Symmetries II: Non-Abelian

1. Motivation, review of SU(2) basics

Reminder: for Abelian symmetries, sum rule $Q + Q' = Q''$ led to block-diagonal Hamiltonian.

For non-Abelian symmetries, e.g. SU(2), there are more possibilities:

Coupling two spin 1/2: $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$ (1)

Hilbert spaces: $V^{\frac{1}{2}} \otimes V^{\frac{1}{2}} = V^0 \oplus V^1$ (2)

Dimensions: $2 \cdot 2 = 1 + 3$ (3)

If Hamiltonian coupling the two spins is SU(2) invariant, will be block-diagonal in basis of total spin:

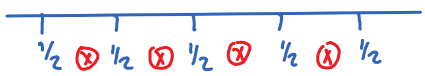
$H =$  (4)

direct product basis — direct sum basis

General: $V^S \otimes V^{S'} = V^{|S-S'|} \oplus V^{|S-S'|+1} \oplus \dots \oplus V^{S+S'}$ (5)

direct product — decomposition into direct sum

Such direct products occur everywhere in tensor networks:



Hamiltonian will be block-diagonal in basis of total spin.

Goal: learn how to systematically construct such a basis in MPS language.
More generally: learn how exploit symmetries for tensor networks, when each leg of each tensor refers to symmetry multiplets, not individual states.

Reminder: SU(2) basics

SU(2) generators: $[\hat{S}^a, \hat{S}^b] = i\varepsilon^{abc}\hat{S}^c \ , \quad \hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ (6)

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

$[\hat{S}^z, \hat{S}^\pm] = \pm \hat{S}^\pm \ , \quad [\hat{S}^+, \hat{S}^-] = 2\hat{S}_z$ (7)

Casimir operator: $\hat{\vec{S}}^2 = (\hat{S}^x)^2 + (\hat{S}^y)^2 + (\hat{S}^z)^2$ (8)

Commuting operators: $[\hat{S}_z, \hat{\vec{S}}^2] = 0$ (9)

Irreducible multiplet: (irrep)

$\hat{\vec{S}}^2 |S, s\rangle = S(S+1)|S, s\rangle \ , \quad S = 0, \tfrac{1}{2}, 1, \dots$ (10)

$\hat{S}_z |S, s\rangle = s\,|S, s\rangle \quad s = -S, -S+1, \dots, S$ (11)

Dimension of multiplet: $d_S = 2S + 1$ (12)

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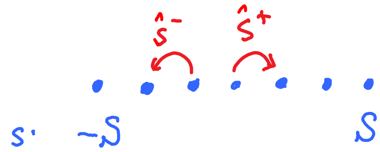
Highest weight state: $\hat{S}^+ |S, S\rangle = 0$ (13)

Lowest weight state: $\hat{S}^- |S, -S\rangle = 0$ (14)



Consider Heisenberg spin chain: $\hat{H} = J \sum_{\ell} \vec{S}_{\ell} \cdot \vec{S}_{\ell+1}$ has SU(2) symmetry. (15)

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, (16)

and $[\hat{H}, \hat{S}^z_{tot}] = 0, \quad [\hat{H}, \hat{\vec{S}}^2_{tot}] = 0$. (17)

Symmetry eigenstates can be labeled $|S, i; s\rangle$ (18)

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

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

'multiplet label' distinguishes different multiplets having same spin S

with

$$\hat{S}^z_{tot} |S, i; s\rangle = s\, |S, i; s\rangle \quad (19)$$

$$\hat{S}^2_{tot} |S, i; s\rangle = S(S+1)\, |S, i; s\rangle \quad (20)$$

$$\langle S', i'; s' | \hat{H} | S, i; s\rangle = \mathbb{1}^{S'}{}_{S}\, \mathbb{1}^{s'}{}_{s}\, [H_{S'}]^{i'}{}_{i} \quad (21)$$

reduced matrix elements in block S'

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.

