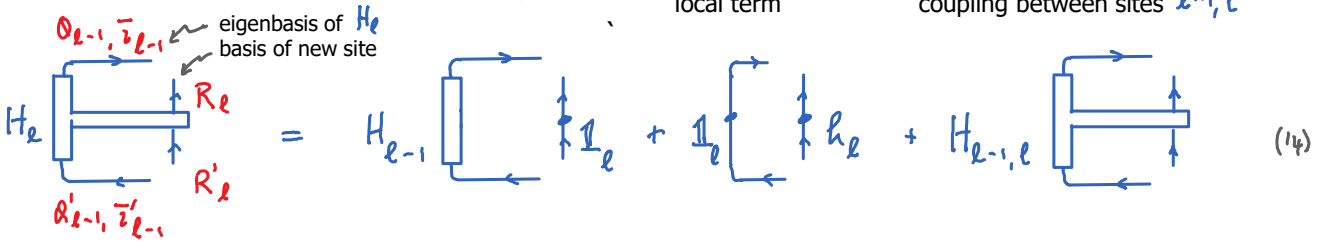
Strategy for iterative diagonalization

(i) Add new site, (ii) transform to symmetry eigenbasis to make Hamiltonian block-diagonal.

(iii) Diagonalize each block, (iv) transform to energy eigenbasis.

(i) $\hat{H}_\ell = \hat{H}_{\ell-1} + \hat{h}_\ell + \hat{H}_{\ell-1,\ell}$ (13)

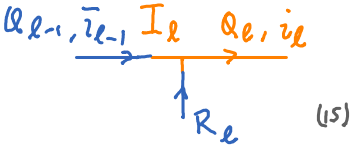
sites $1 \dots \ell$ — sites $1 \dots \ell-1$ — local term — coupling between sites $\ell-1, \ell$



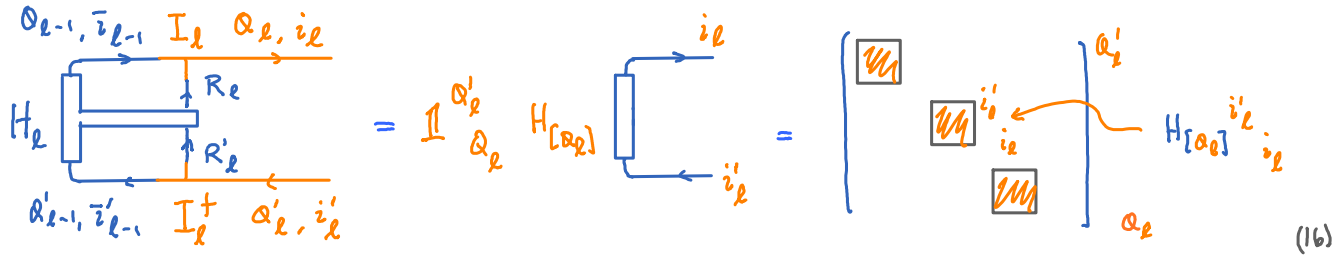
(14)

(ii) Symmetry eigenbasis:

$$|Q_\ell, i_\ell\rangle = |R_\ell\rangle\, |Q_{\ell-1}, \bar{\imath}_{\ell-1}\rangle \left[I_\ell^{Q_{\ell-1}, R_\ell\; Q_\ell}\right]^{\bar{\imath}_{\ell-1}}_{\;\; i_\ell}$$ (15)



To transform to this basis, attach 'identity matrices' to legs of H_ℓ :

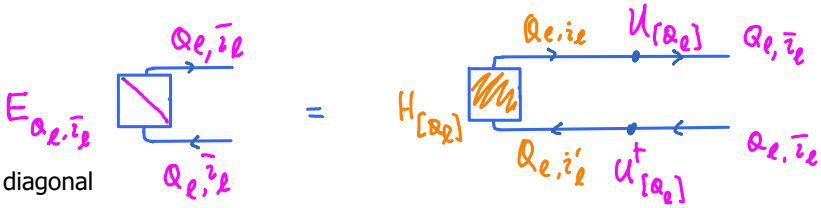


(16)

(iii) Diagonalize block: $H_{[Q_\ell]}\, |Q_\ell, \bar{\imath}_\ell\rangle = E_{Q_\ell, \bar{\imath}_\ell}\, |Q_\ell, \bar{\imath}_\ell\rangle$ (17)

(iv) Transform to energy eigenbasis: $|Q_\ell, \bar{\imath}_\ell\rangle = |Q_\ell, i_\ell\rangle\, U_{[Q_\ell]}{}^{i_\ell}_{\;\; \bar{\imath}_\ell}$ (18)

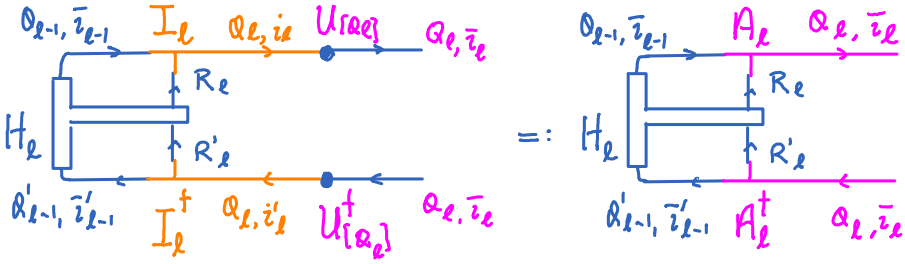
Applying this transformation to H_ℓ yields diagonal representation:



(19)

here we need only those blocks of $H_{\ell-1}$ (see 14) which contribute to total charge Q_ℓ

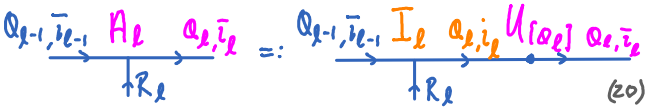
(16) =



So, transformation from old to new eigenbasis is described by A-matrices (only these need to be saved to disk):

determined by group theory (symmetries of Hamiltonian) — determined by dynamics (details of Hamiltonian)

$$\left[A_\ell^{Q_{\ell-1}, R_\ell\; Q_\ell}\right]^{\bar{\imath}_{\ell-1}}_{\;\; \bar{\imath}_\ell} = \left[I_\ell^{Q_{\ell-1}, R_\ell\; Q_\ell}\right]^{\bar{\imath}_{\ell-1}}_{\;\; i_\ell} \left[U_{[Q_\ell]}\right]^{i_\ell}_{\;\; \bar{\imath}_\ell}$$

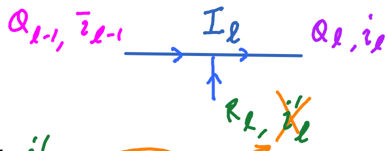


(20)

3. Bookkeeping for 'identity matrices'

'Identity matrix' relates direct product basis of bond $\ell-1$ and site ℓ to basis of bond ℓ :

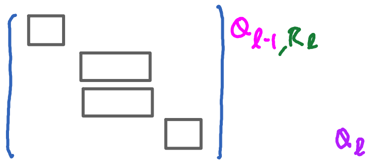
$$\left(I_\ell^{Q_{\ell-1},R_\ell}{}_{Q_\ell}\right)^{\bar{i}_{\ell-1}\,\cancel{i'_\ell}}{}_{i_\ell} := \langle Q_{\ell-1},\bar{i}_{\ell-1}|\langle R_\ell,\cancel{i'_\ell}|Q_\ell,i_\ell\rangle$$



Each site hosts just one spin 1/2, hence physical leg needs no multiplet index i'_ℓ

$|R_\ell\rangle \in \{|+1\rangle, |-1\rangle\}$

$(Q_{\ell-1}, R_\ell)$ (viewed as composite index), Q_ℓ label row, column positions of blocks within I_ℓ =



$\bar{i}_{\ell-1} = 1,\dots,M_{\ell-1}$, $i_\ell = 1,\dots,M_\ell$ } label row, column positions of matrix elements within blocks: $\square^{\bar{i}_{\ell-1}}{}_{i_\ell}$

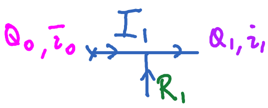
Exploit sparse structure by storing only nonzero blocks, i.e. those with charge labels satisfying $Q_\ell = Q_{\ell-1} + R_\ell$.

Make list in which each row describes one such block, containing $Q_{\ell-1}, R_\ell, Q_\ell$ and the block matrix elements:

List index	incoming bond	physical leg	outgoing bond	block dimension	matrix elements of block
ν :	$Q_{\ell-1}$	R_ℓ	Q_ℓ	$M_{\ell-1}\times 1,\ M_\ell$	$\square^{\bar{i}_{\ell-1}}{}_{i_\ell}$

<u>Sites 0 and 1</u>

$$\left(I_1^{Q_0R_1}{}_{Q_1}\right)^{\bar{i}_0}{}_{i_1} =$$



$Q_0 = 0$
$R_1 \in \{\pm 1\}$
$Q_1 = Q_0 + R_1 \in \{\pm 1\}$

$\langle Q_0,\bar{i}_0|\langle R_1|$ \ $|Q_1,i_1\rangle$		$|+1,1\rangle$	$|-1,1\rangle$
		$\uparrow$	$\downarrow$
$\langle 0,1|\langle +1|$	$\times\uparrow$	1	
$\langle 0,1|\langle -1|$	$\times\downarrow$		1

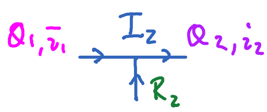
=:

list index ν	bond 0 Q_0	site 1 R_1	bond 1 Q_1	block dim $M_0\times 1, M_1$	block elements $\left(I^{Q_0R_1}{}_{Q_1}\right)^{\bar{i}_0}{}_{i_1}$
1	0	+1	+1	1x1, 1	1
2	0	−1	−1	1x1, 1	1

each grey box is 1x1 matrix, since multiplet indices take only one value, $\bar{i}_0 =$, $i_1 =$ i.e. $M_0 =$, $M_1 =$

<u>Sites 1 and 2</u>

$$\left(I_2^{Q_1R_2}{}_{Q_2}\right)^{\bar{i}_1}{}_{i_2} =$$



$Q_1 \in \{\pm 1\}$
$R_2 \in \{\pm 1\}$
$Q_2 = Q_1 + R_2 \in \{\pm 2, 0\}$

$\langle Q_1,\bar{i}_1|\langle R_2|$ \ $|Q_2,i_2\rangle$		$|2,1\rangle$	$|0,1\rangle$	$|0,2\rangle$	$|-2,1\rangle$
		$\uparrow\uparrow$	$\uparrow\downarrow$	$\downarrow\uparrow$	$\downarrow\downarrow$
$\langle +1,1|\langle +1|$	$\uparrow\uparrow$	1			
$\langle +1,1|\langle -1|$	$\uparrow\downarrow$		1	0	
$\langle -1,1|\langle +1|$	$\downarrow\uparrow$		0	1	
$\langle -1,1|\langle -1|$	$\downarrow\downarrow$				1

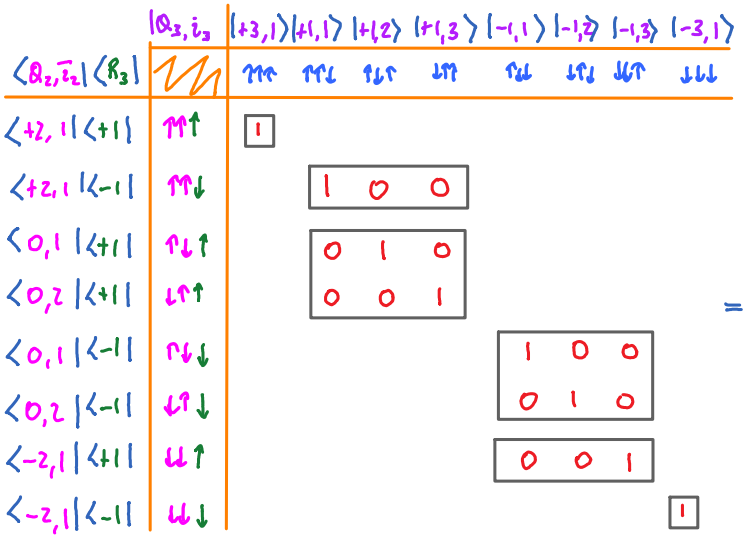
=:

ν	Q_1	R_2	Q_2	$M_1\times 1, M_2$	$\left(I^{Q_1R_2}{}_{Q_2}\right)^{\bar{i}_1}{}_{i_2}$
1	+1	+1	+2	1x1, 1	1
2	+1	−1	0	1x1, 2	1 0
3	−1	−1	0	1x1, 2	0 1
4	−1	−1	−2	1x1, 1	1

Sites 2 and 3

$$\left(I_3^{Q_2 R_3}{}_{Q_3}\right)^{\bar{\imath}_2}{}_{i} = \quad Q_2,\bar{\imath}_2 \rightarrow \overset{I_3}{\bullet} \rightarrow Q_3,i_3 \quad (R_3 \uparrow)$$

$Q_2 \in \{\pm 2, 0\}$
$R_3 \in \{\pm 1\}$
$Q_3 = Q_2 + R_3 \in \{\pm 3, \pm 1\}$



=:

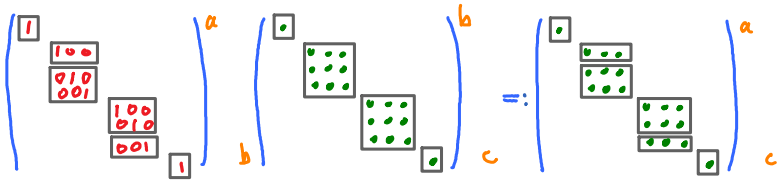
ν	Q_2	R_3	Q_3	$M_2 \times 1, M_3$	$(I^{Q_2 R_3}{}_{Q_3})^{\bar{\imath}_2}{}_{i_3}$
1	+2	+1	+3	1×1, 1	[1]
2	+2	−1	+1	1×1, 3	[1 0 0]
3	0	+1	+1	2×1, 3	[0 1 0; 0 0 1]
4	0	−1	−1	2×1, 3	[1 0 0; 0 1 0]
5	−2	+1	−1	1×1, 3	[0 0 1]
6	−2	−1	−3	1×1, 1	[1]

The scheme for producing such tables can be automated!

A-matrix obtained by diagonalizing H has same structure:

$$Q_2,\bar{\imath}_2 \rightarrow \overset{I_3}{\bullet} \rightarrow \overset{U_3}{\bullet} \rightarrow \bar{Q}_3,\bar{\imath}_3 \quad (R_3 \uparrow, Q_3,i_3) \quad =: \quad Q_2,\bar{\imath}_2 \rightarrow \overset{A_3}{\bullet} \rightarrow Q_3,i_3 \quad (R_3 \uparrow)$$

$$\left(I_{[3]}^{\overbrace{Q_2,R_3}^{a}}{}_{\underbrace{Q_3}_{b}}\right)^{\bar{\imath}_2}{}_{i_3} \left(U^{Q_3}{}_{\bar{Q}_3}\right)^{i_3}{}_{\bar{\imath}_3} \quad (\sim \mathbb{1}^{Q_3}{}_{\bar{Q}_3}) \quad =: \left(A_3{}^{Q_2,R_3}{}_{Q_3}\right)^{\bar{\imath}_2}{}_{\bar{\imath}_3}$$



$\doteq$

ν	Q_2	R_3	Q_3	$M_2 \times 1, M_3$	$(A^{Q_2 R_3}{}_{Q_3})^{\bar{\imath}_2}{}_{i_3}$
1	+2	+1	+3	1×1, 1	[•]
2	+2	−1	+1	1×1, 3	[• • •]
3	0	+1	+1	2×1, 3	[• •; • •]
4	0	−1	−1	2×1, 3	[• •; • •]
5	−2	+1	−1	1×1, 3	[• • •]
6	−2	−1	−3	1×1, 1	[•]