CGC for DMRG

MP

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1 Definition and notation for CGC

Clebsch-Gordon coefficients describe the coupling of irreps of a group. For $SU(2)$ the irreps are labeled by the spin quantum number j, for $U(1)$ the irreps are labeled by an integer n for the amount of particles for example. The CGC depend on three irreps: the two ordered (first j_1 and second j_2) irreps to couple and the total irrep j.

$$C^{j_1,j_2\to j}_{m_1,m_2\to m} \tag{1}$$

For $U(1)$, this simply requires $n_1 + n_2 = n$. Hence the CGc for $U(1)$ are symmetric in n_1 and n_2 but *not* for other permutations. For $SU(2)$ the symmetry relations can be found on wikipedia.

2 $6j$, $9j$ and recoupling symbols

CGC can be multiplied to give recoupling coefficients which are related to Wigner $3nj$-symbols. The $6j$-symbol is related to the recoupling of three irreps:

$$\begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{bmatrix} \delta_{jj'} = \sum_{m_i,m_{ik}} C^{j_1,j_2\to j_{12}}_{m_1,m_2\to m_{12}} C^{j_2,j_3\to j_{23}}_{m_2,m_3\to m_{23}} C^{j_1,j_{23}\to j'}_{m_1,m_{23}\to m'} C^{j_{12}j_3\to j}_{m_{12}m_3\to m} \tag{2}$$

In the first column the CGC share the first irrep and in the second column they share the second irrep. The second and third irrep from the CGC in the first column and first row build the first irrep from the CGC in the second column. The second and thir irreps from the CGC from the first column and second row build the third irreps of the CGC in the second column. It is worthwhile to have this visual structure to identify if the sum over four CGC forms a recoupling coeff or not. The $[\ldots]$-symbol is the recoupling coeff which is related to the $6j$-symbol (curly brackets):

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{Bmatrix} = (-1)^{j_1+j_2+j_3+j} \frac{1}{\sqrt{(2j_{12}+1)(2j_{23}+1)}} \begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{bmatrix} \tag{3}$$

The same quantities exist for four irreps. The recoupling coeff is:

$$\begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{bmatrix} = \sum_{m_i,m_{ik}} C^{j_1,j_2\to j_{12}}_{m_1,m_2\to m_{12}} C^{j_3,j_4\to j_{34}}_{m_3,m_4\to m_{34}} C^{j_{12},j_{34}\to j}_{m_{12},m_{34}\to m} C^{j_1,j_3\to j_{13}}_{m_1,m_3\to m_{13}} C^{j_2,j_4\to j_{24}}_{m_2,m_4\to m_{24}} C^{j_{13},j_{24}\to j}_{m_{13},m_{24}\to m} \tag{4}$$

Notice, that: in the first column the CGC shares the first irrep, in the second column they share the second irrep and in the third column they share the third irrep. Between the first and second column one can draw a cross from $j_2 <--> j_2$ and $j_3 <--> j_3$. In the last column the first and second irrep of each CGC comes from the third irrep in the CGC in the same row but from the first or second column respectively. All m are summed beside the last one from the CGC in the third column. It is worthwhile to have this visual structure to identify if the sum over six CGC forms a recoupling coeff or not. The $9j$-symbol is defined as:

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} = \frac{1}{\sqrt{(2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1)}} \begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{bmatrix} \tag{5}$$

3 Wigner-Eckart

For a tensor operator $O_m^{[k]}$ the following holds:

$$\left\langle j_1, m_1 \middle| O_m^{[k]} \middle| j_2, m_2 \right\rangle = C_{m_2 m \to m_1}^{j_2 k \to j_1} \left\langle j_1 \middle\| O^{[k]} \middle\| j_2 \right\rangle \tag{6}$$

This is convention also used by Mc Culloch. The CGC is build so that the first irrep is the ket, the second irrep is the operator irrep and the total irrep is the bra. For $U(1)$ this means $ket + op = bra$.

For an operator with $k = 0$ (scalar operator), the CGC part is $\delta_{j_2 j_1} \delta_{m_2 m_1}$, so that the reduced matrix elements are the same as the normal matrix elements. If the trace however is calculated from the reduced matrix elements, one needs to take into account that $2j_1 + 1$ copies of the reduced matrix elements appear:

$$\mathrm{tr} O = \sum_j (2j+1) \left\langle j \middle\| O^{[0]} \middle\| j \right\rangle \tag{7}$$

This coefficients is called COEFF_DOT in the implementation. It appears at every situation, where one obtains a scalar quantity. E.g. when contracting the left and right environment to obtain an expectation value.