2. Tensor product decomposition

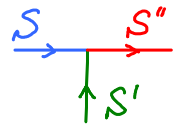
(needed when adding new site to chain) $\boxed{\text{Sym-II.2}}$

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

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

'irrep label' (S) 'internal label' (s)

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 specifying 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. (requiring extra book-keeping effort, see Sym-III.2)

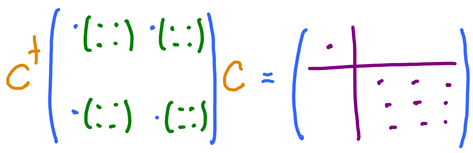
Action of generators:

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

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



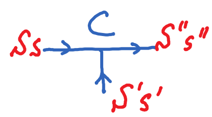
(5)

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

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

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

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



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

" $\hat{\vec{S}}_1^2$ " $S(S+1)$ (8b)

" $\hat{\vec{S}}_2^2$ " $S'(S'+1)$ (8c)

" $\hat{S}_1^z + \hat{S}_2^z$ " 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:

$$\hat{U}(g)|S,s\rangle = |S,s'\rangle [\mathcal{D}^S(g)]^{s'}{}_{s} \tag{0}$$

representation matrix for spin-S irrep, of dimension $(2S+1)\times(2S+1)$

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

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

$$\hat{U}(g)\,\hat{O}^{(S,s)}\,\hat{U}^\dagger(g) = O^{(S,s')}[\mathcal{D}^S(g)]^{s'}{}_{s} \tag{1}$$

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):

$$\hat{S}^{(S=1,s)} = \Big(\underbrace{\tfrac{1}{\sqrt{2}}\hat{S}^+}_{s=1}, \underbrace{\hat{S}^z}_{s=0}, \underbrace{\tfrac{1}{\sqrt{2}}\hat{S}^-}_{s=-1}\Big)^T, \qquad \hat{U}(g)\,\hat{S}^{(1,s)}\,\hat{U}^\dagger(g) = \hat{S}^{(1,s')}[\mathcal{D}^{(1)}(g)]^{s}{}_{s'} \tag{3}$$

Wigner-Eckardt theorem

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

$$\langle S,i;s|\hat{O}^{(S',s')}|S'',i'';s''\rangle = [O^{S,S'}{}_{S''}]^{i}{}_{i''}\,\underbrace{\langle S,s;S',s'|S'',s''\rangle}_{\propto N^{SS'}{}_{S''}\,\mathbb{1}^{s+s'}{}_{s''}} \tag{4}$$

CGCs encode sum rules: $\propto N^{SS'}{}_{S''}\,\mathbb{1}^{s+s'}{}_{s''}$

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

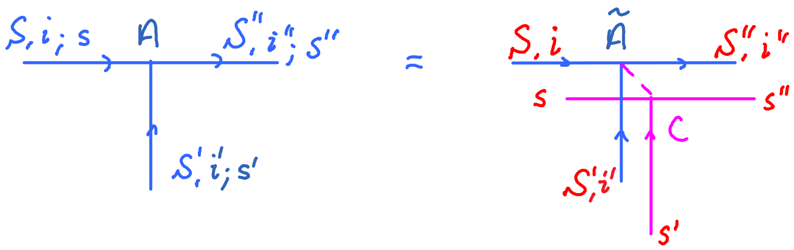
$$\langle S,i;s|\hat{H}|S'',i'';s''\rangle = \underbrace{[H^{S,0}{}_{S''}]^{i}{}_{i''}}_{=:[H_S]^{i}{}_{i''}}\ \underbrace{\langle S,s;0,0|S'',s''\rangle}_{\delta^S{}_{S''}\,\delta^s{}_{s''}} \tag{5, 5'}$$

Hamiltonian matrix for block S $\to =: [H_S]^{i}{}_{i''}$

$\delta^S{}_{S''}\,\delta^s{}_{s''}$: sum rules

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

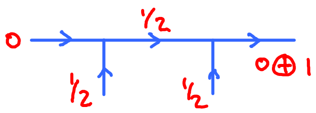
$$A^{(S,i;s),(S',i';s')}{}_{(S'',i'';s'')} = (\tilde{A}^{S,S'}{}_{S''})^{i}{}_{i''}\,(C^{S,S'}{}_{S''})^{s,s'}{}_{s''} \tag{6}$$



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

(self-study: check details!)

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



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:

$$|S,s\rangle = |0,0\rangle = \tfrac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \quad (2)$$

$$= \tfrac{1}{\sqrt{2}}\left(|1/2, 1/2; 1/2, -1/2\rangle - |1/2, -1/2; 1/2, 1/2\rangle\right) \quad (3)$$

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:

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

↖site 2

⟨direct product | direct sum⟩

Transforming operators from direct product to direct sum basis

(self-study: check details!)

