Symmetries I Abelian

NRG: [Wilson1975], [Toth2008], [Weichselbaum2012b] QSpace

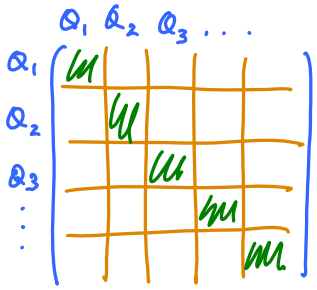
DMRG: [McCulloch2001], [McCulloch2002]

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

Goal: exploit symmetries of Hamiltonian!

If Hamiltonian has symmetries, $[\hat{H}, \hat{Q}] = 0$, then: (1)

(generator of symmetry group)



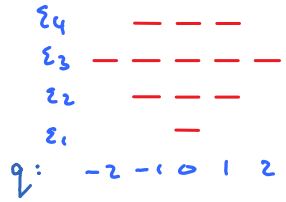
- $\hat{Q}$ and $\hat{H}$ can be diagonalized simultaneously:

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

(overbar will indicate energy eigenbasis)

- H connects only states with same Q , $\Rightarrow$ blockdiagonal
- for non-Abelian symmetries, eigenstates from degenerate multiplets,

$|Q q, \bar{\imath}\rangle$, where q distinguishes states within multiplet,
and $\bar{\imath}$ enumerates distinct multiplets.



Exploiting these structures reduces numerical costs!

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

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

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

This is obvious by inspection. But let us check explicitly:

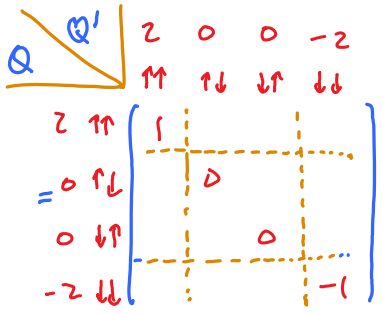
$\hat{Q} = 2\hat{S}^z_{tot}$ "charge" (to avoid ½ ...)

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

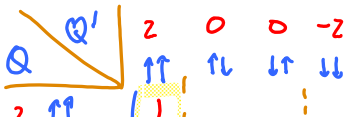
Consider direct-product space of sites 1 and 2, and its Hamiltonian H_{12}

$$\hat{S}^z_1 + \hat{S}^z_2 = \hat{S}^z_1 \otimes \hat{\mathbb{1}}_2 + \hat{\mathbb{1}}_1 \otimes \hat{S}^z_2 \quad (6)$$

$$= \begin{pmatrix} \frac{1}{2}\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & \\ & -\frac{1}{2}\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \end{pmatrix} + \begin{pmatrix} 1\cdot\begin{pmatrix} \frac{1}{2} & \\ & -\frac{1}{2} \end{pmatrix} & \\ & 1\cdot\begin{pmatrix} \frac{1}{2} & \\ & -\frac{1}{2} \end{pmatrix} \end{pmatrix}$$

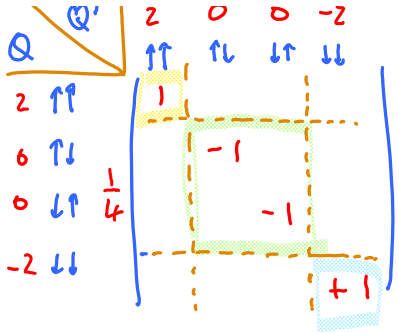


(7)



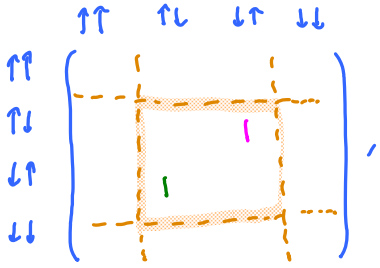
H_{12}

$$\hat{S}_1^z \hat{S}_2^z = \begin{pmatrix} \frac{1}{2}\left(\frac{1}{2}\right) & & & \\ & -\frac{1}{2}\left(\frac{1}{2}\right) & & \\ & & -\frac{1}{2}\left(-\frac{1}{2}\right) & \\ & & & \frac{1}{2}\left(-\frac{1}{2}\right) \end{pmatrix} =$$