3.1 Product of tensor operators

The product of two operators $O_{m_1}^{[k_1]}$ and $S_{m_2}^{[k_2]}$ gives rise to different irreducible tensor operators by the definition:

$$\left[O^{[k_1]} \times S^{[k_2]} \right]_m^{[k]} = \sum_{m_1, m_2} C_{m_1 m_2 \to m}^{k_1 k_2 \to k} O_{m_1}^{[k_1]} S_{m_2}^{[k_2]} \tag{8}$$

One can obtain the reduced matrix elements of the product directly from the reduced matrix elements of the individual operators. To see this, one inserts in Eq. (8) the

CGC as defined in the Wigner-Eckart theorem for all operators, namely $O^{[k_1]}_{m_1}$, $S^{[k_2]}_{m_2}$ and $\left[O^{[k_1]} \times S^{[k_2]}\right]^{[k]}_{m}$. Therefore, one sandwiches the eqation with $\langle j_1, m_{j_1} | \ldots | j_2 m_{j_2}\rangle$ and introduces an identity $\sum_{j_3 m_{j_3}} |j_3 m_{j_3}\rangle \langle j_3 m_{j_3}|$ for the operator product on the right side of Eq. (8). For clearness it is worthwile to omit the reduced matrix elements because they factor out. The CGC part reads then:

$$C^{j_2 k \to j_1}_{m_{j_2} m_k \to m_{j_1}} = \sum_{m_{k_1}, m_{k_2}, m_{j_3}} C^{k_1 k_2 \to k}_{m_{k_1} m_{k_2} \to m_k} C^{j_3 k_1 \to j_1}_{m_{j_3} m_{k_1} \to m_{j_1}} C^{j_2 k_1 \to j_3}_{m_{j_2} m_{k_1} \to m_{j_3}} \tag{9}$$

The CGC at the left side can be brought to the right side by multiplying with $C^{j_2 k \to J_1}_{m_{j_2} m_k \to m_{J_1}}$ and summing over m_{j_2} and m_k. This gives $\delta_{j_1 J_1} \delta_{m_{j_1} m_{J_1}}$ for the left side and for right side:

$$\begin{aligned} \delta_{j_1 J_1} \delta_{m_{j_1} m_{J_1}} = & \sum_{m_{k_1}, m_{k_2}, m_{j_3}, m_{j_2}, m_k} \\ & C^{j_2 k_1 \to j_3}_{m_{j_2} m_{k_1} \to m_{j_3}} C^{k_1 k_2 \to k}_{m_{k_1} m_{k_2} \to m_k} \\ & C^{j_2 k \to j_1}_{m_{j_2} m_k \to m_{j_1}} C^{j_3 k_2 \to j_1}_{m_{j_3} m_{k_2} \to m_{j_1}} \end{aligned} \tag{10}$$

This equation does not fit the definition of the recouple coeff in Eq. (2). To reach this, one has to interchange k_1 and k_2 in the CGC $C^{k_1 k_2 \to k}_{m_{k_1} m_{k_2} \to m_k}$. This leads to a an additional phase factor $(-1)^{k_1 + k_2 - k}$. Afterwards, one can perform the sum over the m quantum numbers to obtain a recouple coeff as in Eq. (2).

$$\begin{aligned} \delta_{j_1 J_1} \delta_{m_{j_1} m_{J_1}} &= (-1)^{k_1 + k_2 - k} \begin{bmatrix} j_2 & k_1 & j_3 \\ k_2 & j_1 & k \end{bmatrix} \delta_{j_1 J_1} \delta_{m_{j_1} m_{J_1}} \\ &= (-1)^{k_1 + k_2 - k} (-1)^{j_2 + k_1 + k_2 + j_1} \sqrt{(2 j_3 + 1)(2k + 1)} \begin{Bmatrix} j_2 & k_1 & j_3 \\ k_2 & j_1 & k \end{Bmatrix} \delta_{j_1 J_1} \delta_{m_{j_1} m_{J_1}} \end{aligned} \tag{11}$$