$S = 1/2$ 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

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

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

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

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

$$\tilde{S}^+ = C^\dagger_{[2]} S^+ C_{[2]} = \begin{pmatrix} 0 & 1/\sqrt2 & 1/\sqrt2 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt2 & -1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt2 & 0 & 1/\sqrt2 & 0 \\ 1/\sqrt2 & 0 & -1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & \sqrt2 & 0 \\ 0 & 0 & 0 & \sqrt2 \\ 0 & 0 & 0 & 0 \end{array}\right) \quad (11)$$

$$\tilde{S}^- = C^\dagger_{[2]} S^- C_{[2]} = \begin{pmatrix} 0 & 1/\sqrt2 & 1/\sqrt2 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt2 & -1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt2 & 0 & 1/\sqrt2 & 0 \\ 1/\sqrt2 & 0 & -1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & \sqrt2 & 0 & 0 \\ 0 & 0 & \sqrt2 & 0 \end{array}\right) \quad (12)$$

$$\tilde{S}^z = C^\dagger_{[2]} S^z C_{[2]} = \begin{pmatrix} 0 & 1/\sqrt2 & 1/\sqrt2 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt2 & -1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/\sqrt2 & 0 & 1/\sqrt2 & 0 \\ 1/\sqrt2 & 0 & -1/\sqrt2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{array}\right) \quad (13)$$

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 $\quad V^0 \oplus V^1$

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

on V^1: $\quad S^+ = \sqrt2 \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad S^- = \sqrt2 \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^z = \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix} \quad (16)$

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

$$S_1^z \otimes S_2^z = \tfrac14 \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \Rightarrow \widetilde{S_1^z \otimes S_2^z} = C^\dagger_{[2]} (S_1^z \otimes S_2^z) C_{[2]} = \tfrac14 \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (17)$$

$$\tfrac12 S_1^+ \otimes S_2^- = \tfrac12 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \tfrac12 \widetilde{S_1^+ \otimes S_2^-} = C^\dagger_{[2]} \tfrac12 (S_1^+ \otimes S_2^-) C_{[2]} = \tfrac14 \begin{pmatrix} -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (18)$$

$$\tfrac12 S_1^- \otimes S_2^+ = \tfrac12 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \tfrac12 \widetilde{S_1^- \otimes S_2^+} = C^\dagger_{[2]} \tfrac12 (S_1^- \otimes S_2^+) C_{[2]} = \tfrac14 \begin{pmatrix} -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (19)$$

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:

$$C^\dagger_{[2]} (\vec{S}_1 \otimes \vec{S}_2) C_{[2]} = C^\dagger_{[2]} \left(S_1^z \otimes S_2^z + \tfrac12 [S_1^+ \otimes S_2^- + S_1^- \otimes S_2^+] \right) C_{[2]} = \tfrac14 \left(\begin{array}{c|ccc} -3 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right) \quad (20)$$

The diagonal entries are consistent with the identity

$$\vec{S}_1 \cdot \vec{S}_2 = \tfrac12 \left[(\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^{\,2} - \vec{S}_2^{\,2} \right] = \begin{cases} \tfrac12 (0 \cdot 1 - \tfrac12 \cdot \tfrac32 - \tfrac12 \cdot \tfrac32) = -\tfrac34 & \text{for } S'' = 0 \\ \tfrac12 (1 \cdot 2 - \tfrac12 \cdot \tfrac32 - \tfrac12 \cdot \tfrac32) = \tfrac14 & \text{for } S'' = 1 \end{cases} \quad (21)$$

In section Sym-II.6 we will need $\mathbb{1}_1 \cdot \vec{S}_2 \cdot \vec{S}_3$. In preparation for that, we here compute

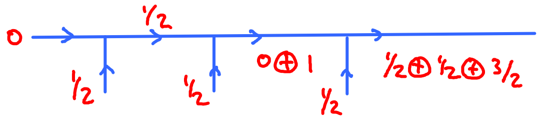
$$\mathbb{1}_1 \otimes S_2^z = \frac{1}{2}\begin{pmatrix} 1 & & & \\ & -1 & & \\ & & +1 & \\ & & & -1 \end{pmatrix} \Longrightarrow \widetilde{\mathbb{1}_1 \otimes S_2^z} = C_{[2]}^\dagger \left(\mathbb{1}_1 \otimes S_2^z\right) C_{[2]} = \frac{1}{2}\begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\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

