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 $\hat{\vec{S}}_{tot} = \sum_\ell \vec{S}_\ell$, then $\hat{S}^x_{tot}, \hat{S}^y_{tot}, \hat{S}^z_{tot}$ are SU(2) generators, (2)

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

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

'spin label' or 'symmetry labe' or 'irrep label' (upper case S)

'spin projection label' or 'internal label' (lower case s), distinguishes states within multiplet

'multiplet label' distinguishes multiplets having same spin S

with

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

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

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

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:
$a, b, c \in \{x, y, z\}$

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

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

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

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

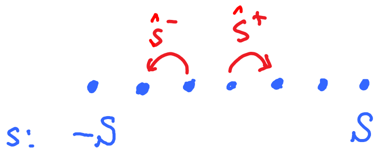
Irreducible multiplet: $\hat{\vec{S}}^2 |S, s\rangle = S(S+1) |S, s\rangle$, $S = 0, \tfrac{1}{2}, 1, \ldots$ (12)

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

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

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

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



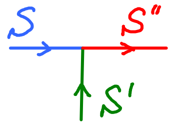
2. Tensor product decomposition

(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:



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

'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.

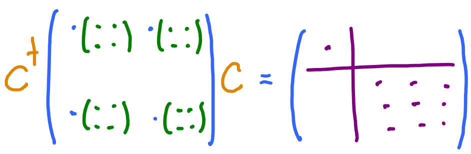
Action of generators:

$$\hat{C}^\dagger \left(\hat{S}^a_1 \otimes \hat{\mathbb{1}}_2 + \hat{\mathbb{1}}_1 \otimes \hat{S}^a_2 \right) \hat{C} = \bigoplus_{S''} \hat{S}^a \qquad (4)$$

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):

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

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

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

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)

" $\hat{S}_1^2$ " S (8b)

" $\hat{S}_2^2$ " S' (8c)

" $\hat{S}^z_1 + \hat{S}^z_2$ " s'' (8d)

3. Tensor operators

Consider an SU(2) rotation, $g \in SU(2)$

A spin multiplet forms an 'irreducible representation' (irrep), i.e. it transforms under this rotation as:

$$\hat U(g)\,|S,s\rangle = |S,s'\rangle\, D(g)^{s'}{}_{s} \qquad \text{representation matrix for spin-S irrep} \tag{0}$$

$$\langle S,s|\,U^\dagger(g) = D^\dagger(g)^{s}{}_{s'}\,\langle S,s'| \tag{0'}$$

An 'irreducible tensor operator' transforms analogously (to bra):

$$\hat U(g)\,\hat T^{(S,s)}\,U^\dagger(g) = D^\dagger(g)^{s}{}_{s'}\,\hat T^{(S,s')} \tag{1}$$

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

$$\hat U(g)\,\hat H\,\hat U^\dagger(g) = \hat H \tag{2}$$

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

$$\hat S^{(S=1,s)} = \left(\tfrac{1}{\sqrt2}\hat S^+,\ \hat S^z,\ \tfrac{1}{\sqrt2}\hat S^-\right)^T \tag{3}$$

<u>Wigner-Eckardt theorem</u>

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

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

CGCs encode sum rules: $\propto N^{SS'}{}_{S''}\,\delta^{s+s'}{}_{s''}$

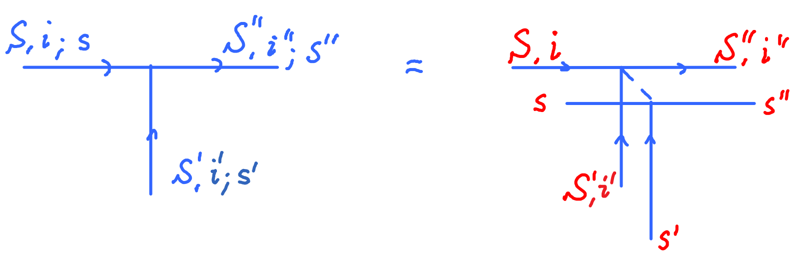
In particular, for Hamiltonian, which is a scalar operator: $(S=0,\ s=0)$

