

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:

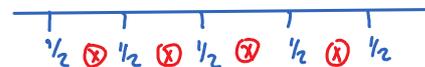
$$H = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix} \longrightarrow \begin{pmatrix} \cdot & & & \\ \cdot & \cdot & & \\ \cdot & & \cdot & \cdot \\ \cdot & & & \cdot \end{pmatrix}$$

direct product basis direct sum basis (4)

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: $[\hat{S}^a, \hat{S}^b] = i\epsilon^{abc} \hat{S}^c$, $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ (6)

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

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

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

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

Irreducible multiplet: $\hat{S}^2 |S, s\rangle = S(S+1) |S, s\rangle$, $S = 0, 1/2, 1, \dots$ (10)

(irrep)

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

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

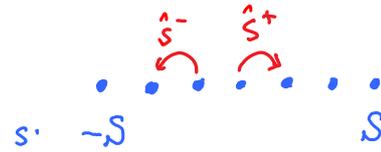
$\hat{S}^+ \dots \hat{S}^- \hat{S}^+$

Dimension of multiplet:

$$a_S = 2S + 1 \quad (14)$$

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

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



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

Define $\hat{S}_{tot} = \sum_{\ell} \vec{S}_{\ell}$, then $\hat{S}_{tot}^x, \hat{S}_{tot}^y, \hat{S}_{tot}^z$ are SU(2) generators, (16)

and $[\hat{H}, \hat{S}_{tot}^z] = 0, [\hat{H}, \hat{S}_{tot}^2] = 0$. (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

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

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

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

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)

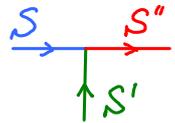
Sym-II.2

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

$$V^S \equiv \text{span} \{ |S, s\rangle \mid s = -S, \dots, S \} \quad (1)$$

↑ 'irrep label'
↑ 'internal label'

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

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


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

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: $\hat{C}^\dagger (\hat{S}_1^a \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{S}_2^a) \hat{C} = \sum_{\oplus S''} \hat{S}^a \quad (4)$

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

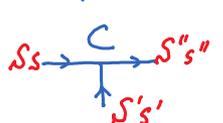
\hat{C} transforms generators into block-diagonal form:

for $S = 1/2, S' = 1/2$: $C^\dagger \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix} C = \begin{pmatrix} \cdot & | & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \quad (5)$

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

completeness in direct product space

$$|S'', s''; S, S'\rangle = \sum_{s, s'} |S, s\rangle \otimes |S', s'\rangle \times \langle S', s' | \langle S, s | |S'', s''; S, S'\rangle \quad (6)$$

$$\text{CGC} = \langle S', s'; S, s | S'', s'' \rangle \equiv (C^{S, S', S''})^{s s'}_{s''} \quad (7)$$


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

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

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

" $\hat{S}_1^2 + \hat{S}_2^2$ " 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:

$$\begin{aligned} \hat{U}(g) |S, s\rangle &= |S, s'\rangle \mathcal{D}(g)^{S'}_{s'} && \text{representation matrix for spin-S irrep,} \\ & && \text{of dimension } (2S'+1) \times (2S'+1) \end{aligned} \tag{0}$$

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

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

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

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):

$$\hat{S}^{(S=1,s)} = \begin{pmatrix} \frac{1}{\sqrt{2}} \hat{S}^+ & \hat{S}^z & \frac{1}{\sqrt{2}} \hat{S}^- \\ s=1 & s=0 & s=-1 \end{pmatrix}, \quad \hat{U}(g) \hat{S}^{(1,s)} \hat{U}^\dagger(g) = \mathcal{D}^\dagger(g)^S_{s'} \hat{S}^{(1,s')} \tag{3}$$

Wigner-Eckardt theorem

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

$$\langle S, i; s | \hat{O}^{(S',s')} | S'', i''; s'' \rangle = [O^{S,S',S''}]^i_{i''} \langle S, s; S', s' | S'', s'' \rangle \tag{4}$$