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

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

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

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



$$|S''=\tfrac12, i=1; s''\rangle: \quad |\tfrac12,\tfrac12\rangle = 1\cdot|0,0\rangle\otimes|\tfrac12,\tfrac12\rangle, \qquad |\tfrac12,-\tfrac12\rangle = 1\cdot|0,0\rangle\otimes|\tfrac12,-\tfrac12\rangle \tag{2}$$

'first doublet'

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

'second doublet'

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

'quartet'

Basis transformation (Clebsch-Gordan coefficients):

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

⟨direct product | direct sum⟩

	first doublet ($i=1$)		second doublet ($i=2$)		quartet			
	$\lvert\tfrac12,\tfrac12\rangle$	$\lvert\tfrac12,-\tfrac12\rangle$	$\lvert\tfrac12,\tfrac12\rangle$	$\lvert\tfrac12,-\tfrac12\rangle$	$\lvert\tfrac32,\tfrac32\rangle$	$\lvert\tfrac32,\tfrac12\rangle$	$\lvert\tfrac32,-\tfrac12\rangle$	$\lvert\tfrac32,-\tfrac32\rangle$
$\langle 0,0;\tfrac12,\tfrac12\rvert$	1	0						
$\langle 0,0;\tfrac12,-\tfrac12\rvert$	0	1						
$\langle 1,1;\tfrac12,\tfrac12\rvert$			0	0	1	0	0	0
$\langle 1,1;\tfrac12,-\tfrac12\rvert$			$\sqrt{2/3}$	0	0	$1/\sqrt3$	0	0
$\langle 1,0;\tfrac12,\tfrac12\rvert$			$-1/\sqrt3$	0	0	$\sqrt{2/3}$	0	0
$\langle 1,0;\tfrac12,-\tfrac12\rvert$			0	$1/\sqrt3$	0	0	$\sqrt{\tfrac23}$	0
$\langle 1,-1;\tfrac12,\tfrac12\rvert$			0	$-\sqrt{2/3}$	0	0	$1/\sqrt3$	0
$\langle 1,-1;\tfrac12,-\tfrac12\rvert$			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, (17-19)) $\otimes\, \mathbb{1}_3$ with (Sym-II.4, (22-24)) $\otimes \vec S_3$, we readily obtain

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

$$C^\dagger_{[3]}\begin{pmatrix} -\tfrac34 & 0 & 0 & \tfrac{1}{2\sqrt2} & -\tfrac14 & 0 & 0 & 0 \\ 0 & -\tfrac34 & 0 & 0 & 0 & \tfrac14 & -\tfrac{1}{2\sqrt2} & 0 \\ 0 & 0 & \tfrac12 & 0 & 0 & 0 & 0 & 0 \\ \tfrac{1}{2\sqrt2} & 0 & 0 & 0 & \tfrac{1}{2\sqrt2} & 0 & 0 & 0 \\ -\tfrac14 & 0 & 0 & \tfrac{1}{2\sqrt2} & \tfrac14 & 0 & 0 & 0 \\ 0 & \tfrac14 & 0 & 0 & 0 & \tfrac14 & \tfrac{1}{2\sqrt2} & 0 \\ 0 & -\tfrac{1}{2\sqrt2} & 0 & 0 & 0 & \tfrac{1}{2\sqrt2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \tfrac12 \end{pmatrix} C_{[3]} = \begin{array}{c|c} & S=\tfrac12 \qquad\qquad S=\tfrac32 \\ \hline \begin{array}{c} S=\tfrac12 \\ \\ S=\tfrac32 \end{array} & \left(\begin{array}{cc|cc|cccc} -\tfrac34 & 0 & \tfrac{\sqrt3}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\tfrac34 & 0 & \tfrac{\sqrt3}{4} & 0 & 0 & 0 & 0 \\ \hline \tfrac{\sqrt3}{4} & 0 & -\tfrac14 & 0 & 0 & 0 & 0 & 0 \\ 0 & \tfrac{\sqrt3}{4} & 0 & -\tfrac14 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \tfrac12 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \tfrac12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \tfrac12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \tfrac12 \end{array}\right) \end{array} \tag{11}$$

$$\begin{bmatrix} 0 & -\frac{1}{2\sqrt{2}} & 0 & 0 & 0 & \frac{1}{2\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \qquad \hat{=} \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{array}\right]$$