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

Hamiltonian matrix for block S $\rightarrow$ $= \left(H_{[S]}\right)^{i}{}_{i''}$ $\delta^{S}{}_{S''}\,\delta^{s}{}_{s''}$ sum rules

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

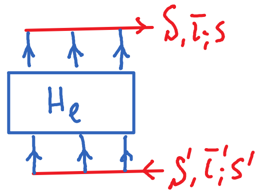
$$A^{(S,i;s),(S',i';s')}{}_{(S'',i'';s'')} = \left(\tilde A^{S,S'}{}_{S''}\right)^{i}{}_{i''}\ \left(C^{S,S'}{}_{S''}\right)^{s,s'}{}_{s''} \tag{6}$$



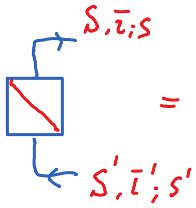
4. A-matrix factorizes

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

Suppose Hamiltonian for sites 1 to ℓ has been diagonalized:

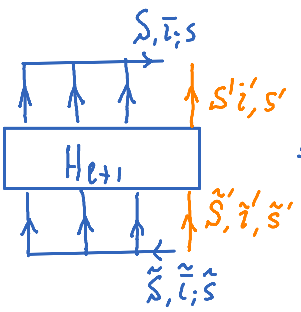


$=$ H_ℓ



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

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:



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

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

sums over all repeated indices implied:

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

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

combine multiplet indices from S, S' to composite multiplet index for S''

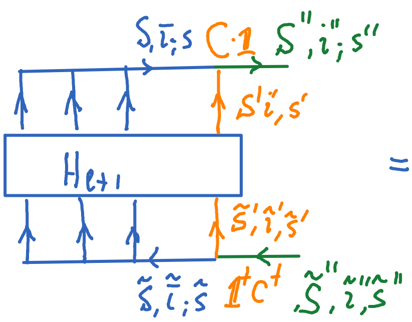
By Wigner-Eckardt theorem:
diagonal in all symmetry labels!

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

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

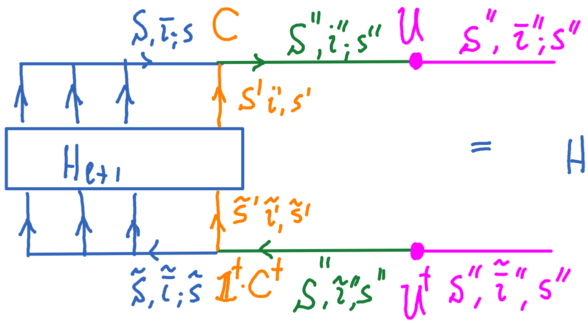
block labeled by S''
with elements labeled by $\tilde{i}''{}_{i''}$

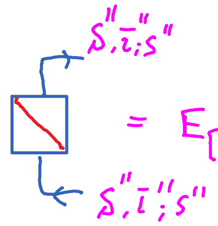
Diagrammatic depiction is more transparent / less cluttered:



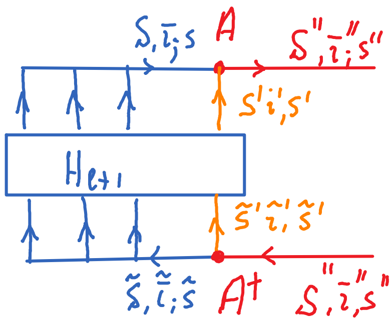
$$= |S'', \tilde{i}'', s''\rangle \left[H_{[S'']}\right]^{\tilde{i}''}{}_{i''} \langle S'' i''; s''| \qquad (11)$$

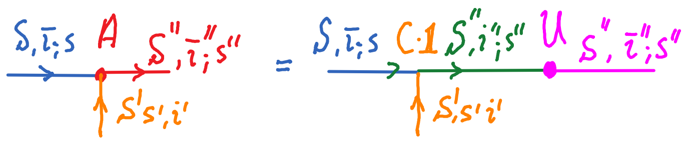
Now diagonalize and make unitary transformation into energy eigenbasis:



