Symmetries II: Non-Abelian

1. Motivation, review of SU(2) basics

Consider Heisenberg spin chain: $\hat{H} = J \sum_\ell \vec{S}_\ell \cdot \vec{S}_{\ell+1}$ has SU(2) symmetry. (1)

Define $\quad \hat{\vec{S}}_{tot} = \sum_\ell \hat{\vec{S}}_\ell \quad , \quad \hat{S}^z_{tot} \quad , \quad \hat{\vec{S}}^2_{tot}$ are SU(2) generators. (2)

then $\quad [\hat{H}, \hat{S}^z_{tot}] = 0, \quad [\hat{H}, \hat{S}^2_{tot}] = 0$ (3)

Symmetry eigenstates can be labeled $|S, i; s\rangle$ (4)

upper case S

'multiplet label' distinguishes multiplets having same spin S

lower case s distinghuises states within multiplet

with

$$\hat{S}^z_{tot} |S, i; s\rangle = s |S, i; s\rangle \quad (5)$$

$$\hat{S}^2_{tot} |S, i; s\rangle = S(S+1) |S, i; s\rangle \quad (6)$$

$$\langle S', i'; s' | \hat{H} | S, i; s\rangle = \delta^{S'}_{S} \, \delta^{s'}_{s} \, [H_{[S]}]^{i'}{}_{i} \quad (7)$$

reduced matrix elements

For each S , we just have to find the reduced Hamiltonian $H_{[S]}{}^{i'}{}_{i}$ and diagonalize it.

Goal: find systematic way of dealing with multiplet structure in a consistent manner.

Reminder: SU(2) basics

SU(2) generators:
$a, b, c \in \{x, y, z\}$

$$[\hat{S}^a, \hat{S}^b] = i\varepsilon^{abc} \hat{S}^c \quad , \quad \hat{S}^\pm = \hat{S}^x \pm i \hat{S}^y \quad (8)$$

$$[\hat{S}^z, \hat{S}^\pm] = \pm \hat{S}^\pm \quad , \quad [\hat{S}^+, \hat{S}^-] = 2 \hat{S}_z \quad (9)$$

Casimir operator: $\quad \hat{\vec{S}}^2 = (\hat{S}^x)^2 + (\hat{S}^y)^2 + (\hat{S}^z)^2$ (10)

Commuting operators: $\quad [\hat{S}_z, \hat{\vec{S}}^2] = 0$ (11)

Irreducible multiplet:

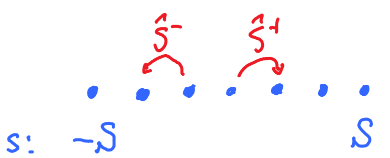
$$\hat{\vec{S}}^2 |S, s\rangle = S(S+1) |S, s\rangle \quad , \quad S = 0, \tfrac{1}{2}, 1, \tfrac{3}{2} \ldots \quad (12)$$

$$\hat{S}_z |S, s\rangle = s |S, s\rangle \qquad s = -S, -S+1, \ldots, S \quad (13)$$

Dimension of multiplet: $\quad d_S = 2S + 1$ (14)

Highest weight state: $\quad \hat{S}^+ |S, S\rangle = 0$ (15)

Lowest weight state: $\quad \hat{S}^- |S, -S\rangle = 0$ (16)

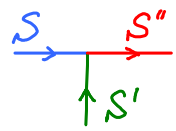


2. Tensor product decomposition (needed when adding new site to chain)

Irreducible representation (irrep) of symmetry group forms a vector space:

$$V^{S} \equiv \mathrm{span}\{\, |S, s\rangle \,|\, s = -S, \dots, S \,\} \qquad (1)$$

Decomposition of tensor product of two irreps into direct sum of irreps:



$$V^{S} \otimes V^{S'} = \sum_{\oplus S'' = |S-S'|}^{S+S'} V^{S''} = \sum_{\oplus S''} N^{SS'}{}_{S''} V^{S''} \qquad (2)$$

'Outer multiplicity' $N^{SS'}{}_{S''}$ is an integer specifiying how often the irrep S'' occurs in the decomposition of the direct product $V^{S} \otimes V^{S'}$.

For SU(2), we have

$$N^{SS'}{}_{S''} = \begin{cases} 1 & \text{for } |S-S'| < S'' < S+S' \\ 0 & \text{otherwise} \end{cases} \qquad (3)$$

For other groups, e.g. $SU(N \geq 3)$, the outer multiplicity can be > 1.

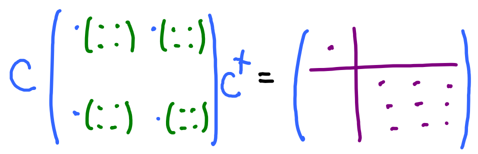
Action of generators:

$$\hat{C}^{\dagger} \left(\hat{S}^{a}_{1} \otimes \hat{\mathbb{1}}_{2} + \hat{\mathbb{1}}_{1} \otimes \hat{S}^{a}_{2} \right) \hat{C} = \sum_{\oplus S''} \hat{S}^{a} \qquad (4)$$

dimensions: $d_S \times d_S$ $\quad d_{S'} \times d_{S'}$ $\quad d_{S''} \times d_{S''}$

$\hat{C}$ transforms generators into block-diagonal form:

For $S = 1/2$, $S' = 1/2$:



(5)

The basis transformation $\hat{C}$ is encoded in Clebsch-Gordan coefficients (CGCs):

$$|S'', s''; S, S'\rangle = \overbrace{\sum_{s,s'} |S', s'\rangle \otimes |S, s\rangle \times \langle S, s| \otimes \langle S', s'|}^{\text{completeness in direct product space}} \, |S'', s''; S, S'\rangle \qquad (6)$$

$$\text{CGC} = \langle S, s | \otimes \langle S', s' | S'', s'', S, S'\rangle \equiv \left(C^{S,S'}{}_{S''} \right)^{s s'}{}_{s''}$$

$$= \sum_{s,s'} |S', s'\rangle \otimes |S, s\rangle \left(C^{S,S'}{}_{S''} \right)^{s s'}{}_{s''} \qquad (7)$$

States in new basis, $|S'', s'', S, S'\rangle$, are eigenstates of $(\hat{\vec{S}}_1 + \hat{\vec{S}}_2)^2$ with eigenvalue $S''(S''+1)$ (8a)