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

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

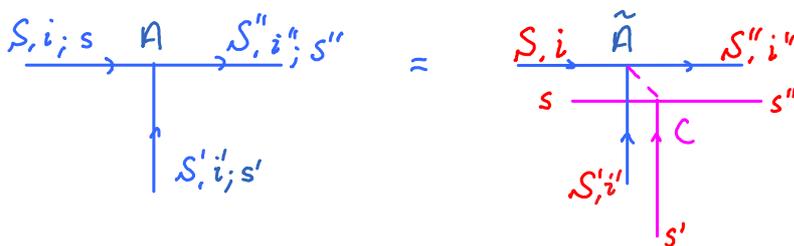
$$\langle S, i; s | \hat{H} | S'', i''; s'' \rangle = [H^{S,0,S''}]^i_{i''} \langle S, s; 0,0 | S'', s'' \rangle \tag{5}$$

Hamiltonian matrix for block $S \rightarrow [H_S]^i_{i''}$ (5')

$\delta^S_{S''} \delta^s_{s''}$ (sum rules)

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

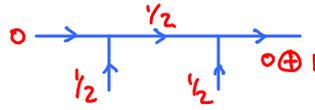
$$A^{(S,i;s), (S',i';s')}_{(S'',i'';s'')} = (\tilde{A}^{S,S',S''})^i_{i''} (C^{S,S',S''})^{s,s'}_{s''} \tag{6}$$



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

(self-study: check details!)

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



Local state space for spin 1/2 :

$$|\uparrow\rangle = |\frac{1}{2}, \frac{1}{2}\rangle, \quad |\downarrow\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle. \quad (1)$$

Singlet: $|S, s\rangle = |0, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ (2)

$$= \frac{1}{\sqrt{2}} (|\frac{1}{2}, \frac{1}{2}; \frac{1}{2}, -\frac{1}{2}\rangle - |\frac{1}{2}, -\frac{1}{2}; \frac{1}{2}, \frac{1}{2}\rangle) \quad (3)$$

Triplet:

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

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

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

Transforming operators from direct product to direct sum basis

(self-study: check details!)

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

In direct product basis, the generators have the form

$$S^+ = S_1^+ \otimes I_2 + I_1 \otimes S_2^+ = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (8)$$

$$S^- = S_1^- \otimes I_2 + I_1 \otimes S_2^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (9)$$

$$S^z = S_1^z \otimes I_2 + I_1 \otimes S_2^z = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (10)$$

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

$$\tilde{S}^+ = C_{\{2\}}^\dagger S^+ C_{\{2\}} = \begin{pmatrix} 0 & \gamma_{12} & \gamma_{12} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \gamma_{12} & -\gamma_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ \gamma_{12} & 0 & \gamma_{12} & 0 \\ \gamma_{12} & 0 & -\gamma_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma_{12} & 0 & 0 \\ 0 & 0 & \gamma_{12} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (11)$$

$$\tilde{S}^- = C_{\{2\}}^\dagger S^- C_{\{2\}} = \begin{pmatrix} 0 & \gamma_{12} & \gamma_{12} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \gamma_{12} & -\gamma_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ \gamma_{12} & 0 & \gamma_{12} & 0 \\ \gamma_{12} & 0 & -\gamma_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \gamma_{12} & 0 & 0 \\ 0 & 0 & \gamma_{12} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (12)$$

$$\tilde{S}^z = C_{\{2\}}^\dagger S^z C_{\{2\}} = \begin{pmatrix} 0 & \gamma_{12} & \gamma_{12} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & \gamma_{12} & -\gamma_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ \gamma_{12} & 0 & \gamma_{12} & 0 \\ \gamma_{12} & 0 & -\gamma_{12} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (13)$$

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 reducible space $V^0 \oplus V^1$

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

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

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

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

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

These matrices are not 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:

$$C_{\{2\}}^\dagger (\vec{S}_1 \cdot \vec{S}_2) C_{\{2\}} = C_{\{2\}}^\dagger (S_1^z \otimes S_2^z + \frac{1}{2} [S_1^+ \otimes S_2^- + S_1^- \otimes S_2^+]) C_{\{2\}} = \frac{1}{4} \begin{pmatrix} -3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (20)$$