$=$ $H_{\ell+1}$  $= E^{\bar i''}_{[S'']}\ \delta^{\bar i''}_{\tilde{\bar i}''}$ (12)

Combined transformation from old energy eigenbasis to new energy eigenbasis:



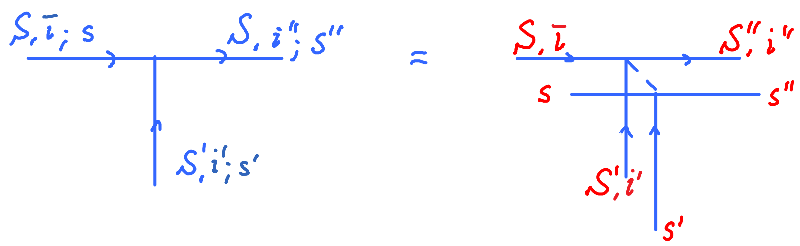


(13)

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

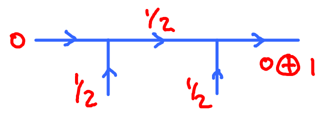
$$\equiv \left[\tilde A^{SS'}{}_{S''}\right]^{\bar i i'}{}_{\bar i''}\left[C^{SS'}{}_{S''}\right]^{ss'}{}_{s''}$$

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 $1/2$: $\quad |\uparrow\rangle = |1/2, 1/2\rangle, \qquad |\downarrow\rangle = |1/2, -\tfrac{1}{2}\rangle.$ (1)

Singlet:
$$|S,s\rangle = |0,0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{2}$$
$$= \tfrac{1}{\sqrt{2}}\left(|1/2, 1/2; 1/2, -1/2\rangle - |1/2, -1/2; 1/2, 1/2\rangle\right) \tag{3}$$

Triplet:
$$|S,s\rangle = \begin{cases} |1,1\rangle = |\uparrow\uparrow\rangle & (4) \\ |1,0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) & (5) \\ |1,-1\rangle = |\downarrow\downarrow\rangle & (6) \end{cases}$$

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

$$\left(C^{1/2\;\;1/2}_{[2]\;\;S''}\right)^{s s'}{}_{s''} = \langle 1/2, s; 1/2, s' | S'', s''\rangle = \begin{array}{cc} & \begin{array}{cccc} |0,0\rangle & |1,1\rangle & |1,0\rangle & |1,-1\rangle \end{array} \\ \begin{array}{cc} \uparrow\uparrow & \langle 1/2, 1/2; 1/2, 1/2| \\ \uparrow\downarrow & \langle 1/2, 1/2; 1/2, -1/2| \\ \downarrow\uparrow & \langle 1/2, -1/2; 1/2, 1/2| \\ \downarrow\downarrow & \langle 1/2, -1/2; 1/2, -1/2| \end{array} & \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt{2} & 0 & +1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 0 & +1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \tag{7}$$

site 2

Check

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

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

In direct product basis, the generators have the form

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

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

$$S^z = S_1^z \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes S_2^z = \tfrac{1}{2}\begin{bmatrix} 1\cdot\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & 0 \\ 0 & -1\cdot\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \end{bmatrix} + \tfrac{1}{2}\begin{bmatrix} 1\cdot\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} & 0 \\ 0 & 1\cdot\begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \end{bmatrix} = \begin{bmatrix} 1+1 & & & \\ & 1-1 & & \\ & & -1+1 & \\ & & & -1-1 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{bmatrix} \tag{10}$$

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

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

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

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

These 4x4 matrices indeed satisfy $[\tilde{S}^{z}, \tilde{S}^{\pm}] = \pm \tilde{S}^{\pm}$, $[\tilde{S}^{+}, \tilde{S}^{-}] = 2\tilde{S}^{z}$ (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}: $S^{+} = S^{-} = S^{z} = 0$ (15)

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

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

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

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

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:

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

The diagonal entries are consistent with the identity

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

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

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

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

$$\mathbb{1}_1 \otimes S_2^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \Rightarrow \widetilde{\mathbb{1}_1 \otimes S_2^-} = C^\dagger_{[2]}\left(\mathbb{1}_1 \otimes S_-^+\right)C_{[2]} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \end{bmatrix} \qquad (24)$$

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

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

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

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

The sum of these three terms yields:

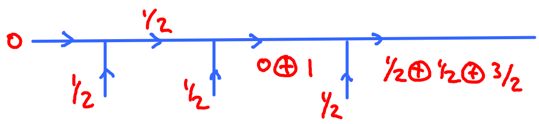
$$\widetilde{\vec{S}_1 \otimes \vec{S}_2} = \left[\begin{array}{cc|cccc} -1 & & & & & \\ & -1 & & & & \\ \hline & & 1/2 & & & \\ & & & 1/2 & & \\ & & & & 1/2 & \\ & & & & & 1/2 \end{array}\right] \qquad (28)$$

The diagonal entries are consistent with the identity

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

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

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



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

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

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

Clebsch-Gordan coefficients:

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

	$\|\tfrac12,\tfrac12\rangle$	$\|\tfrac12,-\tfrac12\rangle$	$\|\tfrac12,\tfrac12\rangle$	$\|\tfrac12,-\tfrac12\rangle$	$\|\tfrac32,\tfrac32\rangle$	$\|\tfrac32,\tfrac12\rangle$	$\|\tfrac32,-\tfrac12\rangle$	$\|\tfrac32,-\tfrac32\rangle$
$\langle 0,0;\tfrac12,\tfrac12\|$	1	0						
$\langle 0,0;\tfrac12,-\tfrac12\|$	0	1						
$\langle 1,1;\tfrac12,\tfrac12\|$			0	0	1	0	0	0
$\langle 1,1;\tfrac12,-\tfrac12\|$			$\sqrt{2/3}$	0	0	$1/\sqrt3$	0	0
$\langle 1,0;\tfrac12,\tfrac12\|$			$-1/\sqrt3$	0	0	$\sqrt{2/3}$	0	0
$\langle 1,0;\tfrac12,-\tfrac12\|$			0	$1/\sqrt3$	0	0	$\sqrt{\tfrac23}$	0
$\langle 1,-1;\tfrac12,\tfrac12\|$			0	$-\sqrt{2/3}$	0	0	$1/\sqrt3$	0
$\langle 1,-1;\tfrac12,-\tfrac12\|$			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.5, (17-19)) $\otimes\, \mathbb{1}_3$ with (Sym-II.5, (22-24)) $\cdot\, \vec S_3$, we readily obtain

$$\widetilde{\vec S_1 \cdot \vec S_2 \cdot \mathbb{1}_3} + \widetilde{\mathbb{1}_1 \cdot \vec S_2 \cdot \vec S_3} = C^\dagger_{[3]} \left(\vec S_1 \cdot \vec S_2 \cdot \mathbb{1}_3 + \mathbb{1}_1 \cdot \vec S_2 \cdot \vec S_3 \right) C_{[3]} \tag{10}$$

$$C^\dagger_{[3]} \begin{pmatrix} -\frac34 & 0 & 0 & \frac{1}{2\sqrt2} & -\frac14 & 0 & 0 & 0 \\ 0 & -\frac34 & 0 & 0 & 0 & \frac14 & -\frac{1}{2\sqrt2} & 0 \\ 0 & 0 & \frac12 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2\sqrt2} & 0 & 0 & 0 & \frac{1}{2\sqrt2} & 0 & 0 & 0 \\ -\frac14 & 0 & 0 & \frac{1}{2\sqrt2} & \frac14 & 0 & 0 & 0 \\ 0 & \frac14 & 0 & 0 & 0 & \frac14 & \frac{1}{2\sqrt2} & 0 \\ 0 & -\frac{1}{2\sqrt2} & 0 & 0 & 0 & \frac{1}{2\sqrt2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac12 \end{pmatrix} C_{[3]} = \begin{array}{c} \\ S=\tfrac12 \\ \\ S=\tfrac32 \end{array} \begin{array}{c} \qquad S=\tfrac12 \qquad\qquad\qquad S=\tfrac32 \\ \left(\begin{array}{cc|cc|cccc} -\frac34 & 0 & \frac{\sqrt3}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac34 & 0 & \frac{\sqrt3}{4} & 0 & 0 & 0 & 0 \\ \hline \frac{\sqrt3}{4} & 0 & -\frac14 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\sqrt3}{4} & 0 & -\frac14 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \frac12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac12 \end{array}\right) \end{array} \tag{11}$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \end{bmatrix} \qquad \left[\begin{array}{ccc|ccc} 0 & 0 & 0 & 0 & 0 & 1/2 \end{array}\right]$$