"	$\hat{\vec{S}}_1^{\,2}$	"	S	(8b)
"	$\hat{\vec{S}}_2^{\,2}$	"	S'	(8c)
"	$\hat{S}^z_1 + \hat{S}^z_2$	"	s''	(8d)

3. Tensor operators

An 'irreducible tensor operator' transforms as follows under a symmetry operation, $\hat{g} \in SU(2)$:

$$\hat{g}\, \hat{T}^{(S,s')}\, \hat{g}^{-1} = \sum_{s=-S}^{S} \underbrace{\mathcal{D}(g)^{s'}{}_{s}}_{\text{spin } S \text{ matrix representation of SU(2)}} \hat{T}^{(S,s)} \tag{1}$$

$$\hat{g}\, |S,s\rangle \to \mathcal{D}(g)^{s'}{}_{s}\, |S,s\rangle$$

Example 1: Heisenberg Hamiltonian is SU(2) invariant, hence transforms in $S = 0$ representation of SU(2): (scalar)

$$\hat{g}\, \hat{H}\, \hat{g}^{-1} = \hat{H} \tag{2}$$

Example 2: SU(2) generators, $\hat{S}^{+}, \hat{S}^{-}, \hat{S}^{z}$, transform in $S = 1$ (vector) representation of SU(2):

$$\hat{S}^{(S=1,\, s)} = \left(\tfrac{1}{\sqrt{2}} \hat{S}^{+},\ \hat{S}^{z},\ \tfrac{1}{\sqrt{2}} \hat{S}^{-} \right)^{T} \tag{3}$$

Wigner-Eckardt theorem

Every matrix element of a tensor operator factorizes as 'reduced matrix elements' times 'CGC':

$$\langle S, i; s \,|\, \hat{T}^{(S',s')} \,|\, S'', i''; s'' \rangle = \left(T^{SS'}{}_{S''} \right)^{i}{}_{i''} \underbrace{\langle S, s; S', s' \,|\, S'', s'' \rangle}_{\propto\, N^{SS'}{}_{S''}\, \delta^{s+s'}{}_{s''}} \tag{4}$$

CGCs encode sum rules:

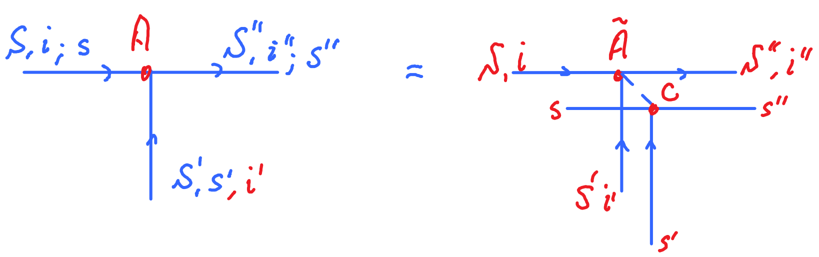
In particular, for Hamiltonian, which is a scalar operator: $(S' = 0,\ s' = 0)$

$$\langle S, i; s \,|\, \hat{H} \,|\, S'', i''; s'' \rangle = \underbrace{\left(H^{S,0}{}_{S''} \right)^{i}{}_{i''}}_{\equiv\, (H_{[S]})^{i}{}_{i''}} \underbrace{\langle S, s; 0, 0 \,|\, S'', s'' \rangle}_{\delta^{S}{}_{S''}\, \delta^{s}{}_{s''}} \tag{5, 5'}$$

Hamiltonian matrix for block S ⟶ $(H_{[S]})^{i}{}_{i''}$; sum rules

We will see: a factorization similar to (4) also holds for A -tensors of an MPS!

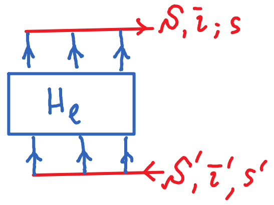
$$A^{(S,i;s),(S',s')}{}_{(S'',i'';s'')} = \left(\tilde{A}^{S,S'}{}_{S''} \right)^{ii'}{}_{i''} \left(C^{SS'}{}_{S''} \right)^{s,s'}{}_{s''} \tag{6}$$



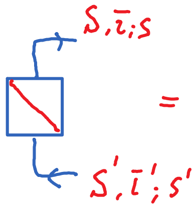
4. A-matrix factorizes

Why does A-matrix factorize? Consider generic step during iterative diagonalization:

Suppose Hamiltonian for sites 1 to ℓ has been diagonalized:

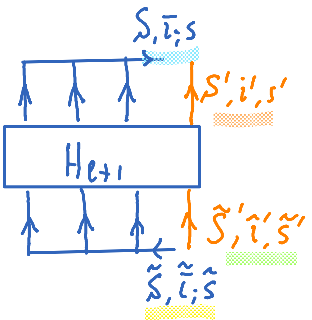


$= H_\ell$



$$= E^{\bar{i}}_{[S,s]}\,\delta^{S'}_{S}\,\delta^{\bar{i}'}_{\bar{i}}\,\delta^{s'}_{s} \qquad (7)$$

Add new site, with Hamiltonian for sites 1 to $\ell+1$ expressed in direct product basis of previous eigenbasis and physical basis of new site:



$$= |\tilde{S}',\tilde{i}';\tilde{s}'\rangle|\tilde{S},\tilde{i};\tilde{s}\rangle\,[H_{\ell+1}]^{(\tilde{S},\tilde{i};\tilde{s}|(\tilde{S}',\tilde{i}';\tilde{s}')}_{(S,\bar{i};s|(S',i';s')}\,\langle S,\bar{i};s|\langle S',i';s'| \qquad (8)$$

Transform to symmetry eigenbasis, i.e. make unitary tranformation into direct sum basis, using CGCs:

sums over all repeated indices implied:

$$\underbrace{\overbrace{|\tilde{S}''\tilde{i}''\tilde{s}''\rangle\langle\tilde{S}''\tilde{i}''\tilde{s}''|}^{\mathbb{1}}\,|S',i',s'\rangle|\tilde{S},\tilde{i};\tilde{s}\rangle\,[H_{\ell+1}]^{(\tilde{S},\tilde{i};\tilde{s}|(\tilde{S}',\tilde{i}';\tilde{s}')}_{(S,\bar{i};s|(S',i';s')}\,\langle S,\bar{i};s|\langle S',i';s'|\overbrace{|S''i''s''\rangle\langle S''i''s''|}^{\mathbb{1}}}_{[C^{\dagger s''}_{s's}]^{S''}_{S'S}\,\mathbb{1}^{\tilde{i}''}_{i'\tilde{i}}\,[H^{\tilde{S}''S''}_{\tilde{s}''s''}]^{\tilde{i}''}_{i''}\,[C^{SS'}_{S''}]^{ss'}_{s''}\,\mathbb{1}^{\bar{i},i'}_{i''}} \qquad (9)$$