The diagonal entries are consistent with the identity

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2} \left[(\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2 \right] = \left. \begin{cases} \frac{1}{2} (0 \cdot 1 - \gamma_{12} \cdot \gamma_{12} - \gamma_{12} \cdot \gamma_{12}) = -3/4 & \text{for } S^z = 0 \\ \frac{1}{2} (1 \cdot 2 - \gamma_{12} \cdot \gamma_{12} - \gamma_{12} \cdot \gamma_{12}) = 1/4 & \text{for } S^z = 1 \end{cases} \right\} \quad (21)$$

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

$$\mathbf{1}_1 \otimes S_2^z = \frac{1}{2} \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \Rightarrow \widetilde{\mathbf{1}_1 \otimes S_2^z} = C_{[2]}^\dagger (\mathbf{1}_1 \otimes S_2^z) C_{[2]} = \frac{1}{2} \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (22)$$

$$\mathbf{1}_1 \otimes S_2^+ = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \widetilde{\mathbf{1}_1 \otimes S_2^+} = C_{[2]}^\dagger (\mathbf{1}_1 \otimes S_2^+) C_{[2]} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (23)$$

$$\mathbf{1}_1 \otimes S_2^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow \widetilde{\mathbf{1}_1 \otimes S_2^-} = C_{[2]}^\dagger (\mathbf{1}_1 \otimes S_2^-) C_{[2]} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \end{pmatrix} \quad (24)$$

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

Sym-II.5

$$(V^0 \oplus V^1) \otimes V^{1/2} = V^{1/2} \oplus V^{3/2} \quad \begin{array}{c} 0 \rightarrow \xrightarrow{1/2} \xrightarrow{1/2} \xrightarrow{0 \oplus 1} \xrightarrow{1/2 \oplus 1/2 \oplus 3/2} \\ \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \\ 1/2 \quad 1/2 \quad 1/2 \quad 1/2 \end{array} \quad (1)$$

$$|S'' = 1/2, i=1; s''\rangle: \begin{array}{l} |1/2, 1/2\rangle = 1 \cdot |0, 0\rangle \otimes |1/2, 1/2\rangle \\ |1/2, -1/2\rangle = 1 \cdot |0, 0\rangle \otimes |1/2, -1/2\rangle \end{array} \quad \text{'first doublet'} \quad (2)$$

$$|S'' = 1/2, i=2; s''\rangle: \begin{array}{l} |1/2, 1/2\rangle = \frac{\sqrt{2}}{3} |1, 1\rangle \otimes |1/2, -1/2\rangle - \frac{1}{\sqrt{3}} |1, 0\rangle \otimes |1/2, 1/2\rangle \\ |1/2, -1/2\rangle = \frac{1}{\sqrt{3}} |1, 0\rangle \otimes |1/2, -1/2\rangle - \frac{\sqrt{2}}{3} |1, -1\rangle \otimes |1/2, 1/2\rangle \end{array} \quad \text{'second doublet'} \quad (3)$$

$$|S'' = 3/2, i=1; s''\rangle: \begin{array}{l} |3/2, 3/2\rangle = 1 \cdot |1, 1\rangle \otimes |1/2, 1/2\rangle \\ |3/2, 1/2\rangle = \frac{1}{\sqrt{3}} |1, 1\rangle \otimes |1/2, -1/2\rangle + \frac{\sqrt{2}}{3} |1, 0\rangle \otimes |1/2, 1/2\rangle \\ |3/2, -1/2\rangle = \frac{\sqrt{2}}{3} |1, 0\rangle \otimes |1/2, -1/2\rangle + \frac{1}{\sqrt{3}} |1, -1\rangle \otimes |1/2, 1/2\rangle \\ |3/2, -3/2\rangle = 1 \cdot |1, -1\rangle \otimes |1/2, -1/2\rangle \end{array} \quad \text{'quartet'} \quad (4)$$

Basis transformation (Clebsch-Gordan coefficients):