(8)

$$\hat{S}_1^+ \hat{S}_2^- + \hat{S}_1^- \hat{S}_2^+ = \begin{pmatrix} 0 & & & \\ & 1\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & & \\ & & 1\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & \\ & & & 0 \end{pmatrix} =$$



(9)

Two observations:

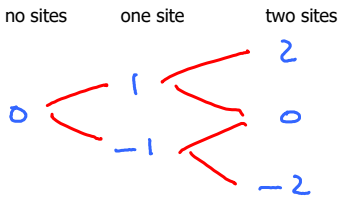
- $[\hat{S}^z_{tot}, \hat{H}_{12}] = 0$, $\Rightarrow$ $\hat{H}_{12}$ does not mix states with different values of S^z_{tot}.
- Eigenstates of $\hat{H}_{12}$ will carry $\hat{S}^z_{tot}$-eigenvalue as one of their quantum numbers. (10)

Programming challenge: exploit this 'sparse' structure to save memory and computation time!
We don't want to store large matrices with many zeros! Instead, store only relevant information!

Bookkeeping Use $Q = 2$ (Eigenvalue of $\hat{S}^z_{tot}$) as label: (11)

Label states as $|Q, i\rangle$, where i enumerate states with same Q.

Record of states needed to describe 2 sites:



record index ν	Q	i	explicit representation	state
1	2	1	1	$\|\uparrow\uparrow\rangle$
2	0	1	$(1,0)^T = \binom{1}{0}$	$\|\uparrow,\downarrow\rangle$
		2	$(0,1)^T = \binom{0}{1}$	$\|\downarrow,\uparrow\rangle$
3	-2	1	1	$\|\downarrow\downarrow\rangle$

(12)

Record of sectors ('blocks') of Hamiltonian for 2 sites:

record index ν	Q'	Q	$\langle Q'\|H\|Q\rangle \sim$
1	2	2	$\frac{1}{4} J_z$
2	0	0	$\frac{J}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{1}{4} J_z \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
3	-2	-2	$\frac{1}{4} J_z$

(13)

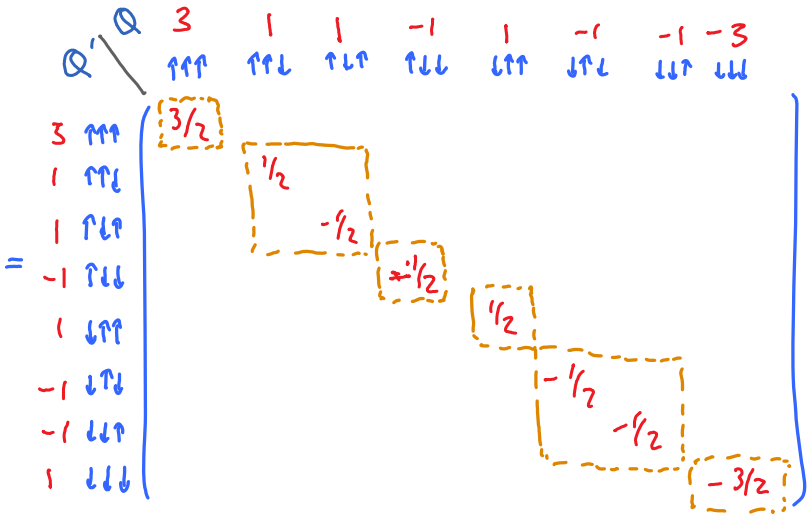
The task of diagonalizing Hamiltonian can be split into three separate tasks (two of which are trivial).

Consider direct-product space of sites 1 and 2 and 3:

Consider direct-product space of sites 1 and 2 and 3:

$$\hat{S}^z_{tot} = \hat{S}^z_1 + \hat{S}^z_2 + \hat{S}^z_3 = \hat{S}^z_1 \otimes \hat{\mathbb{1}}_2 \otimes \hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1 \otimes \hat{S}^z_2 \otimes \hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1 \otimes \hat{\mathbb{1}}_2 \otimes \hat{S}^z_3 \qquad (14)$$