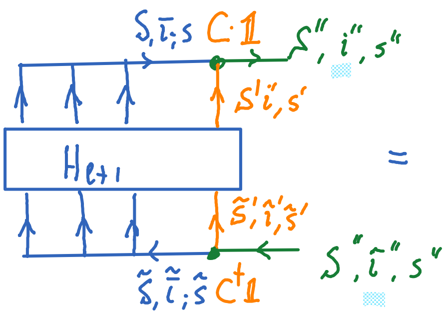
By Wigner-Eckardt theorem:
diagonal in all symmetry labels!

$$= \delta^{\tilde{S}''}_{S''}\,\delta^{\tilde{s}''}_{s''}\,[H_{[S'']}]^{\tilde{i}''}_{i''} \qquad (10)$$

H couples multiplets $\tilde{i}''$, i'' from same symmetry sector,
states within each multiplet are left unchanged/not scrambled

block labeled by S''
with elements labeled by $\tilde{i}''_{\;i''}$

Diagrammatic depiction is more transparent / less cluttered:



$$= |S'',\tilde{i}'',s''\rangle\,[H_{[S'']}]^{\tilde{i}''}_{i''}\,\langle S'',i'';s''| \qquad (11)$$

Now diagonalize and make unitary transformation into energy eigenbasis:

composite index: $i'' = (\bar{i}, i')$

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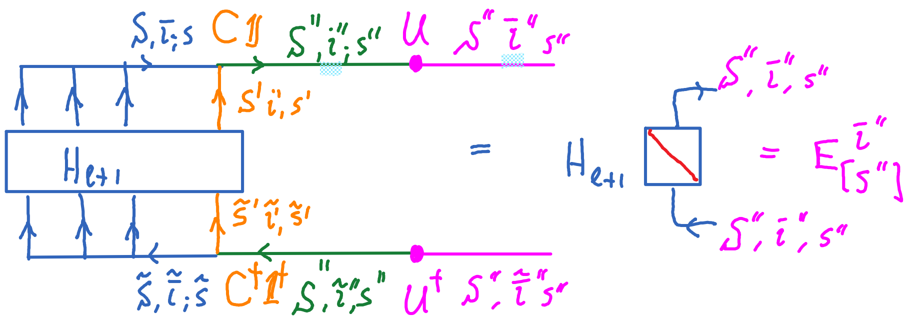
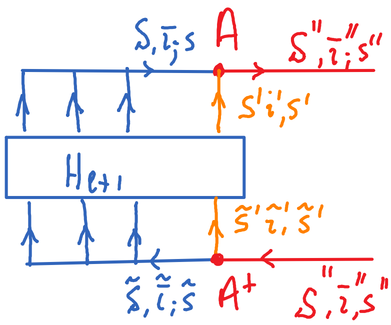
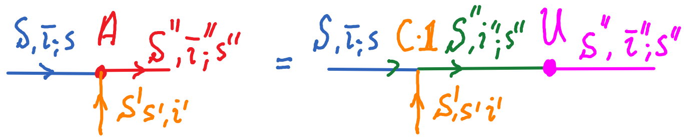


(12)

Combined transformation from old energy eigenbasis to new energy eigenbasis:



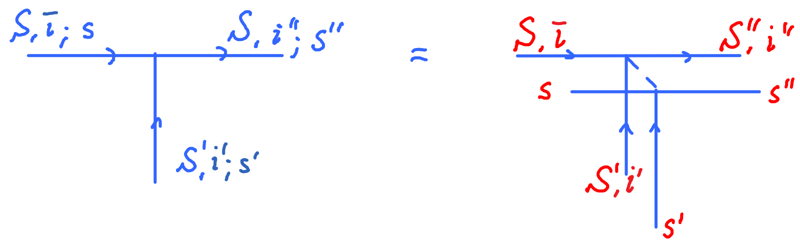


(13)

$$A^{(S,\bar i;s)(S's')}{}_{(S'',\bar i'';s'')} = \left[C^{SS'}{}_{S''}\right]^{ss'}{}_{s''} \mathbb{1}^{\bar i i'}{}_{i''} \left[U_{[S'']}\right]^{i''}{}_{\bar i''} \tag{14}$$

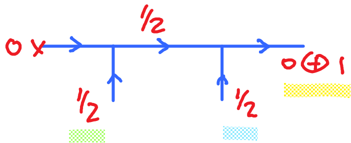
$$\equiv \left[\tilde A^{SS'}{}_{S''}\right]^{\bar i, i'}{}_{\bar i''} \left[C^{SS'}{}_{S''}\right]^{ss'}{}_{s''}$$

A-matrix factorizes, into product of reduced A-matrix and CGC !! $A = \tilde A \cdot C$ (15)



5. Example: direct product of two spin 1/2's

$$V^{1/2} \otimes V^{1/2} = V^{0} \oplus V^{1}$$



Local state space for spin $\frac{1}{2}$: $\quad |\uparrow\rangle = |\tfrac12, \tfrac12\rangle , \qquad |\downarrow\rangle = |\tfrac12, -\tfrac12\rangle .$ (1)

Singlet:
$$|S,s\rangle = |0,0\rangle = \tfrac{1}{\sqrt2}\big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\big) \tag{2}$$
$$= \tfrac{1}{\sqrt2}\big(|\tfrac12,\tfrac12;\tfrac12,-\tfrac12\rangle - |\tfrac12,-\tfrac12;\tfrac12,\tfrac12\rangle\big) \tag{3}$$

Triplet:
$$|S,s\rangle = \begin{cases} |1,1\rangle = |\uparrow\downarrow\rangle & (4) \\ |1,0\rangle = \tfrac{1}{\sqrt2}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big) & (5) \\ |1,-1\rangle = |\downarrow\downarrow\rangle & (6) \end{cases}$$