For sign, one finds:

$$(-1)^{k_1 + k_2 - k - k + k + j_2 + k_1 + k_2 + j_1} = (-1)^{2(k_1 + k_2 - k)} (-1)^{k + j_2 + j_1} = (-1)^{k + j_2 + j_1}, \tag{12}$$

because k_1, k_2 and k fulfil the triangle condition. In summary, the coefficient for the product is:

$$\begin{aligned} \left\langle j_1 \left\| \left[O^{[k_1]} \times S^{[k_2]}\right]^{[k]}_{m} \right\| j_2 \right\rangle = & \sum_{j_3} (-1)^{k + j_2 + j_1} \sqrt{(2 j_3 + 1)(2k + 1)} \begin{Bmatrix} j_2 & k_1 & j_3 \\ k_2 & j_1 & k \end{Bmatrix} \\ & \left\langle j_1 \left\| O^{[k_1]} \right\| j_3 \right\rangle \left\langle j_3 \left\| S^{[k_2]} \right\| j_2 \right\rangle \end{aligned} \tag{13}$$

The corresponding coefficient is called COEFF_PROD.

3.2 Adjoint of tensor operators

The adjoint of tensor operators can be defined with respect to the metric defined in Eq. (8) when coupling two operators of rank k to a singlet operator ($k = 0$). The corresponding CGC is $C^{kk\to 0}_{m_1 m_2 \to 0} = \frac{(-1)^{k-m_1}}{\sqrt{2k+1}} \delta_{m_1,-m_2}$. The adjoint tensor operator is therefore:

$$O^{\dagger[k]}_m = (-1)^{k-m} \left(O^{[k]}_{-m} \right)^\dagger \tag{14}$$

The Wigner Eckart theorem gives:

$$\left\langle j_1 m_1 \middle| O^{\dagger[k]}_m \middle| j_2 m_2 \right\rangle = C^{j_2 k \to j_1}_{m_2 m \to m_1} \left\langle j_1 \middle\| O^{\dagger[k]} \middle\| j_2 \right\rangle \tag{15}$$

The reduced matrix elements of the adjoint are related to the original one. The factor is obained when applying the Wigner Eckart theorem for Eq. (14):

$$C^{j_2 k \to j_1}_{m_2 m \to m_1} = (-1)^{k-m} C^{j_1 k \to j_2}_{m_1, -m \to m_2} \tag{16}$$

Interchanging j_1 and j_2 at the right side leads to the factor $\sqrt{\frac{2j_2+1}{2j_1+1}}(-1)^{k-m}$ and to the subtitution m_1 to $-m_1$ and m_2 to $-m_2$ in the CGC at the right. The sign $(-1)^{k-m}$ cancels and after reverting all signs of the CGC at the right, the two CGC are identical. Reverting all signs give another sign $(-1)^{j_1+k-j_2}$ so that the corresponding coeff reads:

$$\left\langle j_1 \middle\| O^{\dagger[k]} \middle\| j_2 \right\rangle = (-1)^{j_1+k-j_2} \sqrt{\frac{2j_2+1}{2j_1+1}} (-1)^{k-m} \left\langle j_2 \middle\| O^{[k]} \middle\| j_1 \right\rangle^* \tag{17}$$

The corresponding coefficient is called COEFF_ADJOINT in the implementation. Notice that $O^{\dagger^\dagger[k]} = (-1)^{2k} O^{[k]}$.

3.3 Spin operator

3.4 Fermionic operators

4 Convention for MPS, MPO and environments

For an MPS, we choose the following convention for the CGC:

$$A^\sigma_{ij} = A^\sigma_{ij} C^{i\sigma \to j}_{m_i m_\sigma \to m_j} \tag{18}$$

This is different from the convention by Mc Culloch. For $U(1)$ it corresponds to $i + \sigma = j$. i is the left index from A and j the right index.

For an MPO, we choose the following convention for the CGC:

$$W_{ab}^{[k]\sigma_1\sigma_2} = W_{ab}^{[k]\sigma_1\sigma_2} C^{\sigma_2 k\to\sigma_1}_{m_{\sigma_2} m_k \to m_{\sigma_1}} C^{ak\to b}_{m_a m_k \to m_b} \tag{19}$$

For $U(1)$ it corresponds to $a+b=j$ and $\sigma_2+k=\sigma_1$. a is the left index from W and b the right index. σ_2 points in the direction of the ket MPS while σ_1 into the direction of the bra.