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

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

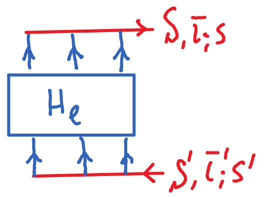
$$\langle S, i; s \,|\, \hat{H} \,|\, S'', i''; s'' \rangle = (H_{[S]})^{i}{}_{i''}\, \delta^{S}{}_{S''}\, \delta^{s}{}_{s''} \tag{13}$$

with reduced matrix elements $$H_{[1/2]} = \boxed{\begin{pmatrix} -3/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & -1/4 \end{pmatrix}} \,, \qquad H_{[3/2]} = \boxed{\tfrac{1}{2}} \tag{14}$$

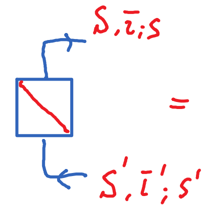
6. A-matrix factorizes

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

Suppose Hamiltonian for sites 1 to ℓ has been diagonalized:

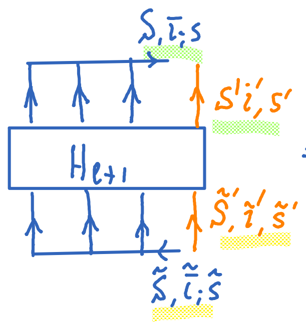


$=$ H_ℓ



$$= E^{\bar{i}}_{[S]}\; 1^{S'}{}_{S}\; 1^{\bar{i}'}{}_{\bar{i}} \qquad (7)$$

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:



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

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

sums over all repeated indices implied:

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

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

specifies which multiplets $\bar{i}, i'$ from S, S' yield the multiplet i'' for S''

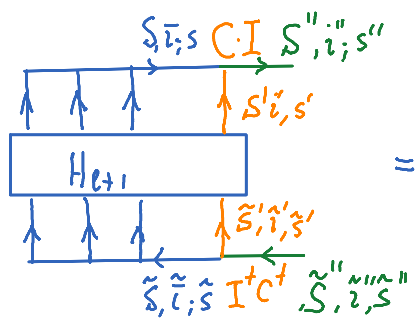
By Wigner-Eckardt theorem:
diagonal in all symmetry labels!

$$= 1^{\tilde{S}''}{}_{S''}\; 1^{\tilde{s}''}{}_{s''}\; \big[H_{S''}\big]^{\tilde{i}''}{}_{i''} \qquad (10)$$

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

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

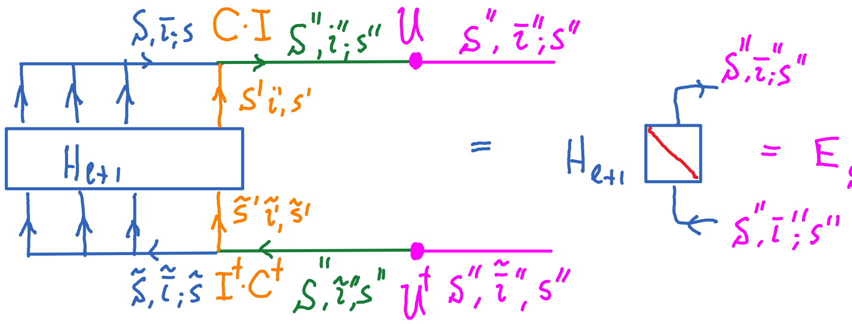
Diagrammatic depiction is more transparent / less cluttered:



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

symmetry ensures that this is diagonal in spin indices!

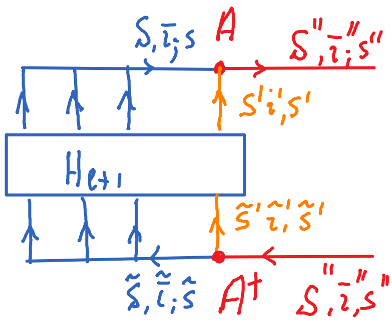
Now diagonalize and make unitary transformation into energy eigenbasis:

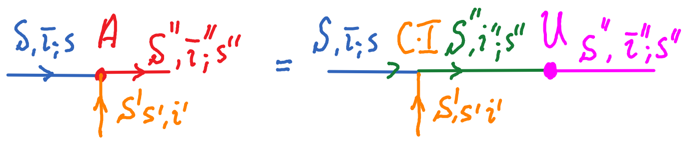


$$= E^{\bar i''}_{S''}\ \delta^{\bar i''}_{\tilde i''} \qquad (12)$$

independent of s'',
hence we have
<u>degenerate</u> multiplets

Combined transformation from old energy eigenbasis to new energy eigenbasis:





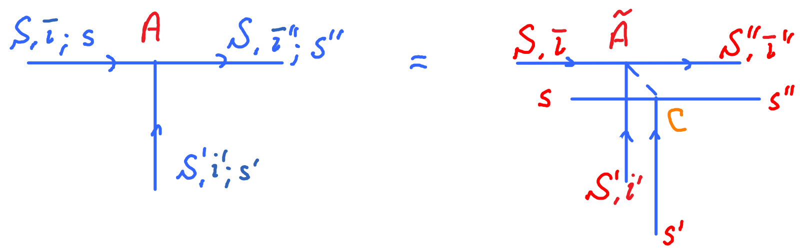
(13)

factorization happens <u>here</u>: CGC are independent of i-indices!

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

$$\equiv \left[\tilde A^{SS'}{}_{S''}\right]^{\bar i i'}{}_{\bar i''} \left[C^{SS'}{}_{S''}\right]^{ss'}{}_{s''} \qquad (15)$$

A-matrix factorizes, into product of reduced A-matrix and CGC !! $\quad A = \tilde A \cdot C \qquad (16)$



7. Bookkeeping: basis transformations spin 1/2 chain

Sym-II.8

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

I specifies which multiplets $\bar{i}_{\ell-1}$ from $Q_{\ell-1}, R_\ell$ yield the multiplet i_ℓ for Q_ℓ

$$\tilde{\mathbb{1}} = C \cdot I$$

$$Q_{\ell-1},\bar{i}_{\ell-1};q_{\ell-1} \xrightarrow{\;\tilde{\mathbb{1}}\;} Q_\ell, i_\ell; q_\ell \quad (\uparrow R_\ell, r_\ell) = \langle Q_{\ell-1},\bar{i}_{\ell-1};q_{\ell-1}; R_\ell r_\ell | Q_\ell, i_\ell; q_\ell\rangle \equiv \Big[C^{Q_{\ell-1}R_\ell}_{Q_\ell}\Big]^{q_{\ell-1}r_\ell}_{q_\ell}\Big[I^{Q_{\ell-1}R_\ell}_{Q_\ell}\Big]^{\bar{i}_{\ell-1}}_{i_\ell} \qquad (1)$$

here, no multiplet label for physical leg hence

CGC encodes sum rules, see Sym-II.3 (4) thus ensuring block-diagonal structure for H

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

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

We will stick with standard notation, though.

Sites 0 and 1

$$Q_0 = 0 \xrightarrow{\;\tilde{\mathbb{1}}_1\;} Q_1 = \tfrac{1}{2}, \qquad R_1 = \tfrac{1}{2}$$

dimensions

$$\begin{array}{c|c} & Q_1 = \tfrac12 \;[2] \\ (Q_0,R_1)\,\bar{i}_0 \backslash i_1 & 1 \\ \hline [1\times2]\;(0,\tfrac12)\;1 & \boxed{\begin{smallmatrix}\bullet & \bullet\\ \bullet & \bullet\end{smallmatrix}} \end{array} = \begin{array}{c|cc} \langle Q_0,q_0;R_1,r_1| \backslash |Q_1,q_1\rangle & |\tfrac12,\tfrac12\rangle & |\tfrac12,-\tfrac12\rangle \\ \hline \langle 0,0;\tfrac12,\tfrac12| & 1 & 0 \\ \langle 0,0;\tfrac12,-\tfrac12| & 0 & 1 \end{array} \qquad (3)$$

$\big[I^{0,R_1}_{Q_1}\big]$ $\quad \big[C^{Q_0,R_1}_{Q_1}\big]^{q_0,r_1}_{q_1}$ $\quad C^{0\,\frac12}_{\frac12} = \mathbb{1}_2$

$\tilde{\mathbb{1}}_1 \doteq$ (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	½	½	1x2, 2	1	$\begin{smallmatrix}1&0\\0&1\end{smallmatrix}$

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

Q_1	$H_{[Q_1]}$	CGC	CGC-dim
½	0	$\mathbb{1}_2$	2

(5)