Transformation matrix for decomposing the direct product representation into direct sum:

$$\Big(C^{\frac12\ \frac12}_{\ \ [2]\ S''}\Big)^{ss'}_{\ \ s''} = \langle \tfrac12, s; \tfrac12, s' | S'' s''\rangle = \begin{array}{cc} & \begin{array}{cccc} |0,0\rangle & |1,1\rangle & |1,0\rangle & |1,-1\rangle \end{array} \\ \begin{array}{c} \uparrow\uparrow\ \langle\frac12,\frac12;\frac12,\frac12| \\ \uparrow\downarrow\ \langle\frac12,\frac12;\frac12,-\frac12| \\ \downarrow\uparrow\ \langle\frac12,-\frac12;\frac12,\frac12| \\ \downarrow\downarrow\ \langle\frac12,-\frac12;\frac12,-\frac12| \end{array} & \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt2 & 0 & 1/\sqrt2 & 0 \\ -1/\sqrt2 & 0 & 1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \tag{7}$$

site 2

<u>Check</u>

Let us transform some operators from direct product basis into direct sum basis:

$S = \frac12$ repr. of SU(2) generators: $\quad S_1^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S_1^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad S_1^z = \begin{pmatrix} \frac12 & \\ & -\frac12 \end{pmatrix}$ (7)

In direct product basis, the generators have the form

$$S^+ = S_1^+ \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes S_2^+ = \begin{bmatrix} 0 & 1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix} \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 1\cdot\begin{pmatrix}0 & 1\\0 & 0\end{pmatrix} & 0 \\ 0 & 1\cdot\begin{pmatrix}0 & 1\\0 & 0\end{pmatrix}\end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{8}$$

$$S^- = S_1^- \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes S_2^- = \begin{bmatrix} 0 & 0 \\ 1\begin{pmatrix}1 & \\ & 1\end{pmatrix} & 0 \end{bmatrix} + \begin{bmatrix} 1\cdot\begin{pmatrix}0 & 0\\1 & 0\end{pmatrix} & 0 \\ 0 & 1\cdot\begin{pmatrix}0 & 0\\1 & 0\end{pmatrix}\end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix} \tag{9}$$

$$S^z = S_1^z \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes S_2^z = \tfrac12\begin{bmatrix} 1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix} & 0 \\ 0 & -1\cdot\begin{pmatrix}1 & \\ & 1\end{pmatrix}\end{bmatrix} + \tfrac12\begin{bmatrix} 1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix} & 0 \\ 0 & 1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix}\end{bmatrix} = \begin{bmatrix} 1+1 & & & \\ & 1-1 & & \\ & & -1+1 & \\ & & & -1-1 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{bmatrix} \tag{10}$$

Transformed into new basis, all operators are block-diagonal:

$$\tilde{S}^+ = C^\dagger_{[2]} S^+ C_{[2]} = \begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 \end{array}\right) \quad (11)$$

$$\tilde{S}^- = C^\dagger_{[2]} S^- C_{[2]} = \begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \end{array}\right) \quad (12)$$

$$\tilde{S}^z = C^\dagger_{[2]} S^z C_{[2]} = \begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{array}\right) \quad (13)$$

These 4x4 matrices indeed satisfy $\quad [\tilde{S}^z, \tilde{S}^\pm] = \pm \tilde{S}^\pm, \quad [\tilde{S}^+, \tilde{S}^-] = 2\tilde{S}^z \quad (14)$

So, they form a representation of the SU(2) operator algebra on the <u>reducible</u> space $V^0 \oplus V^1$

Futhermore, we identify: on V^0: $\quad S^+ = S^- = S^z = 0 \quad (15)$

on V^1: $\quad S^+ = \sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad S^- = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^z = \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix} \quad (16)$

Now consider the coupling between sites 1 and 2, $\vec{S}_1 \cdot \vec{S}_2$. How does it look in the new basis?

$$S_1^z \otimes S_2^z = \frac{1}{4}\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \Rightarrow \widetilde{S_1^z \otimes S_2^z} = C^\dagger_{[2]}(S_1^z \otimes S_2^z)C_{[2]} = \frac{1}{4}\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (17)$$

$$\frac{1}{2} S_1^+ \otimes S_2^- = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \frac{1}{2}\widetilde{S_1^+ \otimes S_2^-} = C^\dagger_{[2]}\frac{1}{2}(S_1^+ \otimes S_2^-)C_{[2]} = \frac{1}{4}\begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (18)$$

$$\frac{1}{2} S_1^- \otimes S_2^+ = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \frac{1}{2}\widetilde{S_1^- \otimes S_2^+} = C^\dagger_{[2]}\frac{1}{2}(S_1^- \otimes S_2^+)C_{[2]} = \frac{1}{4}\begin{pmatrix} -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (19)$$

These matrices are <u>not</u> block-diagonal, since the operators represented by them break SU(2) symmetry.

But their sum, yielding $\vec{S}_1 \cdot \vec{S}_2$, is block-diagonal:

$$C^\dagger_{[2]}(\vec{S}_1 \otimes \vec{S}_2)C_{[2]} = C^\dagger_{[2]}\left(S_1^z \otimes S_2^z + \frac{1}{2}[S_1^+ \otimes S_2^- + S_1^- \otimes S_2^+]\right)C_{[2]} = \frac{1}{4}\left(\begin{array}{c|ccc} -3 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right) \quad (20)$$

The diagonal entries are consistent with the identity

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}\left[(\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^{\,2} - \vec{S}_2^{\,2}\right] = \begin{cases} \frac{1}{2}\left(0 \cdot 1 - \frac{1}{2}\cdot\frac{3}{2} - \frac{1}{2}\cdot\frac{3}{2}\right) = -\frac{3}{4} & \text{for } S'' = 0 \\ \frac{1}{2}\left(1 \cdot 2 - \frac{1}{2}\cdot\frac{3}{2} - \frac{1}{2}\cdot\frac{3}{2}\right) = \frac{1}{4} & \text{for } S'' = 1 \end{cases} \quad (21)$$