$$= \begin{pmatrix} \frac{1}{2}\begin{pmatrix}1 & & \\ & 1 & \\ & & 1\end{pmatrix} & & \\ & -\frac{1}{2}\begin{pmatrix}1 & & \\ & 1 & \\ & & 1\end{pmatrix} & \\ & & \end{pmatrix} + \begin{pmatrix} 1\begin{pmatrix}1/2 & & \\ & 1/2 & \\ & & -1/2\end{pmatrix} & & \\ & -1/2\begin{pmatrix}1 & & \\ & 1 & \\ & & 1\end{pmatrix} & \\ & & 1\begin{pmatrix}1/2 & & \\ & -1/2 & \\ & & -1/2\end{pmatrix}\end{pmatrix} + \begin{pmatrix} 1\begin{pmatrix}1/2 & & \\ & -1/2 & \\ & & -1/2\end{pmatrix} & & \\ & 1\begin{pmatrix}-1/2 & & \\ & 1/2 & \\ & & -1/2\end{pmatrix} & \\ & & 1\begin{pmatrix}-1/2 & & \\ & -1/2 & \\ & & 1/2\end{pmatrix}\end{pmatrix} \qquad (15)$$



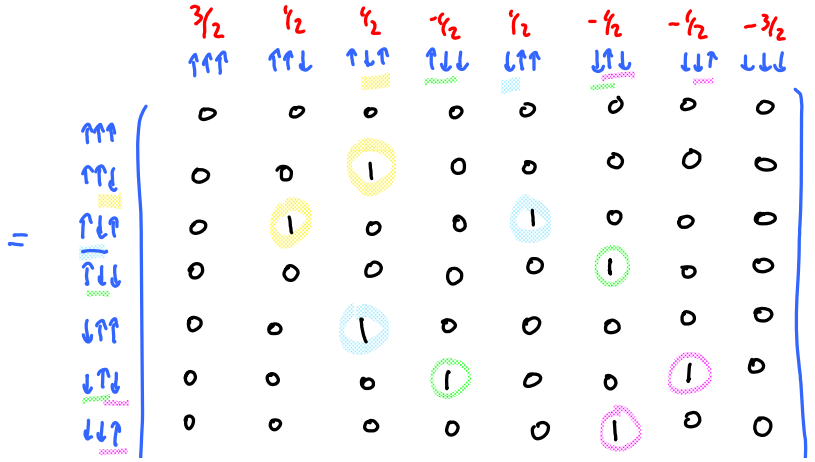
$$S^z_{tot} \in \{3/2, 1/2, -1/2, -3/2\}$$

degeneracy: 1 3 3 1

(16)

$$\frac{\hat{H}_{spin\text{-}flip}}{J/2} = \hat{S}^+_1 \hat{S}^-_2 \hat{\mathbb{1}}_3 + \hat{S}^-_1 \hat{S}^+_2 \hat{\mathbb{1}}_3 + \hat{\mathbb{1}}_1 \hat{S}^+_2 \hat{S}^-_3 + \hat{\mathbb{1}}_1 \hat{S}^-_2 \hat{S}^+_3 \qquad (17)$$

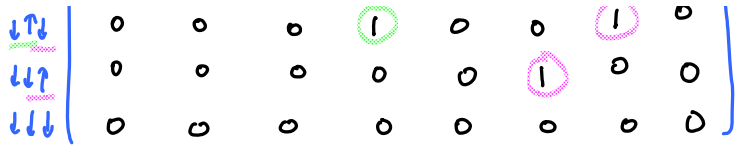
$$= \begin{pmatrix} & 1\cdot\begin{pmatrix}1 & & \\ & 1 & \\ & & 0\end{pmatrix} & \\ 0 & & \end{pmatrix} + \begin{pmatrix} & & 0 \\ 1\cdot\begin{pmatrix}1 & & \\ & 1 & \\ & & 0\end{pmatrix} & & \end{pmatrix} + \begin{pmatrix} 1\begin{pmatrix}0 & 1 & \\ & 0 & \\ & & 0\end{pmatrix} & & \\ & 1\begin{pmatrix}0 & 1 & \\ & 0 & \\ & & 0\end{pmatrix} & \end{pmatrix} + \begin{pmatrix} 1\begin{pmatrix}0 & & \\ & 0 & \\ & & 1\end{pmatrix} & & \\ & 1\begin{pmatrix}0 & & \\ & 0 & \\ & & 1\end{pmatrix} & \end{pmatrix} \qquad (18)$$