Sites 1 and 2

$$Q_1 = \tfrac12 \xrightarrow{\;\tilde{\mathbb{1}}_2\;} Q_2 = 0 \oplus 1, \qquad R_2 = \tfrac12$$

block column index

dimensions

block row index

(see Sym-II.4.7)

$$\begin{array}{c|c|c} & [1] & [3] \\ (Q_1,R_2)\,\bar{i}_1 \backslash Q_2, i_2 & 0,\;1 & 1,\;1 \\ \hline [2\times2]\;(\tfrac12,\tfrac12)\;1 & \begin{smallmatrix}\bullet\\\bullet\\\bullet\\\bullet\end{smallmatrix} & \begin{smallmatrix}\bullet&\bullet&\bullet\\\bullet&\bullet&\bullet\\\bullet&\bullet&\bullet\\\bullet&\bullet&\bullet\end{smallmatrix} \end{array} = \begin{array}{c|c|ccc} & \text{singlet} & & \text{triplet} & \\ \langle Q_1,q_1;R_2,r_2| \backslash |Q_2,q_2\rangle & |0,0\rangle & |1,1\rangle & |1,0\rangle & |1,-1\rangle \\ \hline \langle \tfrac12,\tfrac12;\tfrac12,\tfrac12| & 0 & 1 & 0 & 0 \\ \langle \tfrac12,\tfrac12;\tfrac12,-\tfrac12| & 1/\sqrt2 & 0 & +1/\sqrt2 & 0 \\ \langle \tfrac12,-\tfrac12;\tfrac12,\tfrac12| & -1/\sqrt2 & 0 & +1/\sqrt2 & 0 \\ \langle \tfrac12,-\tfrac12;\tfrac12,-\tfrac12| & 0 & 0 & 0 & 1 \end{array} \qquad (6)$$

$C^{\frac12\frac12}_{0}$ $\quad C^{\frac12\frac12}_{1}$

$$\tilde{\mathbb{1}}_2 = {}_1\Big(\overset{1}{1}\;\; \overset{2}{1}\Big) \odot \Big(\boxed{}\;\; \boxed{}\Big), \qquad \big[I^{Q_1R_2}_{Q_2}\big]^{\bar{i}_1}_{i_2}, \quad \big[C^{Q_1R_2}{}_{,Q_2}\big]^{q_1r_2}_{q_2}$$

For first matrix, rows are labeled by $(Q_1,\bar{i}_1,R_2)$, columns by (Q_2,i_2). Each of its elements must be multiplied by the CG block labeled $Q_1 R_2, Q_2$. To indicate this graphically, arrange these blocks in second matrix, carrying same indices as the

For first matrix, rows are labeled by $(Q_1, \bar{i}_1, R_2)$, columns by $(Q_2, \bar{i}_2)$. Each of its elements must be multiplied by the CG block labeled Q_1, R_2, Q_2. To indicate this graphically, arrange these blocks in second matrix, carrying <u>same</u> indices as the first, but having corresponding CG-blocks as elements. $\odot$ means element-wise multiplication of first & second matrices.

$\tilde{\mathbb{1}}_2 \doteq$

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)]:

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

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>

$$Q_2 = 0 \oplus 1 \xrightarrow{\tilde{\mathbb{1}}_{[3]}} Q_3 = 1/2 \oplus 1/2 \oplus 3/2, \quad R_3 = 1/2$$ (9)

block column index

dimensions		[2]	[2]	[4]
block column index		1	2	3
	Q_3	1/2	1/2	3/2
(Q_2, R_3)	$\bar{i}_2$ \ $\bar{i}_3$	1	2	1
1: [2] $(0, \frac{1}{2})$	1	⁝⁝		
2: [3×2] $(1, \frac{1}{2})$	1		⁝⁝	⁝⁝⁝⁝

block row index

(see Sym-II.5.5)