In section Sym-II.5 we will need $\mathbb{1}_1 \cdot \vec{S}_2 \cdot \vec{S}_3$. In preparation for that, we here compute

$$\mathbb{1}_1 \otimes S_2^z = \tfrac{1}{2}\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & +1 & \\ & & & -1 \end{pmatrix} \Longrightarrow \widetilde{\mathbb{1}_1 \otimes S_2^z} = C^\dagger_{[2]}\left(\mathbb{1}_1 \otimes S_2^z\right)C_{[2]} = \tfrac{1}{2}\begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \quad (22)$$

$$\mathbb{1}_1 \otimes S_2^+ = \tfrac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Longrightarrow \widetilde{\mathbb{1}_1 \otimes S_2^+} = C^\dagger_{[2]}\left(\mathbb{1}_1 \otimes S_2^+\right)C_{[2]} = \tfrac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (23)$$

$$\mathbb{1}_1 \otimes S_2^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \Longrightarrow \widetilde{\mathbb{1}_1 \otimes S_2^-} = C^\dagger_{[2]}\left(\mathbb{1}_1 \otimes S^+_-\right)C_{[2]} = \tfrac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \end{bmatrix} \quad (24)$$

<u>Another example:</u> $V^1 \oplus V^{1/2}$ (not relevant for spin-1/2 chain)

$$S_1^z \otimes S_2^z = \tfrac{1}{2}\begin{pmatrix} 1\cdot\begin{pmatrix}1 & \\ & -1\end{pmatrix} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1\begin{pmatrix}1 & \\ & -1\end{pmatrix} \end{pmatrix} \Longrightarrow C^\dagger\left(S_1^z \otimes S_2^z\right)C = \widetilde{S_1^z \otimes S_2^z} = \begin{bmatrix} -\frac{1}{3} & 0 & 0 & -\frac{1}{\sqrt{18}} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 & 0 & \frac{1}{\sqrt{18}} & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{\sqrt{18}} & 0 & 0 & -\frac{1}{6} & 0 & 0 \\ 0 & \frac{1}{\sqrt{18}} & 0 & 0 & -\frac{1}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \quad (25)$$

$$\tfrac{1}{2} S_1^+ \otimes S_2^- = \tfrac{1}{2}\begin{pmatrix} 0 & \sqrt{2}\begin{pmatrix}0 & 0 \\ 1 & 0\end{pmatrix} & 0 \\ 0 & 0 & \sqrt{2}\begin{pmatrix}0 & 0 \\ 1 & 0\end{pmatrix} \\ 0 & 0 & 0 \end{pmatrix} \Longrightarrow \tfrac{1}{2}\widetilde{S_1^+ \otimes S^-} = \begin{bmatrix} -\frac{1}{3} & 0 & 0 & \sqrt{2/9} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 & 0 & \frac{1}{\sqrt{18}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{18}} & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & -\sqrt{2/9} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (26)$$

$$\tfrac{1}{2} S_1^- \otimes S_2^+ = \tfrac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2}\begin{pmatrix}0 & 1 \\ 0 & 0\end{pmatrix} & 0 & 0 \\ 0 & \sqrt{2}\begin{pmatrix}0 & 1 \\ 0 & 0\end{pmatrix} & 0 \end{pmatrix} \Longrightarrow \tfrac{1}{2}\widetilde{S_1^- \otimes S_2^+} = \begin{bmatrix} -\frac{1}{3} & 0 & 0 & -\frac{1}{\sqrt{18}} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 & 0 & -\sqrt{\frac{2}{9}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{2/9} & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{\sqrt{18}} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (27)$$

The sum of these three terms yields:

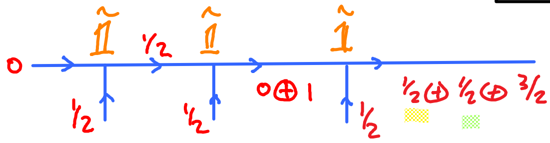
$$\widetilde{\vec{S}_1 \otimes \vec{S}_2} = \left[\begin{array}{cc|cccc} -1 & & & & & \\ & -1 & & & & \\ \hline & & \frac{1}{2} & & & \\ & & & \frac{1}{2} & & \\ & & & & \frac{1}{2} & \\ & & & & & \frac{1}{2} \end{array}\right] \quad (28)$$

The diagonal entries are consistent with the identity

$$\vec{S}_1 \cdot \vec{S}_2 = \tfrac{1}{2}\left[\left(\vec{S}_1 + \vec{S}_2\right)^2 - \vec{S}_1^{\,2} - \vec{S}_2^{\,2}\right] = \begin{cases} \frac{1}{2}\left(\frac{1}{2}\cdot\frac{3}{2} - 1\cdot 2 - \frac{1}{2}\cdot\frac{3}{2}\right) = -1 & \text{for } S'' = \frac{1}{2} \\ \frac{1}{2}\left(\frac{3}{2}\cdot\frac{5}{2} - 1\cdot 2 - \frac{1}{2}\cdot\frac{3}{2}\right) = \frac{1}{2} & \text{for } S'' = \frac{3}{2} \end{cases} \quad (29)$$

6. Example: direct product of three spin-1/2 sites

$$(V^0 \oplus V^1) \otimes V^{1/2} = V^{1/2} \oplus V^{1/2} \oplus V^{3/2} \qquad (1)$$



$$|S''=\tfrac12,\ i=1;\ s''\rangle: \quad \begin{aligned} |\tfrac12,\tfrac12\rangle &= 1.\ |0,0\rangle \otimes |\tfrac12,\tfrac12\rangle \\ |\tfrac12,-\tfrac12\rangle &= 1.\ |0,0\rangle \otimes |\tfrac12,-\tfrac12\rangle \end{aligned} \qquad (2)$$

$$|S''=\tfrac12,\ i=2;\ s''\rangle: \quad \begin{aligned} |\tfrac12,\tfrac12\rangle &= \sqrt{\tfrac23}\,|1,1\rangle \otimes |\tfrac12,-\tfrac12\rangle - \tfrac{1}{\sqrt3}\,|1,0\rangle \otimes |\tfrac12,\tfrac12\rangle \\ |\tfrac12,-\tfrac12\rangle &= \tfrac{1}{\sqrt3}\,|1,0\rangle \otimes |\tfrac12,-\tfrac12\rangle - \sqrt{\tfrac23}\,|1,-1\rangle \otimes |\tfrac12,\tfrac12\rangle \end{aligned} \qquad (3)$$

$$|S''=\tfrac32,\ i=1;\ s''\rangle: \quad \begin{aligned} |\tfrac32,\tfrac32\rangle &= 1.\ |1,1\rangle \otimes |\tfrac12,\tfrac12\rangle \\ |\tfrac32,\tfrac12\rangle &= \tfrac{1}{\sqrt3}\,|1,1\rangle \otimes |\tfrac12,-\tfrac12\rangle + \sqrt{\tfrac23}\,|1,0\rangle \otimes |\tfrac12,\tfrac12\rangle \\ |\tfrac32,-\tfrac12\rangle &= \sqrt{\tfrac23}\,|1,0\rangle \otimes |\tfrac12,-\tfrac12\rangle + \tfrac{1}{\sqrt3}\,|1,-1\rangle \otimes |\tfrac12,\tfrac12\rangle \\ |\tfrac32,-\tfrac32\rangle &= 1.\ |1,-1\rangle \otimes |\tfrac12,-\tfrac12\rangle \end{aligned} \qquad (4)$$