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

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

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

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.

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

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

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

$Q =$ 2(spin) $= 0, 1, 2, \ldots$, $\quad q =$ 2(spin projection) $= -Q, \ldots, Q$ (2)

We will stick with standard notation, though.

Sites 0 and 1

$$Q_0 = 0 \xrightarrow{\ \tilde{\mathbb{1}}_{[1]}\ } Q_1 = \tfrac{1}{2}, \qquad \uparrow R_1 = \tfrac{1}{2}$$

dimensions

$$\tilde{\mathbb{1}}_{[1]}: \quad \begin{array}{c|c} & \begin{array}{c} [2] \\ Q_1 = \tfrac{1}{2} \\ i_1 = 1 \end{array} \\ \hline (Q_0, R_1)\ i_0 & \\ [1\times 2]\ (0, \tfrac{1}{2})\ \ 1 & \boxed{\begin{matrix} \cdot & \cdot \\ \cdot & \cdot \end{matrix}} \end{array} \qquad \begin{array}{c|cc} |Q_1, q_1\rangle & |\tfrac{1}{2}, \tfrac{1}{2}\rangle & |\tfrac{1}{2}, -\tfrac{1}{2}\rangle \\ \hline \langle Q_0, q_0; R_1, r_1| & & \\ \langle 0, 0; \tfrac{1}{2}, \tfrac{1}{2}| & 1 & 0 \\ \langle 0, 0; \tfrac{1}{2}, -\tfrac{1}{2}| & 0 & 1 \end{array} \qquad (3)$$

$$\left[\mathbb{1}^{Q_0 R_1}_{Q_1}\right] \quad \left[C^{Q_0, R_0}_{Q_1}\right]^{S_0, r_1}_{q_1}$$

$\tilde{\mathbb{1}}_{[1]}$: $\doteq$ (4)

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	$\frac{1}{2}$	$\frac{1}{2}$	1×2, 2	1	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

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

Q_1	$H_{[Q_1]}$	CGC	CGC-dim
$\frac{1}{2}$	0	$\mathbb{1}_2$	2

(5)

Sites 1 and 2

$$Q_1 = \tfrac{1}{2} \xrightarrow{\ \tilde{\mathbb{1}}_{[2]}\ } Q_2 = 0 \oplus 1, \qquad \uparrow R_2 = \tfrac{1}{2}$$

(see Sym-II.4.7)

dimensions

$$\tilde{\mathbb{1}}_{[2]} = \begin{array}{c|c|c} & \begin{array}{c} [1] \\ Q_2 = 0 \\ i_2 = 1 \end{array} & \begin{array}{c} [3] \\ 1 \\ 1 \end{array} \\ \hline (Q_1, R_2)\ i_1 & & \\ [2\times 2]\ (\tfrac{1}{2}, \tfrac{1}{2})\ \ 1 & \mathbb{1}\ \boxed{\begin{matrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{matrix}} & \mathbb{1}\ \boxed{\begin{matrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{matrix}} \end{array} = \begin{array}{c|c|ccc} |Q_2, q_2\rangle & |0,0\rangle & |1,1\rangle & |1,0\rangle & |1,-1\rangle \\ \hline \langle Q_1, q_1; R_2, r_2| & & & & \\ \langle \tfrac{1}{2}, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}| & 0 & 1 & 0 & 0 \\ \langle \tfrac{1}{2}, \tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}| & 1/\sqrt{2} & 0 & +1/\sqrt{2} & 0 \\ \langle \tfrac{1}{2}, -\tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}| & -1/\sqrt{2} & 0 & +1/\sqrt{2} & 0 \\ \langle \tfrac{1}{2}, -\tfrac{1}{2}; \tfrac{1}{2}, -\tfrac{1}{2}| & 0 & 0 & 0 & 1 \end{array} \qquad (6)$$