direct-product scheme
does not automatically produce a
manifest block structure

to arrive at a block structure,
switch rows: 4 ⟷ 5
and columns: 4 ⟷ 5

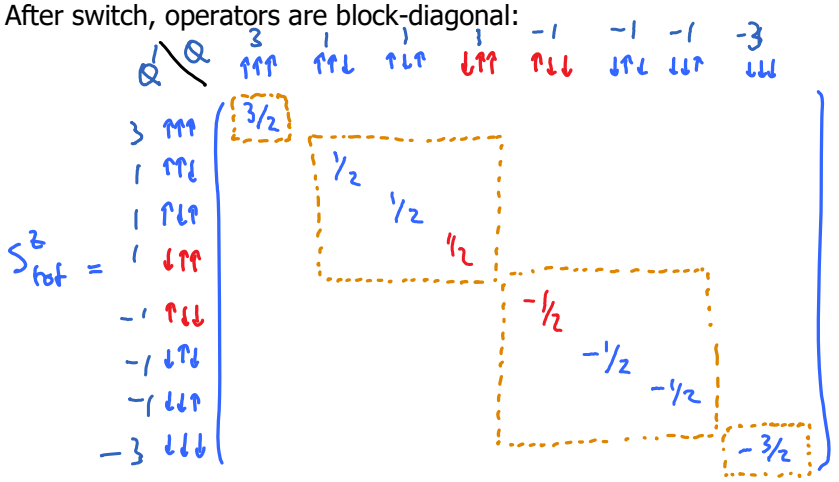
(19)



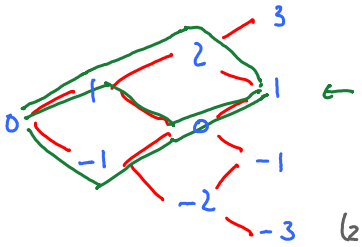
and columns: $4 \longleftrightarrow 5$

(19)

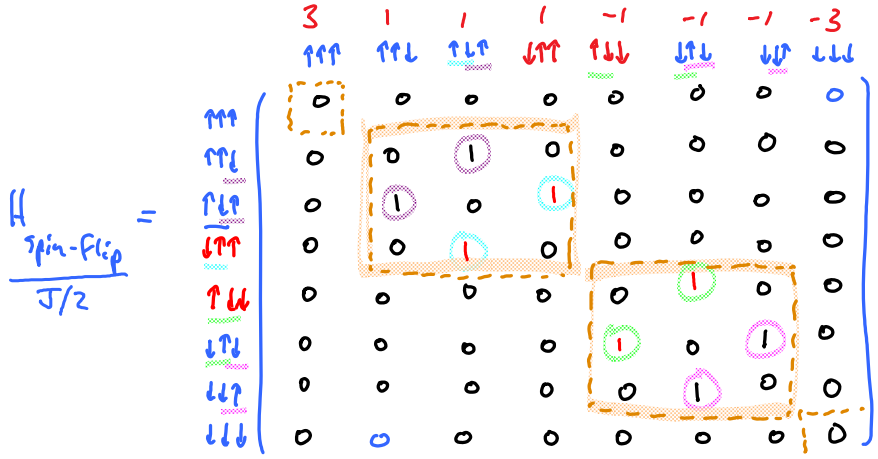
After switch, operators are block-diagonal:



there are several ways to obtain the same S^z_{tot} :



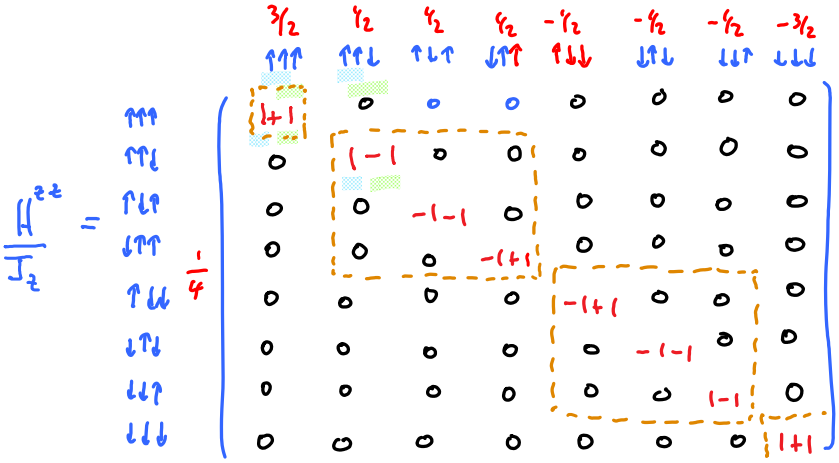
(20)