Clebsch-Gordan coefficients:

$$\left(C^{SS'}_{[3]\,S''}\right)^{ss'}_{\ \ s''} = \langle S,s;S',s'|S'',s''\rangle:$$

	$\vert\frac12,\frac12\rangle$	$\vert\frac12,-\frac12\rangle$	$\vert\frac12,\frac12\rangle$	$\vert\frac12,-\frac12\rangle$	$\vert\frac32,\frac32\rangle$	$\vert\frac32,\frac12\rangle$	$\vert\frac32,-\frac12\rangle$	$\vert\frac32,-\frac32\rangle$
$\langle 0,0;\frac12,\frac12\vert$	1	0						
$\langle 0,0;\frac12,-\frac12\vert$	0	1						
$\langle 1,1;\frac12,\frac12\vert$			0	0	1	0	0	0
$\langle 1,1;\frac12,-\frac12\vert$			$\sqrt{2/3}$	0	0	$1/\sqrt3$	0	0
$\langle 1,0;\frac12,\frac12\vert$			$-1/\sqrt3$	0	0	$\sqrt{2/3}$	0	0
$\langle 1,0;\frac12,-\frac12\vert$			0	$1/\sqrt3$	0	0	$\sqrt{\frac23}$	0
$\langle 1,-1;\frac12,\frac12\vert$			0	$-1/\sqrt3$	0	0	$1/\sqrt3$	0
$\langle 1,-1;\frac12,-\frac12\vert$			0	0	0	0	0	1

(5)

Let us find $H_{12} + H_{23} = \vec{S}_1\cdot\vec{S}_2\cdot\mathbb{1}_3 + \mathbb{1}_1\cdot\vec{S}_2\cdot\vec{S}_3$ in this basis. (6)

Combining (Sym-II.~~4~~5, (17-19)) $\otimes\, \mathbb{1}_3$ with (Sym-II.~~4~~5, (22-24)) $\cdot\, \vec{S}_3$, we readily obtain

$$\vec{S}_1\cdot\vec{S}_2\cdot\mathbb{1}_3 + \mathbb{1}_1\cdot\vec{S}_2\cdot\vec{S}_3 = C^\dagger_{[3]}\left(\vec{S}_1\cdot\vec{S}_2\cdot\mathbb{1}_3 + \mathbb{1}_1\cdot\vec{S}_2\cdot\vec{S}_3\right)C_{[3]} \qquad (10)$$

$$C^\dagger_{[3]} \begin{bmatrix} -\frac34 & 0 & 0 & \frac{1}{2\sqrt2} & -\frac14 & 0 & 0 & 0 \\ 0 & -\frac34 & 0 & 0 & 0 & \frac14 & -\frac{1}{2\sqrt2} & 0 \\ 0 & 0 & \frac12 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2\sqrt2} & 0 & 0 & 0 & \frac{1}{2\sqrt2} & 0 & 0 & 0 \\ -\frac14 & 0 & 0 & \frac{1}{2\sqrt2} & \frac14 & 0 & 0 & 0 \\ 0 & \frac14 & 0 & 0 & 0 & \frac14 & \frac{1}{2\sqrt2} & 0 \\ 0 & -\frac{1}{2\sqrt2} & 0 & 0 & 0 & \frac{1}{2\sqrt2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac12 \end{bmatrix} C_{[3]} = \begin{array}{c} \\ S=\frac12 \\ \\ S=\frac32 \end{array} \overset{\qquad S=\frac12 \qquad\qquad\qquad S=\frac32}{\left[\begin{array}{cc|cc|cccc} -\frac34 & 0 & \frac{\sqrt3}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac34 & 0 & \frac{\sqrt3}{4} & 0 & 0 & 0 & 0 \\ \hline \frac{\sqrt3}{4} & 0 & -\frac14 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt3}{4} & 0 & -\frac14 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \frac12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac12 \end{array}\right]} \qquad (11)$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \end{bmatrix} \sim \begin{bmatrix} 0 & 0 & 0 & | & 0 & 0 & 1/2 \end{bmatrix}$$

$$= \left(\begin{array}{c|c} \boxed{\begin{matrix} -3/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & -1/4 \end{matrix}} \otimes \mathbb{1}_{2\times 2} & \\ \hline & \boxed{\tfrac{1}{2}}\, \mathbb{1}_4 \end{array}\right) \qquad (12)$$

Beautifully blocked, and in agreement with Wigner-Eckardt theorem, cf. Sym-II.3 (5'):

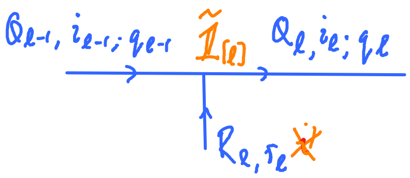
$$\langle \tilde{S}'', \tilde{i}''; \tilde{s}'' | \hat{H} | S'', i''; s'' \rangle = \left(H_{[S]}\right)^{\tilde{i}''}{}_{i''} \, \delta^{\tilde{S}''}{}_{S''} \, \delta^{\tilde{s}}{}_{s''} \qquad (13)$$

with reduced matrix elements

$$H_{[1/2]} = \boxed{\begin{pmatrix} -3/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & -1/4 \end{pmatrix}} , \quad H_{[3/2]} = \boxed{\tfrac{1}{2}} \qquad (14)$$

7. Bookkeeping for unit matrices

General notation: $|Q,q\rangle \equiv |S,s\rangle$ for virtual bonds, $|R,r\rangle \equiv |S,s\rangle$ for physical legs.



$$= \langle Q_{\ell-1}, i_{\ell-1}; q_{\ell-1} | \langle R_\ell, r_\ell | Q_\ell, i_\ell; q_\ell \rangle \equiv \mathbb{1}^{i_{\ell-1}}_{i_\ell} \left(C^{Q_{\ell-1} R_\ell}_{Q_\ell} \right)^{q_{\ell-1} r_\ell}_{q_\ell} \qquad (1)$$