$$\left[\mathbb{1}^{Q_1 R_1}_{Q_2}\right]^{i_1}_{i_2} \qquad \left[C^{Q_1 R_2}_{Q_2}\right]^{q_1 r_2}_{q_2}$$

$$\equiv \left(1 \quad 1 \right) \otimes \left(\boxed{} \quad \boxed{} \right)$$

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

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

$\tilde{\mathbb{1}}_{[2]}: \doteq$

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
1	1/2	1/2	0	2×2, 1	1	
2	1/2	1/2	1	2×2, 3	1	

(7)

sparse way of storing $\mathbb{1}^{Q_1 R_2}_{Q_2}$

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	$-3/4$	$\mathbb{1}_1$	1
1	$1/4$	$\mathbb{1}_3$	3

(8)

<u>Sites 2 and 3</u>

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

(9)

dimensions

$\mathbb{1}_{[3]}:$

dimensions	(Q_2, R_3) \ Q_3, i_3	i_2	[2] 1/2, 1	[2] 1/2, 2	[4] 3/2, 1
[2]	(0, 1/2)	1			
[3x2]	(1, 1/2)	1			

(see Sym-II.5.5)

$\langle Q_2, q_2; R_3, r_3 \vert$ \ $\vert Q_3, q_3 \rangle$	i_2 \ i_3	$\vert\frac{1}{2},\frac{1}{2}\rangle$ 1	$\vert\frac{1}{2},-\frac{1}{2}\rangle$ 1	$\vert\frac{1}{2},\frac{1}{2}\rangle$ 2	$\vert\frac{1}{2},-\frac{1}{2}\rangle$ 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
$\langle 0,0; 1/2, 1/2 \vert$	1	1	0						
$\langle 0,0; 1/2, -1/2 \vert$	1	0	1						
$\langle 1,1; 1/2, 1/2 \vert$	1			0	0	1	0	0	0
$\langle 1,1; 1/2, -1/2 \vert$	1			$\sqrt{2/3}$	0	0	$1/\sqrt{3}$	0	0
$\langle 1,0; 1/2, 1/2 \vert$	1			$-1/\sqrt{3}$	0	0	$\sqrt{2/3}$	0	0
$\langle 1,0; 1/2, -1/2 \vert$	1			0	$1/\sqrt{3}$	0	0	$\sqrt{\frac{2}{3}}$	0
$\langle 1,-1; 1/2, 1/2 \vert$	1			0	$-\sqrt{2/3}$	0	0	$1/\sqrt{3}$	0
$\langle 1,-1; 1/2, -1/2 \vert$	1			0	0	0	0	0	1

first $S = 1/2$ multiplet; second $S = 1/2$ multiplet

(10)

$$\sum \left[\mathbb{1}^{Q_2 R_3}{}_{Q_3}\right]^{i_2}{}_{i_3} \left[C^{Q_2,R_3}{}_{Q_3}\right]^{q_2 r_3}{}_{q_3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \otimes \left(\square \;\; \square \;\; \square \right)$$

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

$\mathbb{1}_{[3]}: \doteq$

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
1	0	1/2	1/2	1×2, 2	1	
2	1	1/2	1/2	3×2, 2	1	
3	1	1/2	3/2	3×2, 4	1	

(11)