	$i=1$ first doublet		$i=2$ second doublet		quartet			
	$ 1/2, 1/2\rangle$	$ 1/2, -1/2\rangle$	$ 1/2, 1/2\rangle$	$ 1/2, -1/2\rangle$	$ 3/2, 3/2\rangle$	$ 3/2, 1/2\rangle$	$ 3/2, -1/2\rangle$	$ 3/2, -3/2\rangle$
$\langle 0, 0; 1/2, 1/2 $	1	0	0	0	0	0	0	0
$\langle 0, 0; 1/2, -1/2 $	0	1	0	0	0	0	0	0
$\langle 1, 1; 1/2, 1/2 $	0	0	$\frac{\sqrt{2}}{3}$	0	1	0	0	0
$\langle 1, 1; 1/2, -1/2 $	0	0	$-\frac{1}{\sqrt{3}}$	0	0	$\frac{1}{\sqrt{3}}$	0	0
$\langle 1, 0; 1/2, 1/2 $	0	0	0	$\frac{1}{\sqrt{3}}$	0	0	$\frac{\sqrt{2}}{3}$	0
$\langle 1, 0; 1/2, -1/2 $	0	0	0	$-\frac{\sqrt{2}}{3}$	0	0	$\frac{1}{\sqrt{3}}$	0
$\langle 1, -1; 1/2, 1/2 $	0	0	0	0	0	0	0	1
$\langle 1, -1; 1/2, -1/2 $	0	0	0	0	0	0	0	0

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

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

$$C_{[3]}^\dagger \begin{pmatrix} -3/4 & 0 & 0 & 1/\sqrt{2} & -1/4 & 0 & 0 & 0 \\ 0 & -3/4 & 0 & 0 & 1/4 & -1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & 0 & 0 & 1/\sqrt{2} & 0 & 0 & 0 \\ -1/4 & 0 & 0 & 1/\sqrt{2} & 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 & 0 & 1/4 & 1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{2} & 0 & 0 & 0 & 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \end{pmatrix} C_{[3]} = \begin{matrix} S=1/2 \\ S=3/2 \end{matrix} \begin{matrix} S=1/2 & S=3/2 \\ \begin{pmatrix} -3/4 & 0 & \sqrt{3}/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3/4 & 0 & \sqrt{3}/4 & 0 & 0 & 0 & 0 \\ \sqrt{3}/4 & 0 & -1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3}/4 & 0 & -1/4 & 0 & 0 & 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 & 0 & 0 & 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1/2 \end{pmatrix} \end{matrix} \quad (11)$$

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

Suppose Hamiltonian for sites 1 to ℓ has been diagonalized:

$$H_e = H_e \begin{matrix} \swarrow \\ \searrow \end{matrix} = E_{[S]}^{i} I_S^{S'} I_{i'}^{i'} \quad (7)$$

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:

$$H_{\ell+1} = |S_{\tilde{i}, \tilde{i}; \tilde{s}}\rangle |S_{i, \bar{i}; s}\rangle |S'_{i', s'}\rangle H_{\ell+1} \begin{matrix} \langle S_{\tilde{i}, \tilde{i}; \tilde{s}} | \langle S_{i, \bar{i}; s} | \langle S'_{i', s'} | \end{matrix} \quad (8)$$

Transform to symmetry eigenbasis, i.e. make unitary transformation into direct sum basis, using CGCs: sums over all repeated indices implied:

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

$$|S_{\tilde{i}, \tilde{i}; \tilde{s}}\rangle \langle S_{\tilde{i}, \tilde{i}; \tilde{s}} | \begin{matrix} [C^{TS} S' S]_{s' s}^{s''} [I^{SS'} S'']_{\tilde{i} \tilde{i}}^{i''} [H_{S''}^{S'' S''}]_{i''}^{i''} [C^{SS'} S'']_{s' s'}^{s''} [I^{S S'} S'']_{\tilde{i} \tilde{i}}^{i''} \end{matrix} \langle S_{i, \bar{i}; s} | \langle S'_{i', s'} | |S_{i, \bar{i}; s''}\rangle \langle S_{i, \bar{i}; s''} | \quad (9)$$