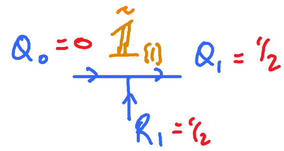
CGC encodes sum rules, see Sym-II.3 (4)

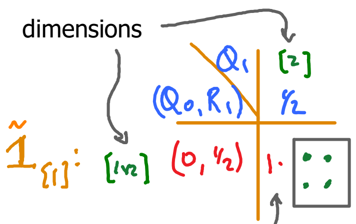
To avoid proliferation of factors of 1/2, Weichselbaum uses the following notation:

$$Q = 2(\text{spin}) = 0, 1, 2, \ldots, \qquad q = 2(\text{spin projection}) = -Q, \ldots, Q \qquad (2)$$

We will stick with standard notation, though.

Sites 0 and 1





$\langle Q_0, q_0; R_1, r_1 \vert$ \ $\vert Q_1, q_1\rangle$	$\vert 1/2, 1/2\rangle$	$\vert 1/2, -1/2\rangle$
$\langle 0, 0; 1/2, 1/2 \vert$	1	0
$\langle 0, 0; 1/2, -1/2 \vert$	0	1

(3)

for the unit matrix, the CGC are multiplied by 1

$\tilde{\mathbb{1}}_{[1]}: \doteq$

record index ν	bond 0 Q_0	site 1 R_1	bond 1 Q_1	dimensions $d_{Q_0} \times d_{R_1}, d_{Q_1}$	data	CGC
1	0	1/2	1/2	1×2, 2	1	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

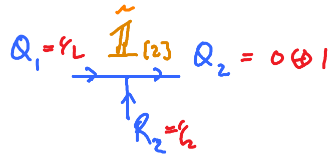
(4)

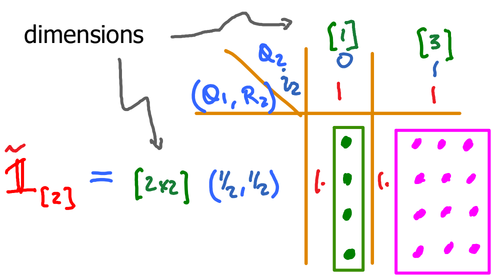
Since Heisenberg Hamiltonian contains only two-site terms, Hamiltonian for a single site is trivially = 0:

Q_1	$H_{[Q_1]}$	CGC	CGC-dim
1/2	0	$\mathbb{1}$	2

(5)

Sites 1 and 2





(see Sym-II.4.7)

$\langle Q_1, q_1; R_2, r_2 \vert$ \ $\vert Q_2, q_2 \rangle$	$\vert 0,0\rangle$	$\vert 1,1\rangle$	$\vert 1,0\rangle$	$\vert 1,-1\rangle$
$\langle 1/2, 1/2; 1/2, 1/2 \vert$	0	1	0	0
$\langle 1/2, 1/2; 1/2, -1/2 \vert$	$1/\sqrt{2}$	0	$+1/\sqrt{2}$	0
$\langle 1/2, -1/2; 1/2, 1/2 \vert$	$-1/\sqrt{2}$	0	$+1/\sqrt{2}$	0
$\langle 1/2, -1/2; 1/2, -1/2 \vert$	0	0	0	1

(6)

$$\equiv \begin{pmatrix} 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} \square & \square \end{pmatrix}$$

for both first matrix and second block matrix, rows are labeled by (Q_1, R_2), columns by Q_2, i_2.

	record index ν	bond 1 Q_1	site 2 R_2	bond 2 Q_2	dimensions $d_{Q_1} \times d_{R_2}, d_{Q_2}$	data	CGC
$\tilde{\mathbb{1}}_{[2]} : \doteq$	1	1/2	1/2	0	2x2 , 1	1	$\square$
	2	1/2	1/2	1	2x2 , 3	1	$\square$

(7)

Hamiltonian for sites 1 to 2 [see Sym-II.5(20)]:

$$\widetilde{\vec{S}_1 \cdot \vec{S}_2} = \left(\begin{array}{c|ccc} \boxed{-3/4} & 0 & 0 & 0 \\ \hline 0 & & & \\ 0 & & \boxed{1/4} \cdot \mathbb{1}_3 & \\ 0 & & & \end{array}\right)$$

Q	$H_{[Q_2]}$	CGC	CGC-dim
0	$\boxed{-3/4}$	$\mathbb{1}_1$	1
1	$\boxed{1/4}$	$\mathbb{1}_3$	3

(8)

<u>Sites 2 and 3</u>

$$Q_2 = 0 \oplus 1 \xrightarrow{\tilde{\mathbb{1}}_{[3]}} Q_3 = \tfrac{1}{2} \oplus \tfrac{1}{2} \oplus \tfrac{3}{2}, \qquad \uparrow R_3 = \tfrac{1}{2}$$

(9)

dimensions

(Q_2, R_3) \ Q_3, i_3	[2] 1/2, 1	[2] 1/2, 1	[4] 3/2, 2
[2] $(0, \frac{1}{2})$	$\square$		
[3x2] $(1, \frac{1}{2})$		$\square$	$\square$

(see Sym-II.5.5)