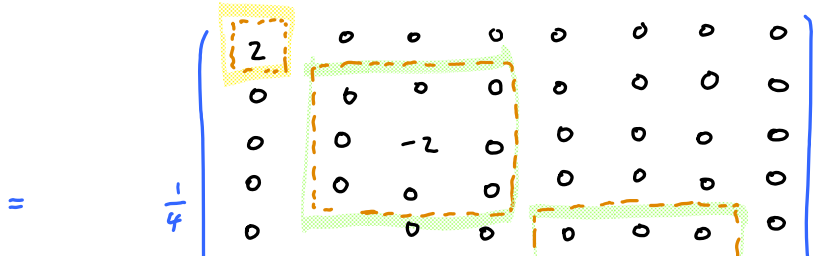
only connects states within block identified by unique total S^z_{tot} !

(21)

$$\frac{H^{zz}}{J_z} = \hat{S}^z_1 \hat{S}^z_2 \hat{\mathbb{1}} + \hat{\mathbb{1}} \hat{S}^z_2 \hat{S}^z_3 \qquad (22)$$



(23)



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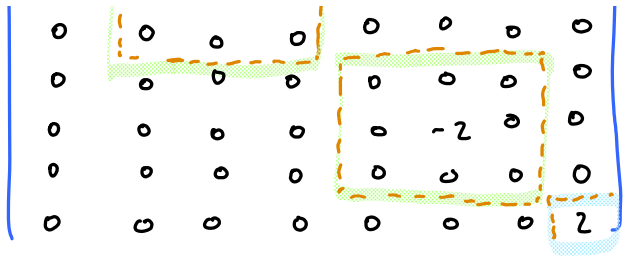
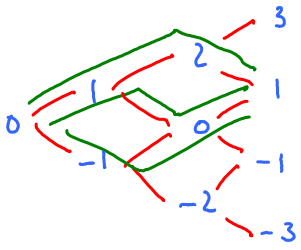
$=$ 

(24)

Bookkeeping Use Q = z(Eigenvalue of S^z_{tot}) as label: (25)

Record of states needed to describe 3 sites:



record index ν	Q	i	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	$\|\downarrow\downarrow\downarrow\rangle$

(26)

Record of sectors ('blocks') of Hamiltonian for 3 sites:

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

record index ν	Q'	Q	$\langle Q'\|H\|Q\rangle \sim \delta_{QQ'}$
1	3	3	$2 \cdot \frac{1}{4} J_z$
2	1	1	$\frac{J}{2}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix} + \frac{1}{4}J_z\begin{pmatrix}0&\\&-2\\&&0\end{pmatrix}$
3	-1	-1	$\frac{J}{2}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix} + \frac{1}{4}J_z\begin{pmatrix}0&\\&-2\\&&0\end{pmatrix}$
4	-3	-3	$2 \cdot \frac{1}{4} J_z$

(27)

Labelling scheme for Abelian symmetry

Suppose $[\hat{H}, \hat{Q}] = 0$, and $\hat{Q}$ -eigenstates are uniquely labeled by a single quantum number:

$\hat{Q}|Q\rangle = Q|Q\rangle$ (e.g. eigenstates of S^z_{tot}) (28)

Then all states in Hilbert space can be labeled by following scheme:

- 'Q-label' or 'symmetry label': Q , eigenvalues of $\hat{Q}$ $|Q, i\rangle$ (29)
- 'i-label' or 'multiplet label': i , enumerates different irreducible multiplets having the same Q (30)

  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: $|Q_\ell, i\rangle$)

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

$$H_{[Q]\,i}^{\;\;i'} = \langle Q,i'|\hat{H}|Q,i\rangle \tag{31}$$

Diagonalizing $H_{[Q]}$ yields symmetry- and energy eigenstates, $|Q,\bar{i}\rangle = |Q,i\rangle U_{[Q]}^{\;\;i}{}_{\bar{i}}$ (32)

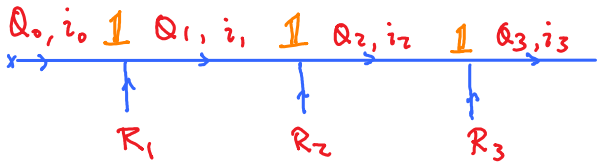
with eigenenergies $E_{[Q]\bar{i}}$ overbar will indicate energy eigenbasis