first $S = 1/2$ doublet, second $S = 1/2$ doublet, quartett

$$\begin{array}{c|cc|cc|cccc}
\langle Q_2, q_2; R_3, r_3| \; \bar{i}_2 \;\backslash\; |Q_3, q_3\rangle \; \bar{i}_3 & |\frac12,\frac12\rangle & |\frac12,-\frac12\rangle & |\frac12,\frac12\rangle & |\frac12,-\frac12\rangle & |\frac32,\frac32\rangle & |\frac32,\frac12\rangle & |\frac32,-\frac12\rangle & |\frac32,-\frac32\rangle \\
 & 1 & 1 & 2 & 2 & 1 & 1 & 1 & 1 \\ \hline
\langle 0,0; \frac12, \frac12| \;\; 1 & 1 & 0 & & & & & & \\
\langle 0,0; \frac12, -\frac12| \;\; 1 & 0 & 1 & & & & & & \\ \hline
\langle 1,1; \frac12, \frac12| \;\; 1 & & & 0 & 0 & 1 & 0 & 0 & 0 \\
\langle 1,1; \frac12, -\frac12| \;\; 1 & & & \sqrt{2/3} & 0 & 0 & 1/\sqrt{3} & 0 & 0 \\
\langle 1,0; \frac12, \frac12| \;\; 1 & & & -\sqrt{1/3} & 0 & 0 & \sqrt{2/3} & 0 & 0 \\
\langle 1,0; \frac12, -\frac12| \;\; 1 & & & 0 & 1/\sqrt{3} & 0 & 0 & \sqrt{2/3} & 0 \\
\langle 1,-1; \frac12, \frac12| \;\; 1 & & & 0 & -\sqrt{2/3} & 0 & 0 & 1/\sqrt{3} & 0 \\
\langle 1,-1; \frac12, -\frac12| \;\; 1 & & & 0 & 0 & 0 & 0 & 0 & 1
\end{array}$$ (10)

$C^{0\,1/2}_{1/2}$, $C^{1\,1/2}_{1/2}$, $C^{1\,1/2}_{3/2}$

$$\{\mathbb{1}^{Q_2 R_3}_{Q_3}\}^{\bar{i}_2}_{\bar{i}_3} \qquad \{C^{Q_2, R_3}_{Q_3}\}^{q_2 r_3}_{q_3}$$

$$\tilde{\mathbb{1}}_3 := \begin{array}{c} \\ 1 \\ 2 \end{array}\begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 1 \end{array}\right) \end{array} \odot \left(\begin{array}{ccc} \square & & \\ & ▯ & ▯ \end{array}\right)$$

for both first matrix and second block matrix, rows are labeled by $(Q_2, \bar{i}_2, R_3)$, columns by $(Q_3, \bar{i}_3)$.

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

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 $1^{Q_2 R_3}{}_{Q_3}$

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

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

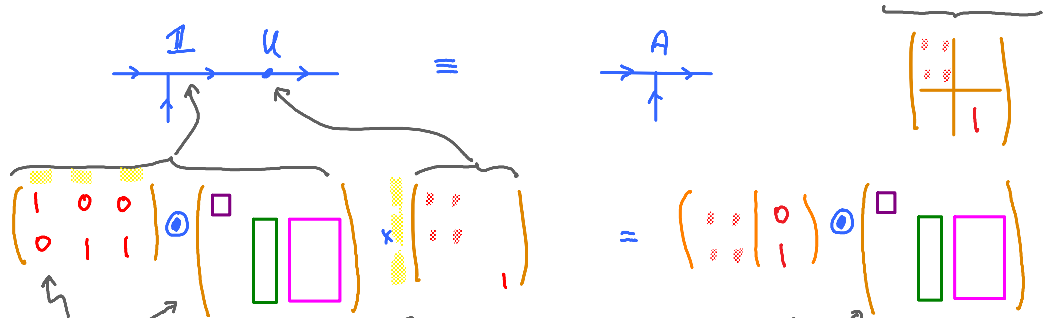
(13)

eigenenergies do not depend on degenerate multiplets!

Diagonalize H:

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

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



(16)

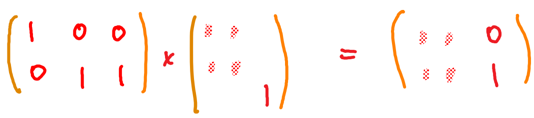
for both first matrix and second block matrix rows are labeled by $(Q_2,\bar i_2,R_3)$, columns by (Q_3,i_3).

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 $(Q_2,\bar i_2,R_3)$, columns by $(Q_3,\bar i_3)$.

sum on i_3 is implied, yielding matrix multiplication:

CGC factor is merely a spectator !



$$\left[1^{Q_2R_2}{}_{Q_3}\right]^{\bar i_2}{}_{i_3}\cdot\left(U_{[Q_3]}\right)^{i_3}{}_{\bar i_3} = \left[A^{Q_2R_3}{}_{Q_3}\right]^{\bar i_2}{}_{\bar i_3}$$

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

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

(18)