Hamiltonian for sites 1 to 3 [see Sym-II.5(12)]: sparse way of storing $1^{Q_2R_3}{}_{Q_3}$

$$\overbrace{\vec S_1\cdot\vec S_2}\cdot 1_3 + 1_1\cdot\overbrace{\vec S_2\cdot\vec S_3} = \begin{pmatrix} \boxed{\begin{pmatrix}-3/4 & \sqrt{3}/4\\ \sqrt{3}/4 & -1/4\end{pmatrix}}\otimes 1_2 & \\ & \boxed{\tfrac12}\otimes 1_4\end{pmatrix} \quad (12)$$

This information can be stored in the format

Q_3	$i'_3 \backslash i_3$	$(H_{[Q_3]})^{i'_3}{}_{i_3}$: 1	2	CGC	CGC-dim
$1/2$	1	$-3/4$	$\sqrt{3}/4$	1_2	2
	2	$\sqrt{3}/4$	$-1/4$		
$3/2$	1	$1/2$		1_4	4

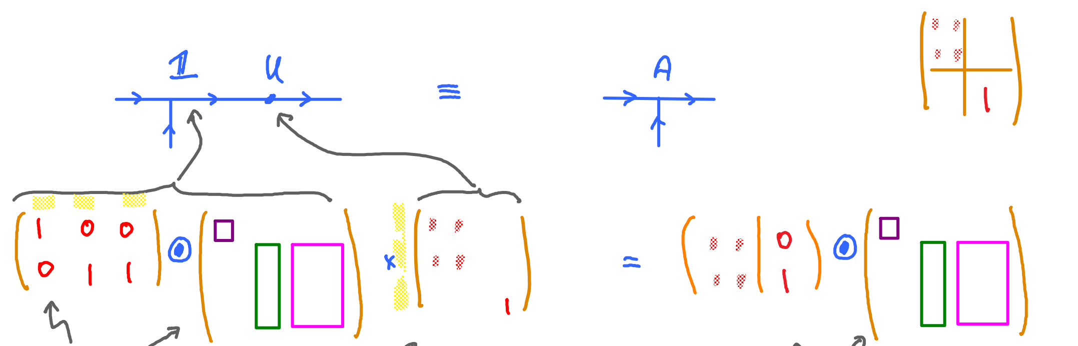
(13)

eigenenergies do not depend on degenerate multiplets!

Diagonalize H:

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

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



(16)

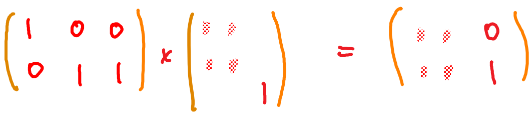
for both first matrix and second block matrix rows are labeled by (Q_2,R_3), columns by (Q_3,i_3).

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 i_3 is implied, yielding matrix multiplication:

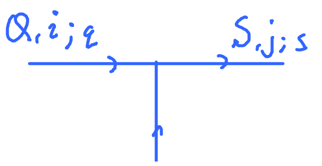
CGC factor is merely a spectator



$$[1^{Q_2,R_3}{}_{Q_3}]^{i_2}{}_{i_3}\cdot(U_{[Q_3]})^{i_3}{}_{\bar i_3} = [A^{Q_2,R_3}{}_{Q_3}]^{i_2}{}_{\bar i_3}$$

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

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



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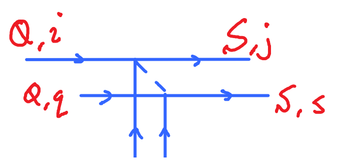
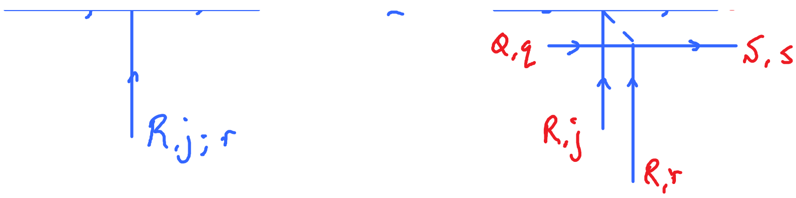


(18)


R, j; r
Q, q
S, s
R, j
R, r