2. Iterative diagonalization with Abelian symmetry

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

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

Ket:

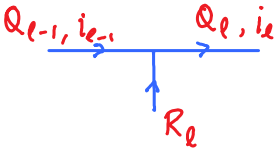


'sum rule' at each vertex:

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

Unit matrix transforms to 'symmetry eigenbasis':

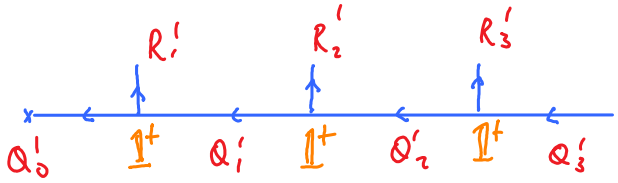
$$|Q_\ell, i_\ell\rangle = |R_\ell\rangle\, |Q_{\ell-1}, i_{\ell-1}\rangle\, \mathbb{1}^{Q_{\ell-1}, i_{\ell-1}; R_\ell}_{Q_\ell, i_\ell}$$



(2)

The i-index is usually not displayed in diagrams, and we will omit it henceforth.

Bra:

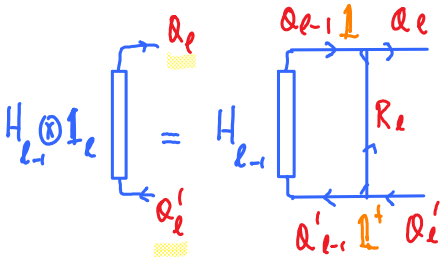


'sum rule' at each vertex:

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

$\mathbb{1}$-matrices encode the sum rules, thereby yielding a block-diagonal Hamiltonian.

Examples: Induction: if $H_{\ell-1}$ is block-diagonal, so is H_ℓ :

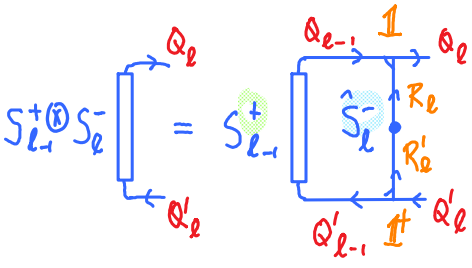


$$\langle Q'_{\ell-1}|H|Q_{\ell-1}\rangle \neq 0 \Rightarrow Q'_{\ell-1} = Q_{\ell-1} \qquad (4)$$

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

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

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)



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

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

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

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

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!

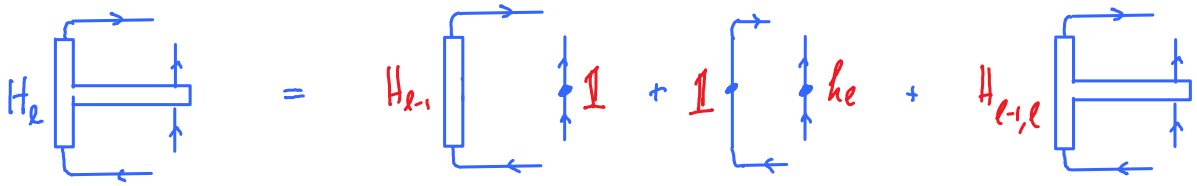
Strategy for iterative diagonalization

(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)

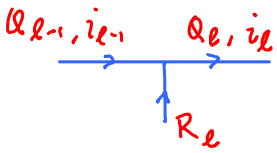
local term coupling between sites $\ell-1, \ell$