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

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

specifies which multiplets from S, S' yield the multiplet i'' for S''

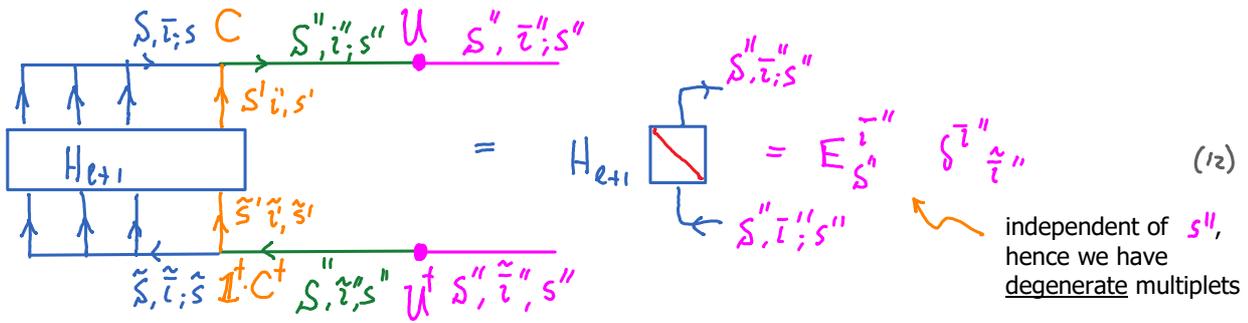
block labeled by S'' with elements labeled by \tilde{i}'', i''

Diagrammatic depiction is more transparent / less cluttered:

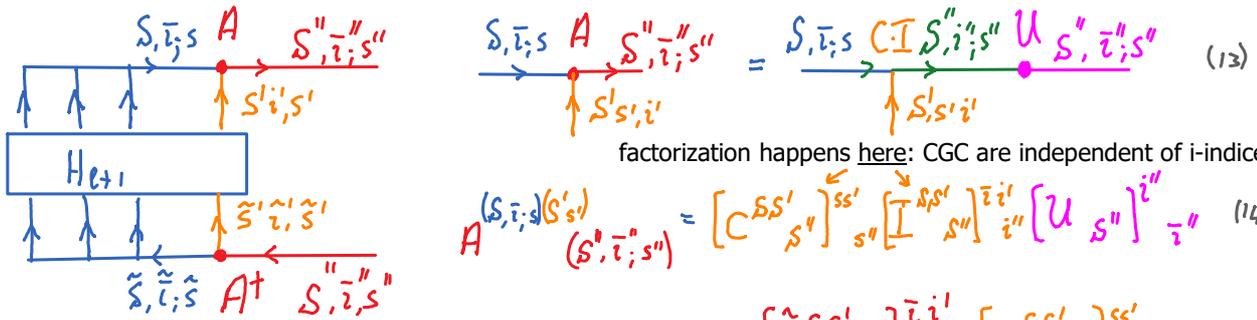
$$H_{\ell+1} = |S''_{i'', s''}\rangle [H_{S''}]_{i''}^{i''} \langle S''_{i'', s''} | \quad (11)$$

symmetry ensures that this is diagonal in spin indices!

Now diagonalize and make unitary transformation into energy eigenbasis:



Combined transformation from old energy eigenbasis to new energy eigenbasis:

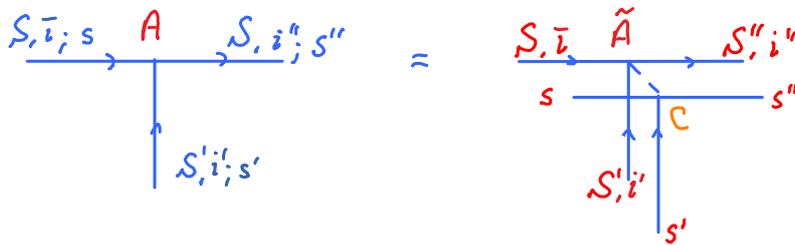


factorization happens here: CGC are independent of i-indices!

$$A_{(S, \bar{i}; s)(S', \bar{i}; s')} = [C^{SS'}]_{s''}^{s'} [I^{SS'}]_{i''}^{i'} [U_{S''}]_{\bar{i}''}^{i''} \quad (14)$$

$$= [\tilde{A}^{SS'}]_{i''}^{i'} [C^{SS'}]_{s''}^{s'} \quad (15)$$

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



7. Bookkeeping: basis transformations spin 1/2

chain

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 i_{e-1} from Q_{e-1}, R_e yield the multiplet i_e for Q_e

$$Q_{e-1, i_{e-1}; q_{e-1}} \tilde{I} = C \cdot I \quad Q_{e, i_e; q_e} = \langle Q_{e-1, i_{e-1}; q_{e-1}} | R_{e, r_e} | Q_{e, i_e; q_e} \rangle \equiv \begin{bmatrix} C^{Q_{e-1}, R_e} & \\ & Q_e \end{bmatrix} \begin{matrix} i_{e-1} \\ q_e \end{matrix} \begin{bmatrix} I^{Q_{e-1}, R_e} \\ & Q_e \end{bmatrix} \begin{matrix} i_e \\ i_e \end{matrix} \quad (1)$$

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:

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

We will stick with standard notation, though.

Sites 0 and 1

$$Q_0 = 0 \quad \tilde{I}_1 \quad Q_1 = 1/2$$

$$R_1 = 1/2 \quad (3)$$

dimensions

$$\begin{matrix} & & [2] \\ & & \begin{matrix} 1/2 \\ 1 \end{matrix} \\ (Q_0, R_1) i_0 & i_1 & \\ \hline [1 \times 2] & (0, 1/2) & 1 \\ & \begin{matrix} \dots \\ \dots \end{matrix} & \\ & [I^{0, 1/2}] & \\ & [C^{0, 0}]^{S_0, \tau_1} & \\ & & q_1 \end{matrix} = \begin{matrix} & & |1/2, 1/2\rangle & |1/2, -1/2\rangle \\ (Q_0, R_1) i_0 & i_1 & & \\ \hline & \langle 0, 0; 1/2, 1/2 | & \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ & \langle 0, 0; 1/2, -1/2 | & \\ & & \uparrow C^{0, 1/2, 1/2} = \mathbb{1}_2 \end{matrix} \quad (4)$$

$$\tilde{I}_1 = \begin{matrix} \text{record} & \text{bond 0} & \text{site 1} & \text{bond 1} & \text{dimensions} & \text{data} & \text{CGC} \\ \text{index } \nu & Q_0 & R_1 & Q_1 & d_{Q_0} \times d_{R_1}, d_{Q_1} & & \\ \hline 1 & 0 & 1/2 & 1/2 & 1 \times 2, 2 & 1 & \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{matrix} \quad (4)$$

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

$$\begin{matrix} Q_1 & H_{[Q_1]} & \text{CGC} & \text{CGC-dim} \\ \hline 1/2 & 0 & \mathbb{1}_2 & 2 \end{matrix} \quad (5)$$

Sites 1 and 2

$$Q_1 = 1/2 \quad \tilde{I}_2 \quad Q_2 = 0 \oplus 1$$

$$R_2 = 1/2$$

block column index

dimensions

block row index

(see Sym-II.4.7)

$$\begin{matrix} & & [1] & [3] \\ & & \begin{matrix} 0 \\ 1 \end{matrix} & \begin{matrix} 1 \\ 1 \end{matrix} \\ (Q_1, R_2) i_1 & i_2 & & \\ \hline [2 \times 2] & (1/2, 1/2) & 1 & \begin{matrix} \dots \\ \dots \end{matrix} \\ & [I^{1/2, 1/2}] & & \\ & [C^{0, 1/2}]^{i_1, i_2} & & \\ & [C^{0, 1/2}]^{j_1, j_2} & & \\ \hline \tilde{I}_2 = & \begin{matrix} (1 & 1) \\ (1 & 1) \end{matrix} \oplus \begin{matrix} \begin{bmatrix} \dots \\ \dots \end{bmatrix} \\ \begin{bmatrix} \dots \\ \dots \end{bmatrix} \end{matrix} \end{matrix} = \begin{matrix} & & \text{singlet} & \text{triplet} \\ (Q_1, R_2) i_1 & i_2 & |0, 0\rangle & |1, 1\rangle |1, 0\rangle |1, -1\rangle \\ \hline & \langle 1/2, 1/2; 1/2, 1/2 | & \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1/2 & 0 & +1/\sqrt{2} & 0 \\ -1/2 & 0 & +1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\ & \langle 1/2, 1/2; 1/2, -1/2 | & \\ & \langle 1/2, -1/2; 1/2, 1/2 | & \\ & \langle 1/2, -1/2; 1/2, -1/2 | & \\ & & \uparrow C^{1/2, 1/2} & \uparrow C^{1/2, 1/2} \end{matrix} \quad (6)$$

For first matrix, rows are labeled by (Q_1, 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, 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 first, but having corresponding CG-blocks as elements. \odot means element-wise multiplication of first & second matrices.

$$\tilde{\mathbb{I}}_2 = \begin{array}{c|cccccc} \text{record index } \nu & \text{bond 1 } Q_1 & \text{site 2 } R_2 & \text{bond 2 } Q_2 & \text{dimensions } d_{Q_1} \times d_{R_2}, d_{Q_2} & \text{data} & \text{CGC} \\ \hline 1 & 1/2 & 1/2 & 0 & 2 \times 2, 1 & 1 & \boxed{} \\ \hline 2 & 1/2 & 1/2 & 1 & 2 \times 2, 3 & 1 & \boxed{} \end{array} \quad (9)$$

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

$$\vec{S}_1 \cdot \vec{S}_2 = \begin{array}{c|ccc} 0 & -3/4 & 0 & 0 & 0 \\ \hline 0 & 0 & 1/4 & 1_3 \\ \hline 1 & 0 & 0 & 0 & 1_3 \end{array}$$

Q	$H[Q_2]$	CGC	CGC-dim
0	$-3/4$	1_1	1
1	$1/4$	1_3	3

(8)

sparse way of storing $\mathbb{I}^{Q_1, R_2, Q_2}$

Sites 2 and 3

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

block column index: 1, 2, 3
 dimensions: [2], [2], [4]
 $(Q_2, R_3)_{i_2}$: 1/2, 1/2, 3/2
 1, 2, 1

(see Sym-II.5.5)

first $S=1/2$ doublet: $|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle$
 second $S=1/2$ doublet: $|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle$
 quartett: $|\frac{3}{2}, \frac{3}{2}\rangle, |\frac{3}{2}, \frac{1}{2}\rangle, |\frac{3}{2}, -\frac{1}{2}\rangle, |\frac{3}{2}, -\frac{3}{2}\rangle$

$\langle Q_2, R_2; R_3, r_3 | i_2$

$\langle 0, 0; 1/2, 1/2 $	1	0		
$\langle 0, 0; 1/2, -1/2 $	0	1		
$\langle 1, 1; 1/2, 1/2 $	0	0	1	0
$\langle 1, 1; 1/2, -1/2 $	0	0	0	1
$\langle 1, 0; 1/2, 1/2 $	0	$1/\sqrt{3}$	0	0
$\langle 1, 0; 1/2, -1/2 $	0	0	$1/\sqrt{3}$	0
$\langle 1, -1; 1/2, 1/2 $	0	0	0	$1/\sqrt{3}$
$\langle 1, -1; 1/2, -1/2 $	0	0	0	0

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

$\tilde{\mathbb{I}}_3 = \begin{array}{c|ccc} 1 & 1 & 0 & 0 \\ \hline 2 & 0 & 1 & 1 \end{array} \odot \begin{array}{c|cc} \boxed{} & \boxed{} \\ \hline \boxed{} & \boxed{} \end{array}$

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

$$\tilde{\mathbb{I}}_{[3]} = \begin{array}{c|cccccc} \text{record index } \nu & \text{bond 2 } Q_2 & \text{site 3 } R_3 & \text{bond 4 } Q_3 & \text{dimensions } d_{Q_2} \times d_{R_3}, d_{Q_3} & \text{data} & \text{CGC} \\ \hline 1 & 0 & 1/2 & 1/2 & 1 \times 2, 2 & 1 & \boxed{} \\ \hline 2 & 1 & 1/2 & 1/2 & 3 \times 2, 2 & 1 & \boxed{} \\ \hline 3 & 1 & 1/2 & 3/2 & 3 \times 2, 4 & 1 & \boxed{} \end{array} \quad (11)$$

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

sparse way of storing $\mathbb{1}^{Q_2 R_3}_{Q_3}$

$$\overbrace{\vec{S}_1 \cdot \vec{S}_2}^{1/2} \cdot \mathbb{1}_3 + \overbrace{\mathbb{1}_1 \cdot \vec{S}_2 \cdot \vec{S}_3}^{3/2} = \frac{1}{2} \left(\begin{array}{c|c} \begin{pmatrix} -3/4 & \sqrt{3}/4 \\ \sqrt{3}/4 & -4/4 \end{pmatrix} \otimes \mathbb{1}_2 & \\ \hline & \frac{1}{2} \otimes \mathbb{1}_4 \end{array} \right) \quad (12)$$

This information can be stored in the format

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

eigenenergies do not depend on degenerate multiplets!

Diagonalize H:

$$H_{[Q_3]} |Q_3, \bar{i}_3; q_3\rangle = E_{[Q_3] \bar{i}_3} |Q_3, \bar{i}_3; q_3\rangle \quad (14)$$

$$|Q_3, \bar{i}_3; q_3\rangle = |Q_3, i_3; q_3\rangle U_{[Q_3] i_3 \bar{i}_3} \quad (15)$$

$$\begin{array}{c} \mathbb{1} \quad U \\ \downarrow \quad \downarrow \\ \left(\begin{array}{ccc|cc} 1 & 0 & 0 & & \\ 0 & 1 & 1 & & \end{array} \right) \otimes \left(\begin{array}{c|c} \square & \\ \hline \square & \square \end{array} \right) \times \left(\begin{array}{ccc|c} \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \\ \dots & \dots & \dots & \end{array} \right) \\ \downarrow \quad \downarrow \quad \downarrow \\ \left(\begin{array}{ccc|c} \dots & \dots & \dots & 0 \\ \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \end{array} \right) \otimes \left(\begin{array}{c|c} \square & \\ \hline \square & \square \end{array} \right) \end{array} = \left(\begin{array}{ccc|c} \dots & \dots & \dots & 0 \\ \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \end{array} \right) \otimes \left(\begin{array}{c|c} \square & \\ \hline \square & \square \end{array} \right) \quad (16)$$

for both first matrix and second block matrix rows are labeled by (Q_2, 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, 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!

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \times \begin{pmatrix} \dots & \dots \\ \dots & \dots \\ \dots & 1 \end{pmatrix} = \begin{pmatrix} \dots & 0 \\ \dots & \dots \\ \dots & 1 \end{pmatrix}$$

$$[\mathbb{1}^{Q_2 R_3}_{Q_3}]_{i_3}^{i_2} \cdot (U_{[Q_2]})_{i_3 \bar{i}_3}^{i_2} = [A^{Q_2 R_3}_{Q_3}]_{\bar{i}_3}^{i_2}$$

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

$$A^{(Q,i; q), (R,j; r)}(S,k; s) = \left(A^{QR} \right)_{ij}^k \left(C^{QR} \right)_{rs}^s \quad (17)$$

$$\begin{array}{c} Q, i; q \quad \rightarrow \quad S, j; s \\ \downarrow R, j; r \\ R, j; r \end{array} = \begin{array}{c} Q, i \quad \rightarrow \quad S, j \\ \downarrow R, j \\ R, j \end{array} \quad (18)$$