$\langle Q_2, q_2; R_3, r_3 \vert$ \ $\vert Q_3, q_3 \rangle$	i_2	$\vert \frac{1}{2}, \frac{1}{2} \rangle$ (first $S=1/2$ multiplet), i_3 = 1	$\vert \frac{1}{2}, -\frac{1}{2} \rangle$ (first $S=1/2$ multiplet), i_3 = 1	$\vert \frac{1}{2}, \frac{1}{2} \rangle$ (second $S=1/2$ multiplet), i_3 = 2	$\vert \frac{1}{2}, -\frac{1}{2} \rangle$ (second $S=1/2$ multiplet), i_3 = 2	$\vert \frac{3}{2}, \frac{3}{2} \rangle$, 1	$\vert \frac{3}{2}, \frac{1}{2} \rangle$, 1	$\vert \frac{3}{2}, -\frac{1}{2} \rangle$, 1	$\vert \frac{3}{2}, -\frac{3}{2} \rangle$, 1
$\langle 0,0; \frac{1}{2}, \frac{1}{2} \vert$	1	1	0						
$\langle 0,0; \frac{1}{2}, -\frac{1}{2} \vert$	1	0	1						
$\langle 1,1; \frac{1}{2}, \frac{1}{2} \vert$	1			0	0	1	0	0	0
$\langle 1,1; \frac{1}{2}, -\frac{1}{2} \vert$	1			$\sqrt{2/3}$	0	0	$1/\sqrt{3}$	0	0
$\langle 1,0; \frac{1}{2}, \frac{1}{2} \vert$	1			$-1/\sqrt{3}$	0	0	$\sqrt{2/3}$	0	0
$\langle 1,0; \frac{1}{2}, -\frac{1}{2} \vert$	1			0	$1/\sqrt{3}$	0	0	$\sqrt{\frac{2}{3}}$	0
$\langle 1,-1; \frac{1}{2}, \frac{1}{2} \vert$	1			0	$-\sqrt{2/3}$	0	0	$1/\sqrt{3}$	0
$\langle 1,-1; \frac{1}{2}, -\frac{1}{2} \vert$	1			0	0	0	0	0	1

$$\equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \otimes \begin{pmatrix} \square & & \\ & \square & \square \end{pmatrix}$$

(10)

for both first matrix and second block matrix, rows are labeled by (Q_2, R_3), columns by (Q_3, i_3).

	record index ν	bond 2 Q_2	site 3 R_3	bond 4 Q_3	dimensions $d_{Q_2} \times d_{R_3}, d_Q$	data	CGC
$\tilde{\mathbb{1}}_{[3]} : \doteq$	1	0	1/2	1/2	1x2 , 2	1	$\square$
	2	1	1/2	1/2	3x2 , 2	1	$\square$
	3	1	1/2	3/2	3x2 , 4	1	$\square$

(11)

<u>Hamiltonian for sites 1 to 3</u> [see Sym-II.5(12)]:

$$\overbrace{\vec S_1\cdot\vec S_2}\cdot 1\!\!1_3 + 1\!\!1_1\cdot\overbrace{\vec S_2\cdot\vec S_3} = \left(\begin{array}{c|c} \boxed{\begin{pmatrix} -3/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & -1/4 \end{pmatrix}} \otimes 1\!\!1_2 & \\ \hline & \boxed{\tfrac{1}{2}} \otimes 1\!\!1_4 \end{array}\right) \tag{12}$$

This information can be stored in the format

Q_3	i_3' \ i_3	$(H_{[Q_3]})^{i_3'}{}_{i_3}$: 1	2	CGC	CGC-dim
$1/2$	1	$-3/4$	$\sqrt{3}/4$	$1\!\!1_2$	2
	2	$\sqrt{3}/4$	$-1/4$		
$3/2$	1	$1/2$		$1\!\!1_4$	4

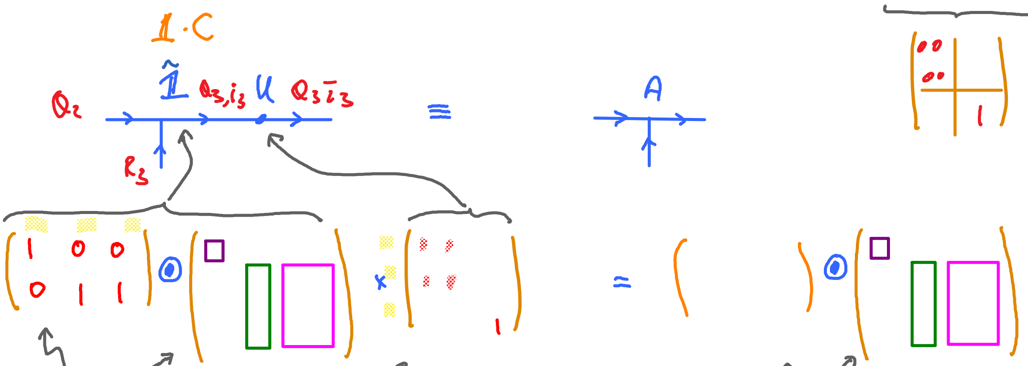
(13)

eigenenergies do not depend on degenerate multiplets!

Diagonalize H:

$$H_{[Q_3]}\,|Q_3,\bar i_3;q_3\rangle = E_{[Q_3]\bar i_3}\,|Q_3,\bar i_3;q_3\rangle \tag{14}$$

$$|Q_3,\bar i_3;q_3\rangle = |Q_3,i_3;q_3\rangle\,\underbrace{U_{[Q_3]}{}^{i_3}{}_{\bar i_3}} \tag{15}$$



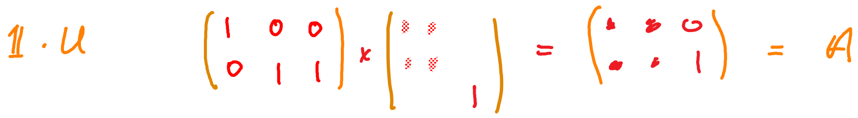
(16)

for both first matrix and second block matrix rows are labeled by (Q_2,R_3), columns by (Q_3,i_3).

for third matrix, rows are labeled by (Q_3,i_3), columns by $(Q_3,\bar i_3)$.

for both matrices, rows are labeled by (Q_2,R_3), columns by $(Q_3,\bar i_3)$.

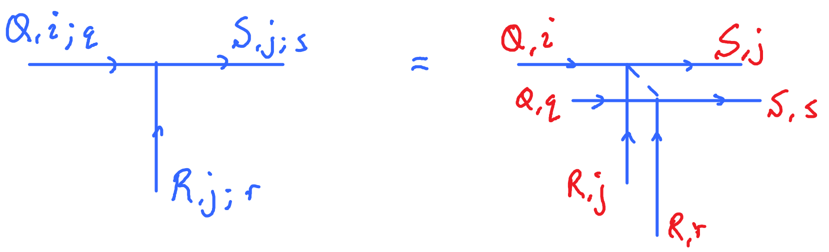
sum on (Q_3,i_3) is implied, yielding matrix multiplication:



CGC factor is merely a spectator

This illustrates the general statement: in the presence of symmetries, A-tensors factorize:

$$A^{(Q,i;q),(R,j;r)}{}_{(S,k;s)} = \left(A^{QR}{}_S\right)^{ij}{}_k \left(C^{QR}{}_S\right)^{qr}{}_s \tag{17}$$



(18)