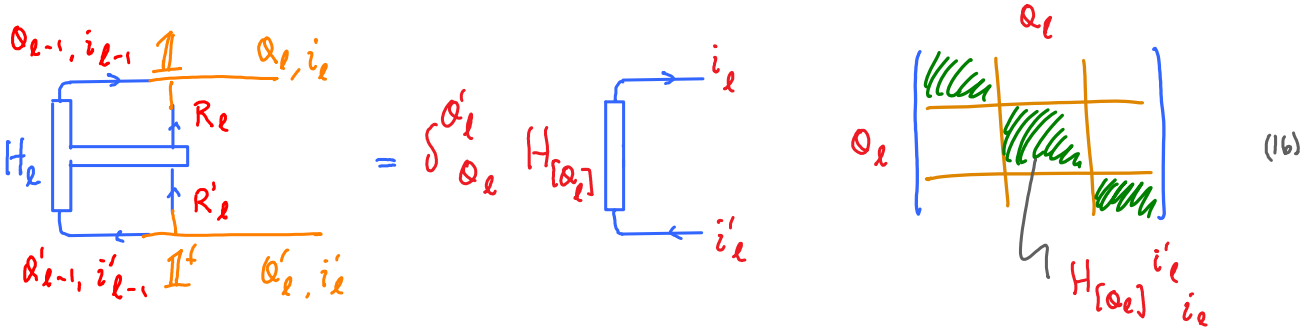
(14)

(ii) Symmetry eigenbasis:

$$|Q_\ell, i_\ell\rangle = |R_\ell\rangle\, |Q_{\ell-1}, i_{\ell-1}\rangle\, \mathbb{1}^{Q_{\ell-1}, i_{\ell-1}; R_\ell}_{Q_\ell, i_\ell}$$ (15)



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



(16)

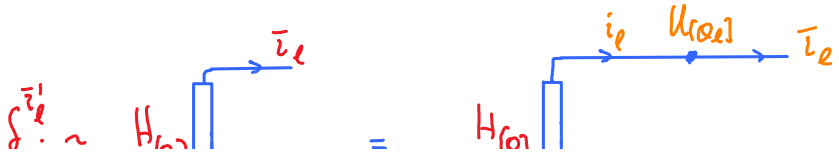
(iii) Diagonalize block:

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

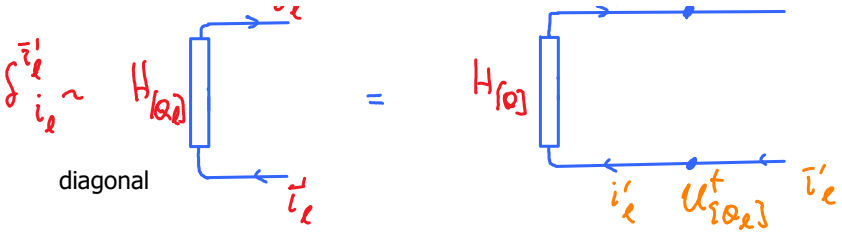
(iv) Transform to energy eigenbasis:

$$|Q_\ell, \bar{\imath}_\ell\rangle = |Q_\ell, i_\ell\rangle\, U^{i_\ell}_{[Q_\ell]\,\bar{\imath}_\ell}$$ (18)

Applying this transformation to H_ℓ yields diagonal representation:

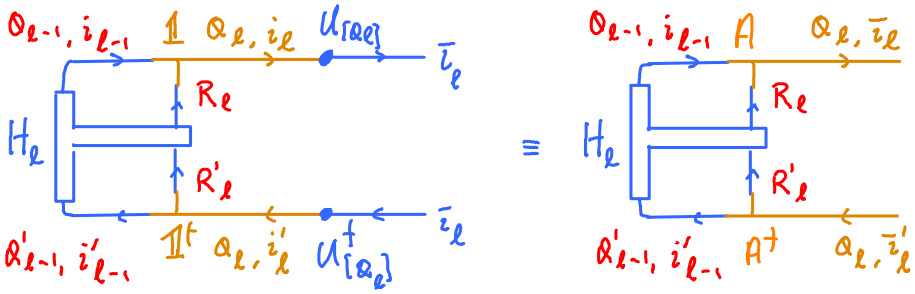


(19)

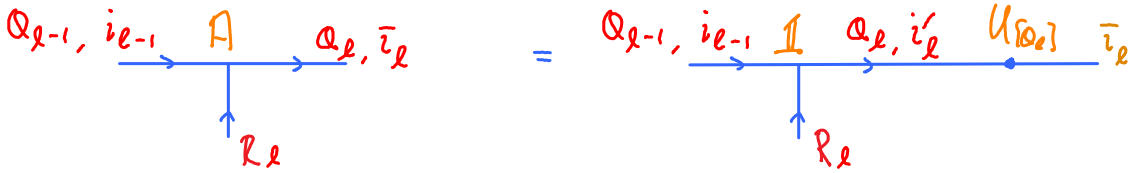


(19)

(16)
=



So, desired transformation from old to new eigenbasis is:

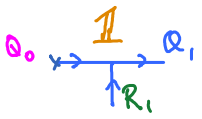


(Only A-matrices need to be saved to disk.)