For the left environment we have:

$$L_{ij}^{a} = L_{ij}^{a} C^{ia\to j}_{m_i m_a \to m_j} \tag{20}$$

For $U(1)$ it corresponds to $i+a=j$. i is pointing to the ket layer, j is pointing to the bra layer.

For the right environment we have:

$$R_{ij}^{a} = R_{ij}^{a} C^{ia\to j}_{m_i m_a \to m_j} \tag{21}$$

For $U(1)$ it corresponds to $i+a=j$. i is pointing to the ket layer, j is pointing to the bra layer.

5 Algorithms

5.1 Sweep and reshape

] Reshaping is is the combination of two indices into a super index. This is essentially an isometry which maps the basis states from the two indices into one. The reshaping process is not unique and a convention is neccesary. E.g. without any symmetries a isometry $\Pi^k_{i\sigma}$ could be chosen as $\Pi^k_{i\sigma}=1$ if $k=i+\dim(i)\sigma$ and $\Pi^k_{i\sigma}=0$ otherwise. For symmetric tensors, the isometry should map on proper irreps of the syymetry. The combination of two irreps into the tensor product is exactly the definition for the CGC, so that the isometry Π needs to be proportional to the CGC.

For a right sweep, we want to left-normalize the A-tensor. Hence the incoming index i get combined with the physical index σ. The symmetry part of isometry Π is chosen as $\Pi = C^{i\sigma\to k}_{m_i m_\sigma \to m_k}$. We have $\Pi\cdot\Pi^\dagger=1$ since:

$$\sum_{m_i m_\sigma} C^{i\sigma\to k}_{m_i m_\sigma \to m_k} C^{i\sigma\to k}_{m_i m_\sigma \to m_k} = 1 \tag{22}$$

is a orthonormality condition for the CGC. Furthermore in the calculation $\Pi\cdot A$, the CGC drop out for the same reason. Hence there is no extra factor for a right sweep step (left-normalization step).

$$A^{\sigma}_{ij} = \tilde{A}^{(i\sigma)}_{j} \tag{23}$$

There is also no extra factor when checking for the left-nomalize condition.

For a left sweep, we want to right-normalize the A-tensor. Hence the outgoing index j get combined with the physical index σ. The symmetry part of isometry Π is chosen as $\Pi \sim C^{k\sigma\to j}_{m_k m_\sigma \to m_j}$. We have $\Pi \cdot \Pi^\dagger \neq 1$ but:

$$\sum_{m_j m_\sigma} C^{k\sigma\to j}_{m_k m_\sigma \to m_j} C^{k\sigma\to j}_{m_k m_\sigma \to m_j} = \frac{2j+1}{2k+1} \tag{24}$$

This can be seen when changing the indices k and j in both CGC which leads to the factor $\sqrt{\frac{2j+1}{2k+1}}(-1)^{\sigma - m_\sigma}$. The phase factor drops out because it appears twice. The CGC after the interchange multiply to one. A proper normalized Π is in fact an isometry: $\Pi = \sqrt{\frac{2k+1}{2j+1}} C^{k\sigma\to j}_{m_k m_\sigma \to m_j}$. When calculating $\Pi \cdot A$, one encounters the same equation as above so there is a factor for the left sweep:

$$A^\sigma_{ij} = \sqrt{\frac{2j+1}{2i+1}} \tilde{A}^{(\sigma j)}_i \tag{25}$$

This factor is called COEFF_LEFTSWEEP in the implementation. Notice that for the inverse reshaping process, one needs the inverse of this factor. This factor has no different name but simply COEFF_LEFTSWEEP is called with reversed quantum numbers. When checking for the right-normalize condition one encounters also Eq. (24). Hence one has to encounter the factor from the CGC when checking the right-normalize condition:

$$\sum_{\sigma j} A^\sigma_{ij} A^{\dagger\sigma}_{ij} \frac{2j+1}{2i+1} \tag{26}$$

This factor is called COEFF_RIGHTORTHO in the implementation.

5.2 Update L

For updating the left environment, we have the following equation:

$$\boldsymbol{L}_{b_l}(l+1) = \sum_{\sigma_l, \sigma'_l, a_l} \boldsymbol{B}^{\sigma_l \dagger}(l) \boldsymbol{L}_{a_l}(l) \boldsymbol{A}^{\sigma'_l}(l) W^{\sigma_l \sigma'_l}_{a_l b_l}(l) \tag{27}$$

Inserting all the CGC for the tensors, the CGC part of this equation reads:

$$C^{i'a'\to j'}_{m_{i'}, m_{a'} \to m_{j'}} = \sum_{m_{\sigma_1}, m_{\sigma_2}, m_i, m_a, m_j, m_k} C^{j,\sigma_1\to j'}_{m_j, m_{\sigma_1}\to m_{j'}} C^{ia\to j}_{m_i, m_a \to m_j} C^{i,\sigma_2\to i'}_{m_i, m_{\sigma_2}\to m_{i'}} C^{\sigma_2, k\to\sigma_1}_{m_{\sigma_2}, m_k \to m_{\sigma_1}} C^{a,k\to a'}_{m_a, m_k \to m_{a'}} \tag{28}$$

We can multiply this equation with $C^{i'a'\to J'}_{m_{i'},m_{a'}\to m_{J'}}$ and sum over $m_{i'}$ and $m_{a'}$. The left hand side is then $\delta_{j'J'}\delta_{m_{j'}m_{J'}}$ and the right side becomes:

$$\begin{aligned}\delta_{j'J'}\delta_{m_{j'}m_{J'}} = &\sum_{m_{\sigma_1},m_{\sigma_2},m_i,m_a,m_j,m_k,m_{i'},m_{a'}} \\ &C^{i,\sigma_2\to i'}_{m_i,m_{\sigma_2}\to m_{i'}} C^{a,k\to a'}_{m_a,m_k\to m_{a'}} C^{i'a'\to j'}_{m_{i'},m_{a'}\to m_{j'}} \\ &C^{ia\to j}_{m_i,m_a\to m_j} C^{\sigma_2,k\to\sigma_1}_{m_{\sigma_2},m_k\to m_{\sigma_1}} C^{j,\sigma_1\to J'}_{m_j,m_{\sigma_1}\to m_{J'}} \\ &= \begin{bmatrix} i & \sigma_2 & i' \\ a & k & a' \\ j & \sigma_1 & j' \end{bmatrix} \delta_{j'J'}\delta_{m_{j'}m_{J'}}\end{aligned} \tag{29}$$

Which is easily obtained when analysing that the visual structure fits the requirements for the recoupling coeff in Eq. (4). This coeffecient is called COEFF_BUILDL.

5.3 Update R

The update of the right environment is similar. Collecting all the CGC for the tensors, the CGC part reads:

$$C^{ia\to j}_{m_i,m_a\to m_j} = \sum_{m_{\sigma_1},m_{\sigma_2},m_j,m_k,m_{i'},m_{a'}} C^{j,\sigma_1\to j'}_{m_j,m_{\sigma_1}\to m_{j'}} C^{i'a'\to j'}_{m_{i'},m_{a'}\to m_{j'}} C^{i,\sigma_2\to i'}_{m_i,m_{\sigma_2}\to m_{i'}} C^{\sigma_2,k\to\sigma_1}_{m_{\sigma_2},m_k\to m_{\sigma_1}} C^{a,k\to a'}_{m_a,m_k\to m_{a'}} \tag{30}$$

We can multiply this equation with $C^{ia\to J}_{m_i,m_a\to m_J}$ and sum over m_i and m_a. The left hand side is then $\delta_{jJ}\delta_{m_j m_J}$ and the right side becomes:

$$\begin{aligned}\delta_{j'J'}\delta_{m_{j'}m_{J'}} = &\sum_{m_{\sigma_1},m_{\sigma_2},m_i,m_a,m_j,m_k,m_{i'},m_{a'}} \\ &C^{i,\sigma_2\to i'}_{m_i,m_{\sigma_2}\to m_{i'}} C^{a,k\to a'}_{m_a,m_k\to m_{a'}} C^{ia\to J}_{m_i,m_a\to m_J} \\ &C^{i'a'\to j'}_{m_{i'},m_{a'}\to m_{j'}} C^{\sigma_2,k\to\sigma_1}_{m_{\sigma_2},m_k\to m_{\sigma_1}} C^{j,\sigma_1\to j'}_{m_j,m_{\sigma_1}\to m_{j'}}\end{aligned} \tag{31}$$

This is not the correct structure for a recoupling coeff. But the following steps will convert this into the form of Eq. (4). Notice, that I will use *coordinates* (i,j) to refer to the CGC in this equation where i is the row and j is the column.

1. interchange i and i' for $(0,0)$. This gives a factor $(-1)^{\sigma_2+m_{\sigma_2}}\sqrt{\frac{2i'+1}{2i+1}}$. Furthermore m_i and $m_{i'}$ goes into $-m_i$ and $-m_{i'}$.

2. interchange j and j' for $(1,2)$. This gives a factor $(-1)^{\sigma_1+m_{\sigma_1}}\sqrt{\frac{2j'+1}{2j+1}}$. Furthermore m_j and $m_{j'}$ goes into $-m_j$ and $-m_{j'}$.

3. interchange a and a' for $(0,1)$. This gives a factor $(-1)^{k+m_k}\sqrt{\frac{2a'+1}{2a+1}}$. Furthermore m_j and $m_{j'}$ goes into $-m_j$ and $-m_{j'}$.

4. Flip all signs of the m quantum numbers for the CGC in $(0,0)$, $(1,1)$, $(1,2)$ and $(0,1)$. This gives four phase factors: $(-1)^{i'+\sigma_2-i}$, $(-1)^{\sigma_2+k-\sigma_1}$, $(-1)^{j'+\sigma_1-j}$ and $(-1)^{a'+k-a}$.

5. The signs $(-1)^{\sigma_2+m_{\sigma_2}}$, $(-1)^{\sigma_1+m_{\sigma_1}}$, $(-1)^{k+m_k}$ and $(-1)^{\sigma_2+k-\sigma_1}$ gives in total $+1$. This can be seen when noting that $m_{\sigma_1} = m_{\sigma_2} + m_k$ (because of the corresponding CGC) and $(-1)^{2(j+m_j)} = 1$ for any j and m_j which belong together.

6. All m-dependent factors disappear and the sum over the resulting CGC give a recoupling coeff:
$$\begin{bmatrix} i' & \sigma_2 & i \\ a' & k & a \\ j' & \sigma_1 & j \end{bmatrix} \tag{32}$$
together with the factor:
$$(-1)^{i'+\sigma_2-i}(-1)^{j'+\sigma_1-j}(-1)^{a'+k-a}\sqrt{\frac{(2i'+1)(2j'+1)(2a'+1)}{(2i+1)(2j+1)(2a+1)}} \tag{33}$$

7. Convert the recoupling coeff to a $9j$-symbol by Eq. (5). Interchange the first and the last column of the $9j$-symbol. This gives a phase factor given by the sum af all quantum numbers in the $9j$-symbol. Converting back to a recoupl coeff giv the final coefficient used for the update of the right environment:
$$\frac{2j'+1}{2j+1}\begin{bmatrix} i & \sigma_2 & i' \\ a & k & a' \\ j & \sigma_1 & j' \end{bmatrix} \tag{34}$$
This coefficient is called COEFF__BUILDR in the implementation.

5.4 Apply H_{eff}

For the effective Hamiltonian the CGC part reads:

$$C^{j,\sigma_1\to j'}_{m_j,m_{\sigma_1}\to m_{j'}} = \sum_{m_{\sigma_1},m_{\sigma_2},m_i,m_a,m_j,m_k} C^{i'a'\to j'}_{m_{i'},m_{a'}\to m_{j'}} C^{ia\to j}_{m_i,m_a\to m_j} C^{i,\sigma_2\to i'}_{m_i,m_{\sigma_2}\to m_{i'}} C^{\sigma_2,k\to\sigma_1}_{m_{\sigma_2},m_k\to m_{\sigma_1}} C^{a,k\to a'}_{m_a,m_k\to m_{a'}} \tag{35}$$

We can multiply this equation with $C^{j,\sigma_1\to J'}_{m_j,m_{\sigma_1}\to m_{J'}}$ and sum over m_j and m_{σ_1}. The left hand side is then $\delta_{j'J'}\delta_{m_{j'}m_{J'}}$ and the right side becomes:

$$\begin{aligned}\delta_{j'J'}\delta_{m_{j'}m_{J'}} = & \sum_{m_{\sigma_1},m_{\sigma_2},m_i,m_a,m_j,m_k,m_{i'},m_{a'}} \\ & C^{i,\sigma_2\to i'}_{m_i,m_{\sigma_2}\to m_{i'}} C^{a,k\to a'}_{m_a,m_k\to m_{a'}} C^{i'a'\to j'}_{m_{i'},m_{a'}\to m_{j'}} \\ & C^{ia\to j}_{m_i,m_a\to m_j} C^{\sigma_2,k\to\sigma_1}_{m_{\sigma_2},m_k\to m_{\sigma_1}} C^{j,\sigma_1\to J'}_{m_j,m_{\sigma_1}\to m_{J'}} \\ = & \begin{bmatrix} i & \sigma_2 & i' \\ a & k & a' \\ j & \sigma_1 & j' \end{bmatrix} \delta_{j'J'}\delta_{m_{j'}m_{J'}}\end{aligned} \tag{36}$$

Which is easily obtained when analysing that the visual structure fits the requirements for the recoupling coeff in Eq. (4). This coeffecient is called COEFF_HPSI. It is identical to COEFF_BUILDL.

5.5 MPS product

The product of two MPS is obtained by the product over the auxiliary space and the combination of σ_1 and σ_2 to a combined index σ. The CGC part of this operation reads:

$$C^{i,\sigma\to j}_{m_i,m_\sigma\to m_j} = \sum_{m_{\sigma_1},m_{\sigma_2},m_{i'}} C^{i,\sigma_1\to i'}_{m_i,m_{\sigma_1}\to m_{i'}} C^{i',\sigma_2\to j}_{m_{i'},m_{\sigma_2}\to m_j} C^{\sigma_1\sigma_2\to\sigma}_{m_{\sigma_1}m_{\sigma_2}\to m_\sigma} \tag{37}$$

Again we bring the CGC from the left side to the right side by using a orthonormality equation for the CGC and obtain:

$$\begin{aligned}\delta_{jJ}\delta_{m_jm_J} = & \sum_{m_{\sigma_1},m_{\sigma_2},m_{i'},m_i,m_\sigma} \\ & C^{i,\sigma_1\to i'}_{m_i,m_{\sigma_1}\to m_{i'}} C^{i',\sigma_2\to j}_{m_{i'},m_{\sigma_2}\to m_j} \\ & C^{i,\sigma\to J}_{m_i,m_\sigma\to m_J} C^{\sigma_1\sigma_2\to\sigma}_{m_{\sigma_1}m_{\sigma_2}\to m_\sigma} \\ = & \begin{bmatrix} i & \sigma_1 & i' \\ \sigma_2 & j & \sigma \end{bmatrix} \delta_{jJ}\delta_{m_jm_J}\end{aligned} \tag{38}$$

The recoupl coeff is related to the $6j$-symbol and this coefficient for the product of two A-tensors is called COEFF_APAIR in the implementation. Notice, that this is different to COEFF_PROD (Eq. (13)). This is because of our convention for the A-tensors.

5.6 MPO product

Multiplying two MPOs means the product in the auxiliary space and the tensor product in the physical space. Since our convention for the auxiliary indices is the same as for the MPS, the coefficient for the product in the auxiliary space is exactly coeff_Apair. The tensor product in the physical space is identical to coeff_tensorProd (which is not included in the doc yet) since the convention for the physical part of the MPO is $C^{\sigma_2,k\to\sigma_1}_{m_{\sigma_2},m_k\to m_{\sigma_1}}$ which is as for normal tensor operators (Eq. (6)). The total coefficient is simply the product of both.

5.7 MPO times MPS

For this operation, the structure is completely identical to the action of the effective Hamiltonian. This is due to our definition of the CGC structure of the environment. The coefficient is therefore identical to coeff_HPsi. In the implementation, it has an extra name: coeff_AW.

6 Todo

1. Add graphical visualizations of the different contractions.

2. Describe the local operators and their reduced matrix elements.

3. Describe the trace, product, tensor product and adjoint of tensor operators for the coefficients coeff_dot, coeff_prod coeff_tensorProd and coeff_adjoint respectively.

4. Think about recoupling of five irreps and $12j$-symbols. What is problem here?