3. Bookkeeping for unit matrices

Sym-I.3

Sites 0 and 1



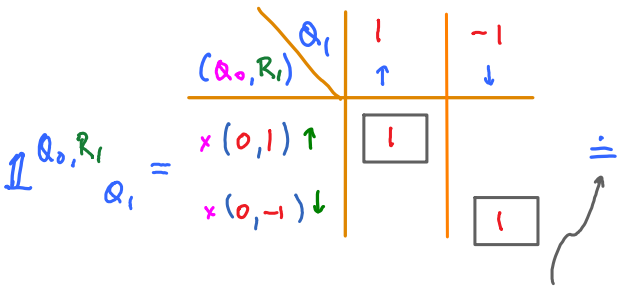


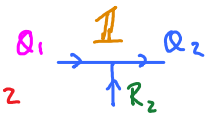
Table lists (Q_0, R_1) combinations yielding Q_1

record index ν	bond 0 Q_0	site 1 R_1	bond 1 Q_1	data
1	0	1	1	1
2	0	−1	−1	1

Green arrows indicate R_1, blue arrows Q_1

save only nonzero entries (as when dealing with sparse matrices)

Sites 1 and 2



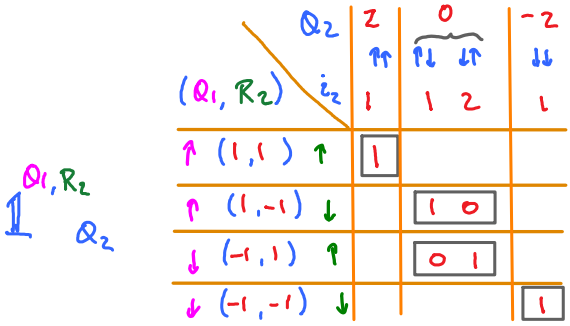
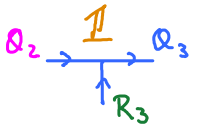


Table lists (Q_1, R_2) combinations yielding Q_2

record index ν	bond 1 Q_1	site 2 R_2	bond 2 Q_2	data
1	1	1	2	1
2	1	−1	0	1 0
3	−1	1	0	0 1
4	−1	−1	−2	1

Magenta arrows indicate Q_1, green,arrows R_2, blue arrows Q_2

Sites 2 and 2



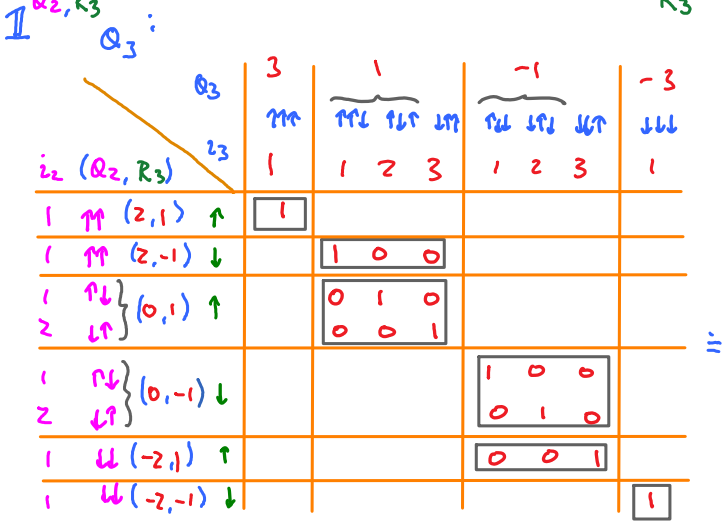


Table lists (Q_2, R_3) combinations yielding Q_3

record index ν	bond 2 Q_2	site 3 R_3	bond 3 Q_3	data
1	2	1	3	1
2	2	−1	1	1 0 0
3	0	1	1	0 1 0 0 0 1
4	0	−1	−1	1 0 0 0 1 0
5	−2	1	−1	0 0 1
6	−2	−1	−3	1

Magenta arrows indicate Q_2, green,arrows R_3, blue arrows Q_3

The scheme for producing such tables can be automated!

Full A-matrix obtained by diagonalizing H has similar structure: