Coupling coeffients for matrix product states

I. P. McCulloch

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1 Clebsch-Gordan coefficients

We use the notation of Biedenharn:

$$C^{j_1\ j_2\ j_3}_{m_1 m_2 m_3} \tag{1}$$

For fixed j_1 and j_2, these coefficients form a unitary matrix of dimension $(2j_1+1)(2j_2+1)$, with rows labelled by m_1, m_2 and columns labelled by j, m. An explicit form is:

$$\begin{aligned} C^{j_1\ j_2\ j}_{m_1 m_2 m} &= \delta_{m_1+m_2,m} \\ &\times \left[\frac{(2j+1)(j+j_1-j_2)!(j-j_1+j_2)!(j_1+j_2-j)!}{(j+j_1+j_2+1)!} \right]^{\frac{1}{2}} \\ &\times \left[\frac{(j+m)!(j-m!)}{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!} \right]^{\frac{1}{2}} \\ &\times \sum_s \frac{(-1)^{j_2+m_2+s}(j_2+j+m_1+s)!(j_1-m_1+s)!}{s!(j-j_1+j_2-s)!(j+m-s)!(j_1-j_2-m+s)!} \,. \end{aligned} \tag{2}$$

Orthogonality of rows

$$\sum_{m_1 m_2} C^{j_1\ j_2\ j}_{m_1 m_2 m} C^{j_1\ j_2\ j'}_{m_1 m_2 m'} = \delta_{jj'}\delta_{mm'} \tag{3}$$

and orthogonality of columns

$$\sum_{jm} C^{j_1\ j_2\ j}_{m_1 m_2 m} C^{j_1\ j_2\ j}_{m_1' m_2' m} = \delta_{m_1 m_1'}\delta_{m_2 m_2'} \tag{4}$$

The 'classical' symmetries form a group of order 12 and until the work of Regge[**?**] it was believed that these exhausted the symmetries. The true symmetry group is of order 72. The symmetry relations are (the group is generated by the first 4, the remainder are for reference),

$$\begin{aligned} C^{j_1\ j_2\ j}_{m_1 m_2 m} &= (-1)^{j_1+j_2-j} C^{j_1\ \ j_2\ \ j}_{-m_1,-m_2,-m} \,, \\ C^{j_1\ j_2\ j}_{m_1 m_2 m} &= (-1)^{j_1+j_2-j} C^{j_2\ j_1\ j}_{m_2 m_1 m} \,, \\ C^{j_1\ j_2\ j}_{m_1,m_2,m_1+m_2} &= C^{\frac{1}{2}(j_1+j_2+m_1+m_2)\ \frac{1}{2}(j_1+j_2-m_1-m_2)\ j}_{\frac{1}{2}(j_1-j_2+m_1-m_2),\frac{1}{2}(j_1-j_2-m_1+m_2),j_1-j_2} \,, \\ C^{j_1\ j_2\ j}_{m_1 m_2 m} &= (-1)^{j_2+m_2}\sqrt{\tfrac{2j+1}{2j_1+1}} C^{j\ \ j_2\ \ j_1}_{-m,m_2,-m_1} \,, \\ C^{j_1\ j_2\ j}_{m_1 m_2 m} &= (-1)^{j_1-m_1}\sqrt{\tfrac{2j+1}{2j_2+1}} C^{j_1\ \ j\ \ j_2}_{m_1,-m,-m_2} \,, \\ C^{j_1\ j_2\ j}_{m_1 m_2 m} &= (-1)^{j_2+m_2}\sqrt{\tfrac{2j+1}{2j_1+1}} C^{j_2\ \ j\ \ j_1}_{-m_2,m,m_1} \,, \\ C^{j_1\ j_2\ j}_{m_1 m_2 m} &= (-1)^{j_1-m_1}\sqrt{\tfrac{2j+1}{2j_2+1}} C^{j\ \ j_1\ \ j_2}_{m\,-m_1\,m_2} \end{aligned} \tag{5}$$

A useful special case is

$$C^{j_1\ 0j}_{m_1\,0m} = \delta_{j_1 j}\delta_{m_1 m} \tag{6}$$

Alternate notation (Edmonds 1957):

$$C^{j_1\ j_2\ j}_{m_1 m_2 m} \equiv \langle j_1 m_1 j_2 m_2 | j_1 j_2 j m\rangle \tag{7}$$

Alternate notation (Varshalovich *et al.*) [**?**]:

$$C^{j_1\ j_2\ j}_{m_1 m_2 m} \equiv C^{jm}_{j_1 m_1 j_2 m_2} \tag{8}$$

As is apparant from the phase factors and normalizations arising in the symmetry relations, the Clebsch-Gordan coefficients have a mixed symmetry. This is also clear from the notation Eq. (**??**) where j_1 and j_2 transform as bras, but j transforms as a ket. To see how this works, we can interpret the special coefficient $C^{j'\ j\ 0}_{m' m 0}$ as a metric tensor $\eta_{j'j}$, that couples spins j' and j to a scalar. Here, j' is the conjugate spin to j. For $SU(2)$, we have numerically $j' = j$, but for $U(1)$ we have $m' = -m$. In this form, the Clebsh-Gordan coefficient has mixed symmetry $C_{j_1 j_1}{}^{j}$. This is convenient because Eq. (7) is usually exactly what we want, but it is important to keep this detail in mind. The 'symmetric' version of the Clebsch-Gordan coefficient is the $3j$ coefficient (an unfortunate name because it is a rather different object to the $N-j$ coefficients for $N > 3$), and has the form

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = (-1)^{j+m+2j_1} \frac{1}{\sqrt{2j+1}} C^{j_1\ \ j_2\ \ j}_{-m_1 -m_2 m} \tag{9}$$

The inverse form is

$$C^{j_1\ j_2\ j}_{m_1 m_2 m} = (-1)^{j_1 - j_2 + m}\sqrt{2j+1}\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix} \tag{10}$$

The phase factors are chosen so that any cyclic permutation of columns leaves the $3j$ symbol unchanged. Under an odd permutation of columns, the symbol picks up a phase factor $(-1)^{j_1+j_2+j}$, which is the same phase factor from the transformation $(m_1, m_2, m) \to (-m_1, -m_2, -m)$.

2 $6j$ Symbols

The simplest known explitit form is due to Racah[**?**, **?**],

$$\begin{aligned} \begin{Bmatrix} j_1 & j_2 & j \\ k_1 & k_2 & k \end{Bmatrix} &= \Delta(j_1 j_2 j)\Delta(k_1 k_2 j)\Delta(j_1 k_2 k)\Delta(k_1 j_2 k) \\ \times \sum_z & \frac{(-1)^z (z+1)!}{(z-j_1-j_2-j)!(z-k_1-k_2-j)!(z-j_1-k_2-k)!(z-k_1-j_2-k)!} \\ & \times \frac{1}{(j_1+j_2+k_1+k_2-z)!(j_1+k_1+j+k-z)!(j_2+k_2+j+k-z)!}, \end{aligned} \tag{11}$$

where $\Delta(abc)$ is the *triangle coefficient*,

$$\Delta(abc) = \epsilon_{abc}\left[\frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!}\right]^{\frac{1}{2}}. \tag{12}$$

Here ϵ_{abc} enforces the *triangle condition*,

$$\epsilon_{abc} = \begin{cases} 1, & \text{if } c \in \{|a-b|, |a-b|+1, \ldots, a+b\} \\ 0, & \text{otherwise} \end{cases}. \tag{13}$$

This is, despite the apparent asymmetry, in fact symmetric in all permutations of a, b, c. The definition of the $6j$ symbols seems to be universal, with just one common alternate, the Racah coefficient W, that differs by a simple phase factor (note also the change in ordering of the indices),

$$W(j_1, j_2, j_5, j_4; j_3, j_6) = \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{array} \right\} (-1)^{j_1+j_2+j_3+j_4} \tag{14}$$

The $6j$ symbol is invariant under permutations of its columns, and swapping the elements of *two* columns. *i.e.*

$$\left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{array} \right\} = \left\{ \begin{array}{ccc} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \end{array} \right\} = \left\{ \begin{array}{ccc} j_1 & j_3 & j_2 \\ j_4 & j_6 & j_5 \end{array} \right\} = \left\{ \begin{array}{ccc} j_4 & j_5 & j_3 \\ j_1 & j_2 & j_6 \end{array} \right\} \tag{15}$$

and so on. The full symmetry group is bigger, 144 elements, but the remaining symmetries are not pure permutations. They also satisfy an orthogonality constraint,

$$\sum_{j_3} (2j_3+1) \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{array} \right\} \left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6' \end{array} \right\} = \frac{\delta_{j_6 j_6'}}{2j_6+1} \tag{16}$$

and a special case where one of the j's is zero,

$$\left\{ \begin{array}{ccc} j_1 & j_2 & j_3 \\ j_4 & j_5 & 0 \end{array} \right\} = \delta_{j_2 j_4} \delta_{j_1 j_5} \frac{(-1)^{j_1+j-2+j_3}}{\sqrt{(2j_1+1)(2j_2+1)}} \,. \tag{17}$$

The $6j$ symbol gives the recoupling of three angular momenta,

$$\begin{aligned} &\langle j_1(j_2 j_3) j_{23}; j'm' | (j_1 j_2) j_{12} j_3; jm \rangle \\ &= \delta_{j'j} \delta_{m'm} (-1)^{j_1+j_2+j_3+j} \sqrt{(2j_{12}+1)(2j_{23}+1)} \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{array} \right\} \end{aligned} \tag{18}$$

This is different to Eq. (2.121) in my thesis, I think the ordering of the $j's$ in that equation is incorrect. Alternative couplings:

$$\begin{aligned} &\langle (j_1 j_2) j_{12} j_3; j'm' | (j_1 j_3) j_{13} j_2; jm \rangle \\ &= \delta_{j'j} \delta_{m'm} (-1)^{j_2+j_3+j_{12}+j_{13}} \sqrt{(2j_{12}+1)(2j_{23}+1)} \left\{ \begin{array}{ccc} j_2 & j_1 & j_{12} \\ j_3 & j & j_{13} \end{array} \right\} \end{aligned} \tag{19}$$

$$\begin{aligned} &\langle j_1(j_2 j_3) j_{23}; j'm' | (j_1 j_3) j_{13} j_2; jm \rangle \\ &= \delta_{j'j} \delta_{m'm} (-1)^{j_1+j_3+j_{23}} \sqrt{(2j_{13}+1)(2j_{23}+1)} \left\{ \begin{array}{ccc} j_1 & j_3 & j_{13} \\ j_3 & j & j_{23} \end{array} \right\} \end{aligned} \tag{20}$$

This is simply a notation change from the recoupling of tensor operators,

$$\begin{aligned} ((\boldsymbol{P}^{[j_1]} \times \boldsymbol{Q}^{[j_2]})^{[j_{12}]} \times \boldsymbol{R}^{[j_3]})^{[j]} &= (-1)^{j_1+j_2+j_3+j} \textstyle\sum_{j_{23}} \sqrt{(2j_{12}+1)(2j_{23}+1)} \\ \times \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{array} \right\} (\boldsymbol{P}^{[j_1]} \times (\boldsymbol{Q}^{[j_2]} \times \boldsymbol{R}^{[j_3]})^{[j_{23}]})^{[j]} \end{aligned} \tag{21}$$

and so on.

For tensors that commute, there is a phase factor from the coupling;

$$(\boldsymbol{P}^{[j_1]} \times \boldsymbol{Q}^{[j_2]})^{[j]} = (-1)^{j_1+j_2-j} (\boldsymbol{Q}^{[j_2]} \times \boldsymbol{P}^{[j_1]})^{[j]} \tag{22}$$

The definition of the $6j$ symbols in terms of the Clebsch-Gordan coefficients is

$$\begin{aligned} &\sum_{m m_i m_{ij}} C^{j_{12}\ j_3\ j}_{m_{12} m_3 m} C^{j_1\ j_2\ j_{12}}_{m_1 m_2 m_{12}} C^{j_1\ j_{23}\ j'}_{m_1 m_{23} m'} C^{j_2\ j_3\ j_{23}}_{m_2 m_3 m_{23}} \\ &= \delta_{j'j} \delta_{m'm} (-1)^{j_1+j_2+j_3+j} \sqrt{(2j_{12}+1)(2j_{23}+1)} \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j & j_{23} \end{array} \right\} \end{aligned} \tag{23}$$

When one argument is zero, the $6j$ coefficients reduce to a simple form,

$$\left\{ \begin{array}{ccc} a & b & c \\ d & e & 0 \end{array} \right\} = (-1)^{a+b+c} \frac{\delta_{ae}\delta_{bd}}{\sqrt{(2a+1)(2b+1)}} \tag{24}$$

The symmetry relations can be used to shift the zero to any position. There are many formulas for other special cases listed in Varshalovich *et al.* [**?**].

3 $9j$ Symbols

A practical formula for evaluation of $9j$ coefficients is in terms of a summation over $6j$ coeffecients:

$$\left\{ \begin{array}{ccc} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{array} \right\} = \sum_k (-1)^{2k}(2k+1) \left\{ \begin{array}{ccc} j_{11} & j_{21} & j_{31} \\ j_{32} & j_{33} & k \end{array} \right\} \left\{ \begin{array}{ccc} j_{12} & j_{22} & j_{32} \\ j_{21} & k & j_{23} \end{array} \right\} \left\{ \begin{array}{ccc} j_{13} & j_{23} & j_{33} \\ k & j_{11} & j_{12} \end{array} \right\}. \tag{25}$$

From this, it can be shown that the $9j$ coefficient is zero unless the triangle conditions are fulfilled by the entries in each row and each column. There are 72 known symmetries of the $9j$ coefficent. The $9j$ coefficient is invarant under even permutations of its rows, even permutation of its columns and under interchange of rows and columns (transposition). It is multiplied by a factor $(-1)^{\sum_{ik} j_{ik}}$ under an odd permutation of its rows or columns.

The $9j$ symbols are related to the recoupling of 4 angular momenta,

$$\begin{aligned} &\langle (j_1 j_2) j_{12} (j_3 j_4) j_{34}\ j'm' | (j_1 j_3) j_{13} (j_2 j_4) j_{24}\ jm \rangle \\ &= \delta_{jj'} \delta_{mm'} \left[\begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right] \end{aligned} \tag{26}$$

where

$$\begin{aligned} &\left[\begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right] = \\ &\sqrt{(2j_{12}+1)(2j_{13}+1)(2j_{24}+1)(2j_{34}+1)} \left\{ \begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right\} \end{aligned} \tag{27}$$

As follows from the definition, a $9j$ symbol can also be expressed as a sum of products of Clebsch-Gordan coefficients,

$$\begin{aligned} &\sum_{m_i, m_{ik}} C^{j_1\ j_2\ j_{12}}_{m_1 m_2 m_{12}} C^{j_3\ j_4\ j_{34}}_{m_3 m_4 m_{34}} C^{j_{12}\ j_{34}\ j}_{m_{12} m_{34} m} C^{j_1\ j_3\ j_{13}}_{m_1 m_3 m_{13}} C^{j_2\ j_4\ j_{24}}_{m_2 m_4 m_{24}} C^{j_{13}\ j_{24}\ j'}_{m_{13} m_{24} m'} \\ &= \delta_{jj'} \delta_{mm'} \left[\begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right] \end{aligned} \tag{28}$$

If we sum over all of the m's, then we get an additional factor $2j+1$ on the right hand side.

We will encounter this $[\cdots]$ symbol quite a lot, so it is worthwhile to examine a bit its symmetries. From the symmetries of the $9j$ coefficient, the $[\cdots]$ is symmetric under transpose of all indices.

$$\left[\begin{array}{ccc} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{array} \right] = \left[\begin{array}{ccc} j_1 & j_3 & j_{13} \\ j_2 & j_4 & j_{24} \\ j_{12} & j_{34} & j \end{array} \right] \tag{29}$$

Under a swap of the first two rows or first two columns, it picks up a phase factor of $(-1)^{\sum j}$, being the sum of all 9 quantum numbers. Hence it is invariant under the combined swap of the first two rows and first two columns,

$$\begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{bmatrix} = \begin{bmatrix} j_4 & j_3 & j_{34} \\ j_2 & j_1 & j_{12} \\ j_{24} & j_{13} & j \end{bmatrix} \tag{30}$$

Other symmetries are more complicated as they involve non-unitary prefactors.

4 Irreducible Tensors

Using the normalization convention of Beidenharn, we define

$$\langle\, j'm' \,|\, T^{[k]}_M \,|\, jm \,\rangle = \langle\, j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \,\rangle \; C^{j\;k\;j'}_{m\,M\,m'} \tag{31}$$

Using the orthogonality of the CG coefficients, this defines the reduced matrix elements[1],

$$\langle\, j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \,\rangle = \sum_{mM} C^{j\;k\;j'}_{m\,M\,m'} \langle\, j'm' \,|\, T^{[k]}_M \,|\, jm \,\rangle \tag{32}$$

where m' is arbitrary. Alternatively, we can sum over m' and divide by $(2m'+1)$,

$$\langle\, j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \,\rangle = \sum_{mMm'} \frac{1}{2j'+1} C^{j\;k\;j'}_{m\,M\,m'} \langle\, j'm' \,|\, T^{[k]}_M \,|\, jm \,\rangle \tag{33}$$

This is a hint that this normalization of the reduced matrix elements is not as symmetric as one might like; however using this normalization the reduced and full matrix elements of scalar operators coincide. In particular, the reduced matrix elements of the identity operator are

$$\langle\, j' \,\|\, I \,\|\, j \,\rangle = \delta_{j'j} \tag{34}$$

and those of the angular momentum operator are

$$\langle\, j' \,\|\, J \,\|\, j \,\rangle = \sqrt{j(j+1)}\; \delta_{j'j} \tag{35}$$

But the trace of a scalar operator needs to be normalized properly;

$$\mathrm{Tr}\, X = \sum_j (2j+1) \langle\, j \,\|\, X \,\|\, j \,\rangle \tag{36}$$

The normalization used here is *not* equivalent to that of Edmonds, who instead defines

$$\langle\, j'm' \,|\, T^{[k]}_M \,|\, jm \,\rangle = \langle\, j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \,\rangle_{\text{Edmonds}} \frac{(-1)^{j-m}}{\sqrt{2k+1}} C^{j'\;\;j\;\;\;k}_{m'\,-m\,M} \tag{37}$$

This normalization is also used by Varshalovich *et al.* [**?**], thus it is important to distinguish properties that explicitly depend on the normalization choice for the reduced matrix elements versus intrinsic properties.

4.1 Tensor multiplication

The coupling of two operators is just as for ordinary spins;

$$\left[\boldsymbol{S}^{[k_1]} \times \boldsymbol{T}^{[k_2]} \right]^{[k]} \tag{38}$$

[1]That this factorization exists is precisely the celebrated Wigner-Eckart theorem.

which denotes the set of operators with components

$$\left[\boldsymbol{S}^{[k_1]} \times \boldsymbol{T}^{[k_2]}\right]^{[k]}_{\mu} = \sum_{\mu_1\mu_2} C^{k_1\,k_2\,k}_{\mu_1\,\mu_2\,\mu} S^{[k_1]}_{\mu_1} T^{[k_2]}_{\mu_2} \tag{39}$$

Applying the Wigner-Eckart gives, after a few lines of algebra,

$$\begin{aligned} &\langle\, j' \,\|\, \left[\boldsymbol{S}^{[k_1]} \times \boldsymbol{T}^{[k_2]}\right]^{[k]} \,\|\, j \,\rangle \\ &= (-1)^{j+j'+k} \textstyle\sum_{j''} \sqrt{(2j''+1)(2k+1)} \begin{Bmatrix} j' & k_1 & j'' \\ k_2 & j & k \end{Bmatrix} \\ &\times \langle\, j' \,\|\, \boldsymbol{S}^{[k_1]} \,\|\, j'' \,\rangle \langle\, j'' \,\|\, \boldsymbol{T}^{[k_2]} \,\|\, j \,\rangle \end{aligned} \tag{40}$$

Note that multiplication of a tensor operator by a *scalar* is a special case where $k_2 = 0$, and Eq. (17) implies the coupling coefficient is identically 1.

4.2 Direct product

A special case of the above product rule is when the tensors $\boldsymbol{S}^{[k_1]}$ and $\boldsymbol{T}^{[k_2]}$ live in different spaces, that is

$$\begin{array}{ccccc} \boldsymbol{S}^{[k_1]} & = & \boldsymbol{S_1}^{[k_1]} & \otimes & I_2 \\ \boldsymbol{T}^{[k_2]} & = & I_1 & \otimes & \boldsymbol{T_2}^{[k_2]} \end{array} \tag{41}$$

The angular momentum of this combined system is $J = J_1 + J_2$. Thus we can write the coupling as $\boldsymbol{S_1}^{[\boldsymbol{k_1}]} \otimes \boldsymbol{T_2}^{[\boldsymbol{k_2}]\,[k]}$. Repeated application of the Wigner-Eckart theorem gives

$$\begin{aligned} &\langle\, j' \,(j_1' j_2' \alpha_1' \alpha_2') \,\|\, \left[\boldsymbol{T}^{[k_1]}(1) \otimes \boldsymbol{T}^{[k_2]}(2)\right]^{[k]} \,\|\, j \,(j_1 j_2 \alpha_1 \alpha_2) \,\rangle \\ &= \begin{bmatrix} j_1 & j_2 & j \\ k_1 & k_2 & k \\ j_1' & j_2' & j' \end{bmatrix} \langle\, j_1' \,(\alpha_1') \,\|\, \boldsymbol{T}^{[k_1]}(1) \,\|\, j_1 \,(\alpha_1) \,\rangle \langle\, j_2' \,(\alpha_2') \,\|\, \boldsymbol{T}^{[k_2]}(2) \,\|\, j_2 \,(\alpha_2) \,\rangle\ . \end{aligned} \tag{42}$$

5 Conjugate Tensors

It is sometimes useful to consider the *tensor conjugate* of an irreducible operator, $\bar{\boldsymbol{T}}^{[k]}$, defined by

$$\bar{T}^{[k]}_M = (-1)^{k-M} T^{[k]}_{-M} \tag{43}$$

This transforms differently under a rotation (*i.e.* it isn't the same as an irreducible tensor operator). This construction occurs when taking the hermitian conjugate of a tensor (see below), but its main usefulness is in constructing scalar products. That is,

$$\bar{\boldsymbol{S}}^{[k]} \cdot \boldsymbol{T}^{[k]} = \sum_M \bar{S}^{[k]}_M T^{[k]}_M \tag{44}$$

is a scalar. Note that tensor conjugation isn't an involution; applying conjugation twice to an operator gives back the original operator multiplied by a phase of $(-1)^{2k}$, so for a half-integer representation we need to conjugate *four* times to get back to the original operator.

The matrix elements of $\bar{\boldsymbol{T}}^{[k]}$ are

$$\begin{aligned} \langle\, j'm' \,|\, \bar{T}^{[k]}_M \,|\, jm \,\rangle &= (-1)^{k-M} C^{j\;\;k\;\;\;j'}_{m\,-M\,m'} \langle\, j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \,\rangle \\ &= (-1)^{j'+k-j} \sqrt{\frac{2j'+1}{2j+1}} C^{j'\,k\,j}_{m'\,M\,m} \langle\, j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \,\rangle \end{aligned} \tag{45}$$

We can regard the reduced matrix elements of $\bar{\boldsymbol{T}}^{[k]}$ as being the same as those of $\boldsymbol{T}^{[k]}$ itself, but with a different coupling coefficient used to obtain the full matrix elements.

With the metric interpretation of the CG coefficients, this operator transforms in the opposite sense. Note that there is a phase ambiguity in the tensor conjugate; here we have chosen $(-1)^{k-M}$ but $(-1)^{k+M}$ would also be a valid choice, and in some ways simply $(-1)^M$ would be more convenient. However for fermionic operators where k, M are half-integral this would imply the conjugate of a real tensor is purely imaginary. With the $(-1)^k$ factor inserted, the operator is real at the expense of having a sign ambiguity.

5.1 Hermitian conjugate

If we define the *hermitian conjugate* $\boldsymbol{T}^{\dagger[k]}$, with matrix elements

$$\begin{aligned} \langle\, j'm' \,|\, T^{\dagger}{}^{[k]}_{M} \,|\, jm \,\rangle &= \langle\, jm \,|\, T^{[k]}_{M} \,|\, j'm' \,\rangle^* \\ &= C^{j'}_{m'}{}^{k}_{M}{}^{j}_{m} \langle\, j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j' \,\rangle^* \end{aligned} \tag{46}$$

this transforms as a conjugate tensor. We may define reduced matrix elements of $\boldsymbol{T}^{\dagger[k]}$, via

$$\langle\, j' \,\|\, \boldsymbol{T}^{\dagger[k]} \,\|\, j \,\rangle = \langle\, j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j' \,\rangle^* \,. \tag{47}$$

This gives the matrix elements as

$$\langle\, j'm' \,|\, T^{\dagger}{}^{[k]}_{M} \,|\, jm \,\rangle = C^{j'}_{m'}{}^{k}_{M}{}^{j}_{m} \langle\, j' \,\|\, \boldsymbol{T}^{\dagger[k]} \,\|\, j \,\rangle \,. \tag{48}$$

Compare Eq. (31).

5.2 Adjoint

If we apply both tensor conjugation and Hermitian conjugation, we get the tensor operator $\bar{\boldsymbol{T}}^{\dagger[k]}$, which has matrix elements

$$\langle\, j' \,\|\, \bar{\boldsymbol{T}}^{\dagger[k]} \,\|\, j \,\rangle = (-1)^{j+k-j'} \sqrt{\frac{2j+1}{2j'+1}} \langle\, j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j' \,\rangle^* \tag{49}$$

That is, the reduced matrix elements of $\bar{\boldsymbol{T}}^{\dagger[k]}$ are simply related to the reduced matrix elements of $\boldsymbol{T}^{[k]}$, and both objects transform as ordinary tensors. At the risk of confusion, we call $\bar{\boldsymbol{T}}^{\dagger[k]}$ the *adjoint* of $\boldsymbol{T}^{[k]}$, also denoted here by $\boldsymbol{T}^{\ddagger[k]}$ (note that neither this terminology nor notation is standard). Applying the adjoint twice does not in general give the original operator, but there is a phase factor factor;

$$\boldsymbol{T}^{\ddagger\ddagger[k]} = (-1)^{2k} \boldsymbol{T}^{[k]} \tag{50}$$

Hence it is also useful to define the 'inverse adjoint', which is denoted here by the rather cumbersome notation $\boldsymbol{T}^{\ddagger\ddagger\ddagger[k]}$.

Note: In previous versions of these notes, the phase factor here was different, and written as $(-1)^{j+k-j'}$. The above convention agrees with my thesis, and also with what is currently implemented in the toolkit.

We now determine the scalar product of $S \cdot T^\dagger$ and $S^\dagger \cdot T$ forms. Expanding in reduced matrix elements, this is

$$\langle\, j'm' \,|\, ST^\dagger \,|\, jm \,\rangle = \sum_{q,j'',m''} \langle\, j'm' \,|\, S^{[k]}_q \,|\, j''m'' \,\rangle \langle\, jm \,|\, T^{[k]}_q \,|\, j''m'' \,\rangle^* \tag{51}$$

Consider first the right hand side,

$$\begin{aligned} &\textstyle\sum_{j''} \langle\, j' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j'' \,\rangle \langle\, j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j'' \,\rangle^* \sum_{q,m''} C^{j''}_{m''}{}^{k}_{q}{}^{j'}_{m'} C^{j''}_{m''}{}^{k}_{q}{}^{j}_{m} \\ &\quad = \textstyle\sum_{j''} \langle\, j' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j'' \,\rangle \langle\, j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j'' \,\rangle^* \delta_{jj'} \delta_{mm'} \end{aligned} \tag{52}$$

which shows we have a scalar operator. Thus,

$$\langle j \,\|\, ST^\dagger \,\|\, j \rangle = \sum_{j''} \langle j \,\|\, \boldsymbol{S}^{[k]} \,\|\, j'' \rangle \langle j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j'' \rangle^* \tag{53}$$

because the CG coefficient that determines the reduced matrix element of $ST^\dagger$ is $C^{j\ 0j}_{m\,0m} = 1$. It follows from this that $TT^\dagger$ is positive definite.

Note that the scalar product differs from the coupling

$$\left[\boldsymbol{S}^{[k]} \times \boldsymbol{T}^{\ddagger\,[k]}\right]^{[0]} \tag{54}$$

which has matrix elements

$$\begin{array}{l} (-1)^{j+j'} \sum_{j''} \sqrt{2j''+1} \left\{ \begin{array}{ccc} j' & k & j'' \\ k & j & 0 \end{array} \right\} (-1)^{j+k-j''} \sqrt{\dfrac{2j+1}{2j''+1}} \\ \quad \times \langle j' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j'' \rangle \langle j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j'' \rangle^* \end{array} \tag{55}$$

The coefficient of $\langle j' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j'' \rangle \langle j \,\|\, \boldsymbol{T}^{[k]} \,\|\, j'' \rangle^*$ is

$$\begin{array}{l} (-1)^{j+j'} \sqrt{2j''+1} (-1)^{j'+k+j''} \frac{\delta_{j'j}}{\sqrt{(2j'+1)(2k+1)}} (-1)^{j+k-j''} \sqrt{\frac{2j+1}{2j''+1}} \\ = (-1)^{2k} \frac{1}{\sqrt{2k+1}} \delta_{j'j} \end{array} \tag{56}$$

giving,

$$\left[\boldsymbol{S}^{[k]} \times \boldsymbol{T}^{\ddagger\,[k]}\right]^{[0]} = (-1)^{2k} \frac{1}{\sqrt{2k+1}} \quad \boldsymbol{S}^{[k]} \cdot \boldsymbol{T}^{\dagger\,[k]} \tag{57}$$

Taking the conjugation other way around,

$$\langle j'm' \,|\, S^\dagger T \,|\, jm \rangle = \sum_{q,j'',m''} \langle j''m'' \,|\, S^{[k]}_q \,|\, j'm' \rangle^* \langle j''m'' \,|\, T^{[k]}_q \,|\, jm \rangle \tag{58}$$

Now

$$\begin{array}{l} \sum_{j''} \langle j'' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j' \rangle^* \langle j'' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle \sum_{q,m''} C^{j'\ kj''}_{m'\,q\,m''} C^{j\ kj''}_{m\,q\,m''} \\ \quad = \sum_{j''} \langle j'' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j' \rangle^* \langle j'' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle \frac{2j''+1}{2j'+1} \delta_{jj'} \delta_{mm'} \end{array} \tag{59}$$

giving

$$\langle j \,\|\, S^\dagger T \,\|\, j \rangle = \sum_{j''} \frac{2j''+1}{2j+1} \langle j'' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j \rangle^* \langle j'' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle \tag{60}$$

This compares with

$$\left[\boldsymbol{S}^{\ddagger\,[k]} \times \boldsymbol{T}^{[k]}\right]^{[0]} \tag{61}$$

which has matrix elements

$$\begin{array}{l} (-1)^{j+j'} \sum_{j''} \sqrt{2j''+1} \left\{ \begin{array}{ccc} j' & k & j'' \\ k & j & 0 \end{array} \right\} (-1)^{j''+k-j'} \sqrt{\dfrac{2j''+1}{2j'+1}} \\ \quad \times \langle j'' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j' \rangle^* \langle j'' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle \end{array} \tag{62}$$

The coefficient of $\langle j'' \,\|\, \boldsymbol{S}^{[k]} \,\|\, j' \rangle^* \langle j'' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle$ is

$$\begin{array}{l} (-1)^{j+j'} \sqrt{2j''+1} (-1)^{j''+k+j'} \frac{\delta_{j'j}}{\sqrt{(2j'+1)(2k+1)}} (-1)^{j''+k-j'} \sqrt{\frac{2j''+1}{2j'+1}} \\ = \frac{2j''+1}{2j+1} \frac{1}{\sqrt{2k+1}} \delta_{j'j} \end{array} \tag{63}$$

Note that $\left[\boldsymbol{T}^{\ddagger\,[k]} \times \boldsymbol{T}^{[k]}\right]^{[0]}$ is always positive-definite, whereas $\left[\boldsymbol{T}^{[k]} \times \boldsymbol{T}^{\ddagger\,[k]}\right]^{[0]}$ is only positive-definite for integral k, otherwise it is negative-definite. Thus, it is more realistic to take instead $\left[\boldsymbol{T}^{[k]} \times \boldsymbol{T}^{\ddagger\ddagger\ddagger\,[k]}\right]^{[0]}$ and restore the positivity properties.

5.3 Flip Conjugation

Another variant of the conjugation operation that we will need corresponds to flipping the direction of all of the spins *without* taking any kind of transpose of the indices. This interchanges

$$\langle j', m' \,|\, \hat{T}^{[k]}_{M} \,|\, j, m \rangle = \langle j', -m' \,|\, T^{[k]}_{-M} \,|\, j, -m \rangle \tag{64}$$

For a MPS, this corresponds to a spin reflection (or charge reflection) of the physical state. Note that this operator transforms as an ordinary tensor operator, not as a conjugate. The reduced matrix elements are

$$\langle j', -m' \,|\, T^{[k]}_{-M} \,|\, j, -m \rangle = \langle j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle \, C^{j \;\; k \;\; j'}_{-m -M -m'} \tag{65}$$

From the symmetries of the CG coefficient, $C^{j \;\; k \;\; j'}_{-m -M -m'} = (-1)^{j+k-j'} C^{j \, k \, j'}_{m M m'}$. Therefore,

$$\langle j' \,\|\, \hat{\boldsymbol{T}}^{[k]} \,\|\, j \rangle = (-1)^{j+k-j'} \langle j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle \tag{66}$$

so the *flip conjugate* introduces a phase factor. For an irreducible MPS, this is pure gauge; after coarse-graining, an MPS will have $j = 0$, and $j' = k$, so the phase factor vanishes.

TODO: we probably should prove that all of these conjugation operations survive coarse-graining...

6 Norms

We can define an operator norm, corresponding to the usual Frobenius norm, such that

$$||\boldsymbol{X}^{[k]}||^2_{\text{frob}} = \operatorname{Tr} \boldsymbol{X}^{[k]} \cdot \boldsymbol{X}^{\dagger[k]} = \operatorname{Tr} \boldsymbol{X}^{\dagger[k]} \cdot \boldsymbol{X}^{[k]} \,. \tag{67}$$

From either Eq. (53) or Eq. (60), we see that

$$||\boldsymbol{X}^{[k]}||^2_{\text{frob}} = \sum_{j'j} (2j'+1) |\langle j' \,\|\, \boldsymbol{T}^{[k]} \,\|\, j \rangle|^2 \tag{68}$$

7 Triple products

An operation that we will find useful is the triple product

$$\boldsymbol{E}^{[a]} = \boldsymbol{A}^{\dagger\,[s']} \boldsymbol{E'}^{[a']} \boldsymbol{B}^{[s]} [sk \to s'; ak \to a'] \tag{69}$$

and couple

$$\langle j'm' \,|\, E^{[a]}_{\alpha} \,|\, jm \rangle = \langle i'n' \,|\, A^{[s']}_{\sigma'} \,|\, j'm' \rangle \langle i'n' \,|\, E'^{[a']}_{\alpha'} \,|\, in \rangle \langle in \,|\, B^{[s]}_{\sigma} \,|\, jm \rangle \tag{70}$$

via the reduced matrix elements

$$\begin{aligned} \langle j' \,\|\, \boldsymbol{E}^{[a]} \,\|\, j \rangle \quad &= \quad \frac{1}{2j'+1} \sum_{m'm\alpha'\alpha n'n\sigma'\sigma M} \langle i' \,\|\, \boldsymbol{A}^{[s']} \,\|\, j' \rangle^* \, \langle i' \,\|\, \boldsymbol{E'}^{[a']} \,\|\, i \rangle \langle i \,\|\, \boldsymbol{B}^{[s]} \,\|\, j \rangle \\ &\quad \times C^{j \; a \; j'}_{m \alpha m'} C^{j' \; s' \; i'}_{m' \sigma' n'} C^{i \; a' \; i'}_{n \alpha' n'} C^{j \; s \; i}_{m \sigma n} C^{s \; k \; s'}_{\sigma M \sigma'} C^{a \; k \; a'}_{\alpha M \alpha'} \end{aligned} \tag{71}$$

Identifying $j \to i_1$, $s \to j_2$, $i \to j_{12}$, $a \to j_3$, $k \to j_4$, $a' \to j_{34}$, $j' \to j_{13}$, $s' \to j_{24}$, $i' \to j$, we get a $9j$ coefficient,

$$\begin{aligned} \langle j' \,\|\, \boldsymbol{E}^{[a]} \,\|\, j \rangle \quad &= \quad \langle i' \,\|\, \boldsymbol{A}^{[s']} \,\|\, j' \rangle^* \, \langle i' \,\|\, \boldsymbol{E'}^{[a']} \,\|\, i \rangle \langle i \,\|\, \boldsymbol{B}^{[s]} \,\|\, j \rangle \\ &\quad \times \frac{2i'+1}{2j'+1} \begin{bmatrix} j & s & i \\ a & k & a' \\ j' & s' & i' \end{bmatrix} \end{aligned} \tag{72}$$

Lets go in the other direction;

$$\boldsymbol{F'}^{[a']} = \boldsymbol{A}^{[s']}\boldsymbol{F}^{[a]}\boldsymbol{B}^{\dagger[s]}[sk \to s'; ak \to a'] \tag{73}$$

which gives the reduced matrix elements

$$\begin{aligned}\langle\, j' \,\|\, \boldsymbol{F'}^{[a']} \,\|\, j \,\rangle \quad &= \quad \frac{1}{2j'+1} \sum_{m'm\alpha'\alpha n'n\sigma'\sigma M} \langle\, j' \,\|\, \boldsymbol{A}^{[s']} \,\|\, i' \,\rangle \,\langle\, i' \,\|\, \boldsymbol{F}^{[a]} \,\|\, i \,\rangle\langle\, j \,\|\, \boldsymbol{B}^{[s]} \,\|\, i \,\rangle^* \\ &\quad \times C^{j\ a\ j'}_{m\alpha m'} C^{i'\ s'\ j'}_{n'\sigma' m'} C^{i\ a\ i'}_{n\alpha n'} C^{j\ s\ i}_{m\sigma n} C^{s\ k\ s'}_{\sigma M \sigma'} C^{a\ k\ a'}_{\alpha M \alpha'}\end{aligned} \tag{74}$$

Identifying $i \to i_1$, $s \to j_2$, $j \to j_{12}$, $a \to j_3$, $k \to j_4$, $a' \to j_{34}$, $i' \to j_{13}$, $s' \to j_{24}$, $j' \to j$, we get a $9j$ coefficient,

$$\begin{aligned}\langle\, j' \,\|\, \boldsymbol{F'}^{[a']} \,\|\, j \,\rangle \quad &= \quad \langle\, j' \,\|\, \boldsymbol{A}^{[s']} \,\|\, i' \,\rangle\langle\, i' \,\|\, \boldsymbol{F}^{[a]} \,\|\, i \,\rangle\langle\, j \,\|\, \boldsymbol{B}^{[s]} \,\|\, i \,\rangle^* \\ &\quad \times \begin{bmatrix} i & s & j \\ a & k & a' \\ i' & s' & j' \end{bmatrix}\end{aligned} \tag{75}$$

8 Matrix Product States

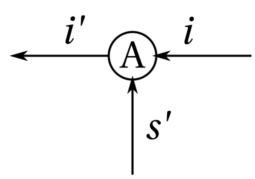
A matrix product state is a set of irreducible tensors ${\boldsymbol{A}^{[s]}}_{ij}$, where $i, j = 1, 2, \ldots, m$ and s runs over the d-dimensional local basis. Here we don't distinguish the state label from its quantum number, this should not cause confusion. A matrix product operator is an array of bi-irreducible tensors, ${\boldsymbol{M}^{[k]}}^{s's}_{i'i}$. We are free to choose how the indices of the operator transform. In upstairs-downstairs notation, the matrix element $\langle\, j' \,\|\, \boldsymbol{A}^{[s]} \,\|\, j \,\rangle$ of an irreducible tensor operator looks like

$$A^{[s]\,i}_{i'} \tag{76}$$

i.e. , the rank index is upstairs. This is consistent with the analagous case for $U(1)$, where one would have the sum rule $i' = i + s$. We could of course define our operators differently, for example having all indices at the same level. This would correspond to replacing the Clebsch-Gordan coefficient with the more symmetric $3j$ symbol, analagous to the $U(1)$ sum rule $i' + i + s = 0$. Here I choose the conventional route of having mixed symmetry tensors. The reduced matrix elements are

$$\langle\, i'\iota' \,|\, A^{[s]}_{sigma} \,|\, i\iota \,\rangle = \langle\, i' \,\|\, \boldsymbol{A}^{[s]} \,\|\, i \,\rangle \; C^{i\,s\,i'}_{\iota\sigma\iota'} \tag{77}$$

Here we follow the convention that z-axis projections are denoted by the corresponding Greek symbol. The associated tensor network diagram is



The directional arrows indicate the symmetry of the coupling coefficients.

8.1 Bra versus ket

An MPS constructed in this way actually looks like a bra vector, since the physical indices are pointing inwards, which, in the conventional picture indicates a bra. This is consistent with the quantum numbers in the auxiliary Hilbert space being 0 (vacuum) on the right-hand side and q on the left. Since the overall tensor network is a rotational invariant (scalar), the physical quantum number is therefore the conjugate of q, which is correct for a bra state. The Hermitian conjugate would correspond to a ket state with physical quantum number q and transforming as the conjugate of q in the auxiliary space.

However, we raraly need to consider mixing the physical and auxiliary Hilbert spaces, so we are free to choose any convention we like for the physical index. Hence we are free to call it a ket. To construct a bra vector, we will construct explicitly the Hermitian conjugate:

$$\langle A|B\rangle \sim A^\dagger B \tag{78}$$

Note that later on, we will see that the contraction of an MPS via E and F-matrices, naturally leads to F being in the conjugate representation and E being normal, leading to

$$\langle A|B\rangle \sim EF^\dagger \tag{79}$$

8.2 Normalization

The normalization constraints for the right and left sides are

$$N = \sum_s \boldsymbol{A}^{[s]} \boldsymbol{A}^{\dagger\,[s]} \tag{80}$$

$$N = \sum_s \boldsymbol{A}^{\dagger\,[s]} \boldsymbol{A}^{[s]} \tag{81}$$

respectively. Typically we will want to find a transformation such that $N = I$. This notation arises from how we apply the matrices. If the right-hand basis is orthonormal, then multiplying on the left by an A matrix that satisfies the right orthogonality constraint, $AA^\dagger = 1$, preserves orthonormality. Conversely, if the left-hand basis is orthonormal, then multiplying on the right with a left-normal matrix, $A^\dagger A = 1$, preserves orthonormality. Expanding Eq. (80) in reduced matrix elements, this is

$$\langle\, j'm' \,|\, N \,|\, jm \,\rangle = \sum_{s,q,j'',m''} \langle\, j'm' \,|\, A_q^{[s]} \,|\, j''m'' \,\rangle \langle\, jm \,|\, A_q^{[s]} \,|\, j''m'' \,\rangle^* \tag{82}$$

Consider first the right hand side,

$$\begin{aligned} &\sum_{s,j''} \langle\, j' \,\|\, \boldsymbol{A}^{[s]} \,\|\, j'' \,\rangle \langle\, j \,\|\, \boldsymbol{A}^{[s]} \,\|\, j'' \,\rangle^* \sum_{q,m''} C^{j''}_{m''}{}^{s}_{q}{}^{j'}_{m'} C^{j''}_{m''}{}^{s}_{q}{}^{j}_{m} \\ &\quad = \sum_{s,j''} \langle\, j' \,\|\, \boldsymbol{A}^{[s]} \,\|\, j'' \,\rangle \langle\, j \,\|\, \boldsymbol{A}^{[s]} \,\|\, j'' \,\rangle^* \delta_{jj'} \delta_{mm'} \end{aligned} \tag{83}$$

which shows that N is a scalar (as it should be). Thus,

$$\langle\, j \,\|\, N \,\|\, j \,\rangle = \sum_{s,j''} \langle\, j \,\|\, \boldsymbol{A}^{[s]} \,\|\, j'' \,\rangle \langle\, j \,\|\, \boldsymbol{A}^{[s]} \,\|\, j'' \,\rangle^* \tag{84}$$

because the CG coefficient that determines the reduced matrix element of N is $C^{j}_{m}{}^{0}_{0}{}^{j}_{m} = 1$.

Alternatively, we could calculate the product

$$\sum_s \boldsymbol{A}^{\dagger\,[s]} \boldsymbol{A}^{[s]} \tag{85}$$

Expanding the matrix elements, this is

$$\langle\, j'm' \,|\, N \,|\, jm \,\rangle = \sum_{s,q,j'',m''} \langle\, j''m'' \,|\, A_q^{[s]} \,|\, j'm' \,\rangle^* \langle\, j''m'' \,|\, A_q^{[s]} \,|\, jm \,\rangle \tag{86}$$

The CG coefficient is

$$\sum_{q,m''} C^{j'}_{m'}{}^{s}_{q}{}^{j''}_{m''} C^{j}_{m}{}^{s}_{q}{}^{j''}_{m''} = \frac{2j''+1}{2j+1} \delta_{j'j} \delta_{m'm} \tag{87}$$

giving the final result of

$$\langle\, j \,\|\, N \,\|\, j \,\rangle = \sum_{s,j''} \frac{2j''+1}{2j+1} \langle\, j'' \,\|\, \boldsymbol{A}^{[s]} \,\|\, j \,\rangle^* \langle\, j'' \,\|\, \boldsymbol{A}^{[s]} \,\|\, j \,\rangle \tag{88}$$

For the center-matrix formalism, we need the transformation

$$\boldsymbol{A}^{[s]}{}_{ij} \to \sum_k \; C_{ik} \; \boldsymbol{A'}^{[s]}{}_{kj} \tag{89}$$

where k is a $d \times m$ dimensional index that encapsulates both a s' and a j' index[2] : $k \simeq (s', j')$. Requiring $\boldsymbol{A'}^{[s]}{}_{kj}$ to satisfy the right orthogonality constraint, $A'A'^{\dagger} = 1$, this requires

$$\boldsymbol{A'}^{[s]}{}_{kj} = \delta_{j'j}\delta_{s's} \quad [\text{with } k \simeq (s', j')] \tag{90}$$

with

$$C_{ik} = \boldsymbol{A}^{[s']}{}_{ij'} \tag{91}$$

In the other direction, we need

$$\boldsymbol{A}^{[s]}{}_{ij} \to \sum_k \; \boldsymbol{A'}^{[s]}{}_{ik} \, C_{kj} \tag{92}$$

where $k \simeq (s', i')$. Requiring $\boldsymbol{A'}^{[s]}{}_{ik}$ to satisfy the left orthogonality constraint, $A'^{\dagger}A' = 1$, this requires

$$\boldsymbol{A'}^{[s]}{}_{ik} = \delta_{s's}\delta_{i'i}\sqrt{\frac{2k+1}{2i+1}} \quad [\text{with } k \simeq (s', i')] \tag{93}$$

and

$$C_{kj} = \boldsymbol{A}^{[s]}{}_{j'j}\sqrt{\frac{2i+1}{2k+1}} \tag{94}$$

8.3 MPS Contraction

The contraction of MPS, given by

$$\boldsymbol{F}^{[k]} = \boldsymbol{A}^{[s']}\boldsymbol{B}^{\dagger [s]} \, \langle\, s' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s \,\rangle \tag{95}$$

is an irreducible tensor that transforms as rank $[k]$. To prove this, we expand

$$\begin{aligned} \langle\, j' \,\|\, \boldsymbol{F}^{[k]} \,\|\, j \,\rangle \;=\; \sum_{s'si;mn\sigma'\sigma\mu} & \langle\, j'm' \,|\, A^{[s']}_{\sigma'} \,|\, in \,\rangle \\ \times\;& \langle\, jm \,|\, B^{[s]}_{\sigma} \,|\, in \,\rangle^* \\ \times\;& \langle\, s'\sigma' \,|\, M^{[k]}_{\mu} \,|\, s\sigma \,\rangle \\ \times\;& C^{i\; s'\; j'}_{n\sigma' m'} C^{i\; s\; j}_{n\sigma m} \\ \times\;& C^{s\; k\; s'}_{\sigma\mu\sigma'} C^{j\; k\; j'}_{m\mu m'} \end{aligned} \tag{96}$$

where the value of m' is arbitary. Upon the identification $i \to j_1$, $s \to j_2$, $j \to j_{12}$, $k \to j_3$, $j' \to j'$, $s' \to j_{23}$, we get, from Eq. (23), the relation

$$\begin{aligned} \langle\, j' \,\|\, \boldsymbol{F}^{[k]} \,\|\, j \,\rangle \;=\; & \textstyle\sum_{s'si} \langle\, j' \,\|\, \boldsymbol{A}^{[s']} \,\|\, i \,\rangle \langle\, j \,\|\, \boldsymbol{B}^{[s]} \,\|\, i \,\rangle^* \langle\, s' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s \,\rangle \\ & \times(-1)^{i+s+k+j'}\sqrt{(2j+1)(2s'+1)} \begin{Bmatrix} i & s & j \\ k & j' & s' \end{Bmatrix} \end{aligned} \tag{97}$$

[2] or more precisely, k runs over the Clebsch-Gordan expansion of $s' \otimes j'$.

Alternatively, we could substitute in Eq. (95) $\langle\, s' \,\|\, \boldsymbol{M}^{\dagger\,[k]} \,\|\, s \,\rangle^*$, and we get exactly the same operator.

Another operation that we will need is when we commute the A, B operators, giving the E matrix,

$$\boldsymbol{E}^{[k]} = \boldsymbol{A}^{\dagger\,[s']} \boldsymbol{B}^{[s]} \,\langle\, s' \,\|\, \boldsymbol{M}^{\dagger\,[k]} \,\|\, s \,\rangle \tag{98}$$

This is also an irreducible tensor of rank $[k]$. Expanding, we get

$$\begin{aligned} \langle\, j' \,\|\, \boldsymbol{E}^{[k]} \,\|\, j \,\rangle \quad = \sum_{s'si;mn\sigma'\sigma\mu} & \quad \langle\, in \,|\, A_{\sigma'}^{[s']} \,|\, j'm' \,\rangle^* \\ \times & \quad \langle\, in \,|\, B_{\sigma}^{[s]} \,|\, jm \,\rangle \\ \times & \quad \langle\, s\sigma \,|\, M_{\mu}^{[k]} \,|\, s'\sigma' \,\rangle^* \\ \times & \quad C_{m'\sigma' n}^{j'\ s'\ i} C_{m \sigma n}^{j\ s\ i} \\ \times & \quad C_{\sigma'\mu\sigma}^{s'\ k\ s} C_{m \mu m'}^{j\ k\ j'} \end{aligned} \tag{99}$$

where again m' is arbitary. Using the symmetries of the CG coefficients, we rewrite

$$\begin{aligned} & C_{m'\sigma' n}^{j'\ s'\ i} C_{m \sigma n}^{j\ s\ i} C_{\sigma'\mu\sigma}^{s'\ k\ s} = \\ & (-1)^{s'+\sigma'} \sqrt{\tfrac{2i+1}{2j'+1}} C_{-n\sigma'-m'}^{i\ \ s'\ j'} (-1)^{s+\sigma} \sqrt{\tfrac{2i+1}{2j+1}} C_{-n\sigma-m}^{i\ \ s\ j} (-1)^{k+\mu} \sqrt{\tfrac{2s+1}{2s'+1}} C_{-\sigma\mu-\sigma'}^{s\ \ k\ s'} \end{aligned} \tag{100}$$

We are free to change the sign of the dummy indices σ', σ, which then gives the same set of CG coefficients that we had previously, except for a factor which we can write as

$$(-1)^{\sigma'+\mu-\sigma} (-1)^{s'+k-s} \frac{2i+1}{2j'+1} \sqrt{\frac{2j'+1}{2j+1}} \sqrt{\frac{2s+1}{2s'+1}} \,. \tag{101}$$

Since, with our negated dummy indices, $\sigma = \sigma' + \mu$, we get

$$\begin{aligned} \langle\, j' \,\|\, \boldsymbol{E}^{[k]} \,\|\, j \,\rangle \quad = \quad & \textstyle\sum_{s'si} \langle\, i \,\|\, \boldsymbol{A}^{[s']} \,\|\, j' \,\rangle^* \langle\, i \,\|\, \boldsymbol{B}^{[s]} \,\|\, j \,\rangle \langle\, s' \,\|\, \boldsymbol{M}^{\dagger\,[k]} \,\|\, s \,\rangle \\ & \times (-1)^{i+s'+k+j} \sqrt{(2j'+1)(2s+1)} \begin{Bmatrix} i & s & j \\ k & j' & s' \end{Bmatrix} \\ & \times (-1)^{j'+k-j} \tfrac{2i+1}{2j'+1} \end{aligned} \tag{102}$$

Which we can see as similar to Eq. (95).

9 Matrix Product Operators

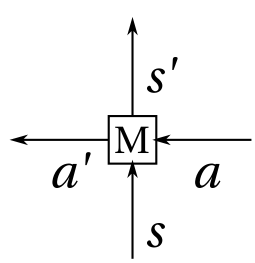
The most natural definition for a matrix product operator has two downstairs indices and three upstairs,

$$M_{s'i'}^{[k]\ si} \tag{103}$$

which transforms as the product of two operators of rank $[k]$, with matrix elements

$$\langle\, s'q'; j'm' \,|\, M_r^{[k]} \,|\, sq; jm \,\rangle = \langle\, s'; j' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; j \,\rangle \; C_{q r q'}^{s\, k\, s'} \; C_{m r m'}^{j\ k\, j'} \tag{104}$$

This has the form



9.1 Normalization

The normalization conditions are

$$
\begin{aligned}
N &= \operatorname{Tr}_k \boldsymbol{M}^{[k]}\boldsymbol{M}^{\dagger[k]} \\
N &= \operatorname{Tr}_k \boldsymbol{M}^{\dagger[k]}\boldsymbol{M}^{[k]}
\end{aligned}
\tag{105}
$$

where we take here the product with respect to both the local and auxilary indices, and trace over the local index. This gives

$$
\langle\, j \,\|\, N \,\|\, j \,\rangle = \sum_{s',s,j'',k} (2s'+1)\langle\, j; s' \,\|\, \boldsymbol{M}^{[k]} \,\|\, j''; s \,\rangle\langle\, j; s' \,\|\, \boldsymbol{M}^{[k]} \,\|\, j''; s \,\rangle^* \tag{106}
$$

or,

$$
\langle\, j \,\|\, N \,\|\, j \,\rangle = \sum_{s',s,j'',k} \frac{(2j''+1)(2s'+1)}{2j+1}\langle\, j''; s' \,\|\, \boldsymbol{M}^{[k]} \,\|\, j; s \,\rangle^*\langle\, j''; s' \,\|\, \boldsymbol{M}^{[k]} \,\|\, j; s \,\rangle \tag{107}
$$

9.2 Operator-State Product

Note that the product of an operator and a state requires a contraction of the index s, which has the symmetry of over two *downstairs* indices, and then shifting the result index s' from upstairs to downstairs. For $SU(2)$, the required phase factor is $(-1)^{s+k-s'}$, giving the rule

$$
\boldsymbol{B}^{[s']} = (\boldsymbol{M}\boldsymbol{A})^{[s']} = \sum_s (-1)^{s+k-s'} {\boldsymbol{M}^{[k]}}^{s's} \otimes \boldsymbol{A}^{[s]} \tag{108}
$$

We can prove this in a variety of ways, here I take the long but solid approach of reverting to the definition of the reduced matrix elements. We apply an operator to a state by contracting over the s index, and taking the tensor product of the matrices,

$$
\begin{aligned}
&\langle\, j_1' j_2'; m_1' m_2' \,|\, B^{[s']}_{q'} \,|\, j_1 j_2; m_1 m_2 \,\rangle \\
&\quad = \sum_{s,q,k,r} \langle\, s' q'; j_1' m_1' \,|\, M^{[k]}_r \,|\, sq; j_1 m_1 \,\rangle\langle\, j_2' m_2' \,|\, A^{[s]}_q \,|\, j_2 m_2 \,\rangle
\end{aligned}
\tag{109}
$$

Now we couple $j_1', j_2' \to j'$ and $j_1, j_2 \to j$, to get the reduced matrix elements of B;

$$
\begin{aligned}
&\langle\, (j_1' j_2') j' \,\|\, \boldsymbol{B}^{[s']} \,\|\, (j_1 j_2) j \,\rangle = \textstyle\sum_{j_1' m_1' j_2' m_2' \; j_1 m_1 j_2 m_2 \; mq} \\
&\quad C^{j_1'\, j_2'\, j}_{m_1' m_2' m'} C^{j_1\, j_2\, j}_{m_1 m_2 m} C^{j\; s'\, j'}_{m q' m'} \langle\, j_1' j_2'; m_1' m_2' \,|\, B^{[s']}_{q'} \,|\, j_1 j_2; m_1 m_2 \,\rangle
\end{aligned}
\tag{110}
$$

where m' is arbitrary. Now expanding B in terms of the reduced matrix elements of M and A,

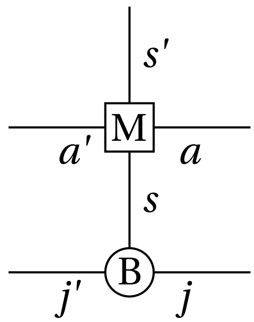
$$
\begin{aligned}
\langle\, (j_1' j_2') j' \,\|\, \boldsymbol{B}^{[s']} \,\|\, (j_1 j_2) j \,\rangle &= \sum C^{j_1'\, j_2'\, j'}_{m_1' m_2' m'} C^{j_1\, j_2\, j}_{m_1 m_2 m} C^{j\; s'\, j'}_{m q' m'} \\
&\times C^{s\,k\,s'}_{q\,r\,q'} C^{j_1\;\, k\, j_1'}_{m_1 r\, m_1'} C^{j_2\;\, s\, j_2'}_{m_2 q\, m_2'} \\
&\times \langle\, s'; j_1' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; j_1 \,\rangle\langle\, j_2' \,\|\, \boldsymbol{A}^{[s]} \,\|\, j_2 \,\rangle
\end{aligned}
\tag{111}
$$

On making the transformation $C^{s\,k\,s'}_{q\,r\,q'} = (-1)^{s+k-s'} C^{k\,s\,s'}_{r\,q\,q'}$, and substituting

$$
\begin{aligned}
k &\to j_3 \\
s &\to j_4 \\
s' &\to j_{34} \\
j_1' &\to j_{13} \\
j_2' &\to j_{24} \\
j' &\to j
\end{aligned}
\tag{112}
$$

we obtain immediately the $[\cdots]$ coefficient from Eq. (28) (remembering that there is no summation over m or m' in either equation), modified by the phase $(-1)^{s+k-s'}$. Thus,

$$(\boldsymbol{MA})^{[s']} = \sum_s (-1)^{s+k-s'} {\boldsymbol{M}^{[k]}}^{s's} \otimes \boldsymbol{A}^{[s]} \tag{113}$$



This corresponds to

$$B'^{s'}_{(j'a'),(ja)} = M^{s's}_{a'a} B^{s}_{j'j} \tag{114}$$

The matrix elements are

$$\langle\, i'\iota'; a'\alpha' \,|\, B'^{[s']}_{\sigma'} \,|\, i\iota; a\alpha \,\rangle = \sum_{s\sigma k r} \langle\, s'a'; \sigma'\alpha' \,|\, \bar{M}^{[k]}_r \,|\, sa; \sigma\alpha \,\rangle \langle\, i'\iota' \,|\, B^{[s]}_{\sigma} \,|\, i\iota \,\rangle \tag{115}$$

In terms of the reduced matrix elements, the right hand side is

$$(-1)^{s'+k-s} \sqrt{\frac{2s'+1}{2s+1}} C^{s'\,k\,s}_{\sigma'\,r\,\sigma} C^{a\,k\,a'}_{\alpha\,r\,\alpha'} \langle\, s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \,\rangle \, C^{i\,s\,i'}_{\iota\,\sigma\,\iota'} \langle\, i' \,\|\, \boldsymbol{B}^{[s]} \,\|\, i \,\rangle \tag{116}$$

and we want to couple $(i'a') \to j'$ and $(ia) \to j$, which gives additional CG coefficients,

$$C^{i'\,a'\,j'}_{\iota'\,\alpha'\,m'} C^{i\,a\,j}_{\iota\,\alpha\,m} \tag{117}$$

and we want to write the final result as

$$\langle\, j' \,\|\, \boldsymbol{B'}^{[s']} \,\|\, j \,\rangle = \sum_{m'\sigma' m} \frac{1}{2j'+1} \langle\, j'm' \,|\, B'^{[s']}_{\sigma'} \,|\, jm \,\rangle C^{j\,\,s'\,j'}_{m\,\sigma'\,m'} \tag{118}$$

9.3 Operator-Operator Product

The action of a matrix-product operator on another matrix product operator is

$$\boldsymbol{X}^{[x]} = \boldsymbol{M}^{[m]} \boldsymbol{N}^{[n]} \tag{119}$$

which corresponds to the ordinary (contraction) product in the local basis and the tensor product in the auxiliary basis.

9.4 Operator Adjoint

Previous versions of these notes included a section on the MPO adjoint; this is now superseded by the section on Hermitian conjugation above. But we note (1) the flip conjugation operation used to be defined without the phase factor - this is unphysical in some sense but is how the toolkit defines it (as of 2015/09/08), and (2) there was an error in the phase factor in the old notes, with a footnote that the toolkit (and my thesis) implemented it differently. In fact the error was in these notes, which is now fixed.

9.5 Operator product

For the evaluation of matrix elements, we need the operation

$$F^{a'}_{i'j'} = \sum_{s',s,i,j,a} M^{s's}_{a'a} A^{*s'}_{i'i} B^{s}_{j'j} E^{a}_{ij} \tag{120}$$

On expanding out the reduced matrix elements, we see immediately that the coupling coefficient is

$$\boldsymbol{F}^{[a']}{}_{i'j'} = \sum_{a,i,j,k,s,s'} \begin{bmatrix} j & s & j' \\ a & k & a' \\ i & s' & i' \end{bmatrix} \boldsymbol{M}^{[k]}{}^{s's}_{a'a} \boldsymbol{A}^{[s']}{}^{*}_{i'i} \boldsymbol{B}^{[s]}{}_{j'j} \boldsymbol{E}^{[a]}{}_{ij} \tag{121}$$

Conversely, from the left hand side,

$$F^{a}_{ij} = \sum_{s',s,i',j',a'} E^{a'}_{i'j'} M^{s's}_{a'a} A^{*s'}_{i'i} B^{s}_{j'j} \tag{122}$$

is

$$\boldsymbol{F}^{[a]}{}_{ij} = \sum_{a',i',j',k,s',s} \frac{2i'+1}{2i+1} \begin{bmatrix} j & s & j' \\ a & k & a' \\ i & s' & i' \end{bmatrix} \boldsymbol{E}^{[a']}{}_{i'j'} \boldsymbol{M}^{[k]}{}^{s's}_{a'a} \boldsymbol{A}^{[s']}{}^{*}_{i'i} \boldsymbol{B}^{[s]}{}_{j'j} \tag{123}$$

On interchanging $A \leftrightarrow E$, $B \leftrightarrow F$, this becomes the equation for a direct operator-matrix-product multiply. But using the center-matrix formalism, we want instead the operation

$$\psi'_{i'i} = \sum_{k'kj'j} E^{k'}_{i'j'} F^{k}_{ij} H_{k'k} \psi_{j'j} \tag{124}$$

where ψ, ψ', and H transform as scalars, *i.e.* the quantum numbers impose $i' = i$, $j' = j$, $k' = k$. H is the center matrix of the operator, and ψ is the center matrix of the wavefunction. This is essentially the scalar product $E \cdot F$, and the coupling coefficients drop out.

For an overlap, the usual scaling applies,

$$\langle A|B \rangle = \sum_{i'i} (2i'+1) A^{*}_{i'i} B_{i'i} \tag{125}$$

which reduces the full overlap equation $\langle\, A \,|\, M \,|\, B \,\rangle$ to

$$\sum_{i'ik'k} (2i'+1) A^{*}_{i'i} E^{k'}_{i'j'} F^{k}_{ij} H_{k'k} B_{j'j} \tag{126}$$

9.6 Alternate notation

It may be better to use the notation of section 8.3. We want to construct

$$\boldsymbol{F'}^{[a']} = \boldsymbol{A}^{[s']} \boldsymbol{F}^{[a]} \boldsymbol{B}^{\dagger}{}^{[s]} \,\langle\, s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \,\rangle \tag{127}$$

The reduced matrix elements of the right hand side are

$$\langle\, j' \,\|\, \boldsymbol{A}^{[s']} \,\|\, i' \,\rangle \langle\, i' \,\|\, \boldsymbol{F}^{[a]} \,\|\, i \,\rangle \langle\, i \,\|\, \boldsymbol{B}^{\dagger}{}^{[s]} \,\|\, j \,\rangle \langle\, s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \,\rangle \tag{128}$$

which leads to the reduced matrix elements $\langle\, j' \,\|\, \boldsymbol{F'}^{[a']} \,\|\, j \,\rangle$, via the coefficients

$$\sum_{\sigma'\sigma n'n\alpha'\alpha mM} C^{i'\ s'\ j'}_{n'\sigma'm'} C^{i\ \ a\ \ i'}_{n'\alpha'n'} C^{i\ s\ j}_{n\sigma m} C^{s\ k\ s'}_{\sigma M\sigma'} C^{a\ k\ a'}_{\alpha M\alpha'} C^{j\ \ a'\ j'}_{m\alpha'm'} \tag{129}$$

where the value of m' is arbitary. Upon identifying $i \to j_1$, $s \to j_2$, $j \to j_{12}$, $a \to j_3$, $k \to j_4$, $a' \to j_{34}$, $i' \to j_{13}$, $s' \to j_{24}$, $j' \to j$, we get immediately

$$\begin{aligned}\langle j' \,\|\, \boldsymbol{F'}^{[a']} \,\|\, j \rangle &= \langle j' \,\|\, \boldsymbol{A}^{[s']} \,\|\, i' \rangle \langle i' \,\|\, \boldsymbol{F}^{[a]} \,\|\, i \rangle \langle j \,\|\, \boldsymbol{B}^{[s]} \,\|\, i \rangle^* \, \langle s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \rangle \\ &\quad \times \begin{bmatrix} i & s & j \\ a & k & a' \\ i' & s' & j' \end{bmatrix}\end{aligned} \tag{130}$$

Compare with the triple product formula, in Eq. (75).

The corresponding E operator is

$$\boldsymbol{E}^{[a]} = \boldsymbol{A}^{\dagger[s']} \boldsymbol{E'}^{[a']} \boldsymbol{B}^{[s]} \, \langle s; a \,\|\, \boldsymbol{M}^{\dagger[k]} \,\|\, s'; a' \rangle \tag{131}$$

The matrix elements are

$$\begin{aligned}\langle j' \,\|\, \boldsymbol{E}^{[e]} \,\|\, j \rangle &= \frac{1}{2j'+1} \sum_{mm'nn'\sigma\sigma'aa'M} \langle i' \,\|\, \boldsymbol{A}^{[s']} \,\|\, j' \rangle^* \, \langle i' \,\|\, \boldsymbol{E'}^{[a']} \,\|\, i \rangle \langle i \,\|\, \boldsymbol{B}^{[s]} \,\|\, j \rangle \langle s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \rangle^* \\ &\quad \times C^{j'\, s'\, i'}_{m'\sigma'n'} C^{i\, a'\, i'}_{n'\alpha'n'} C^{j\, s\, i}_{m\sigma n} C^{s\, k\, s'}_{\sigma M\sigma'} C^{a\, k\, a'}_{\alpha M\alpha'} C^{j\, a'\, j'}_{m\alpha'm'}\end{aligned} \tag{132}$$

from which we identify $j \to j_1$, $s \to j_2$, $i \to j_{12}$, $a \to j_3$, $k \to j_4$, $a' \to j_{34}$, $j' \to j_{13}$, $s' \to j_{24}$, $i' \to j$, to give

$$\begin{aligned}\langle j' \,\|\, \boldsymbol{E}^{[e]} \,\|\, j \rangle &= \langle i' \,\|\, \boldsymbol{A}^{[s']} \,\|\, j' \rangle^* \, \langle i' \,\|\, \boldsymbol{E'}^{[a']} \,\|\, i \rangle \langle i \,\|\, \boldsymbol{B}^{[s]} \,\|\, j \rangle \langle s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \rangle^* \\ &\quad \times \frac{2i'+1}{2j'+1} \begin{bmatrix} j & s & i \\ a & k & a' \\ j' & s' & i' \end{bmatrix}\end{aligned} \tag{133}$$

Compare with the triple product formula, in Eq. (72).

A note on this notation: we have chosen here to have the Hermitian conjugate appear in the E matrix definition, and not in the F matrix. This is consistent in the sense that if we accumulate tensors coming from both the left and the right, the final expectation value is $\mathrm{Tr}\, \boldsymbol{E}^{\dagger[a]} \boldsymbol{F}^{[a]}$. **should check this!**

10 Matrix-vector multiply

If we are not using the center-matrix formalism, then we need to apply the E and F matrices directly to an MPS. This operation is

$$A'^{s'}_{ij} = M^{s's}_{a'a} E^{*a'}_{i'i} A^{s}_{i'j'} F^{a}_{j'j} \tag{134}$$

Since we are treating the local basis elements in A as downstairs indices, we expect similar conjugate phase issues as for the operator-state product.

A contraction that we want to perform is

$$A^{s'}_{i'i} = M^{s',s}_{a'a} E^{a'\dagger}_{i'j'} F^{a}_{ij} B^{s\dagger}_{j'j} \tag{135}$$

To construct the coupling coefficient, we write the matrix elements, which gives the quantum number triples

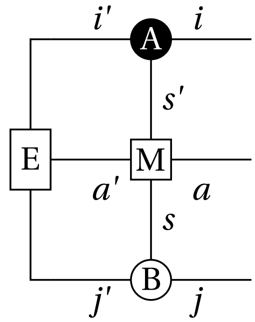
$$(j, s, j')(j, a, i)(j', a', i')(a, k, a')(s, k, s') \to (i, s', i') \tag{136}$$

We can identify this with the $9j$ coefficient,

$$\langle i' \,\|\, \boldsymbol{A}^{[s']} \,\|\, i \rangle = \begin{bmatrix} j & s & j' \\ a & k & a' \\ i & s' & i' \end{bmatrix} \langle s'; a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, s; a \rangle \langle i' \,|\, \boldsymbol{E}^{[a']} \,|\, j' \rangle^* \langle i \,|\, \boldsymbol{F}^{[a]} \,|\, j \rangle \langle j' \,|\, \boldsymbol{B}^{[s]} \,|\, j \rangle^* \tag{137}$$

10.1 E-matrix

We can express the E-matrix contraction as

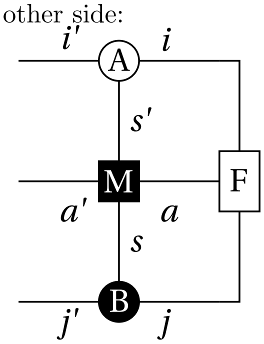


This has two incoming indices, and one out index, and therefore transforms as an ordinary tensor,

$$E'^{a}_{ij} = M^{s's}_{a'a} \bar{B}^{s}_{i'i} E^{a'}_{i'j'} A^{s'}_{j'j} \tag{138}$$

10.2 F-matrix

The F-matrix is the contraction from the other side:



This has two outgoing indices and one in index, and therefore transforms as a conjugate tensor. Hence the tensor that we will actually obtain is $\bar{F}$, which is obtained as

$$\bar{F}'^{a'}_{i'j'} = M^{s's}_{a'a} \bar{B}^{s}_{i'i} A^{s'}_{j'j} \bar{F}^{a}_{ij} \tag{139}$$

Or, conjugating all tensors,

$$F'^{a'}_{i'j'} = \bar{M}^{s's}_{a'a} B^{s}_{i'i} \bar{A}^{s'}_{j'j} F^{a}_{ij} \tag{140}$$

11 Direct SVD

We want to calculate the SVD directly of A-matrices, for the 1-site algorithm, and also for a pair of A-matrices for the 2-site algorithm,

11.1 Single matrix, truncating basis 2

Here we consider the decomposition of an A-matrix into

$$A^s = X = U^s D V \tag{141}$$

where we treat X as a $dm \times m$ matrix. For the subspace expansion technique, A^s is expanded on the right-hand side to be m' states, so that X is $dm \times m'$, then we have U^s as $d \times m \times m'$, and $D.V$ are $m' \times m'$.

This is essentially the same operation that we did in the center-matrix formulation. Phase factors appearing in X are irrelevant since they will cancel out again when we convert back into U^s. Hence section

section 8.2 applies, and we can write $A^s = A'^s X$, where A'^s is a $d \times m \times dm$ MPS that satisfies the left orthogonality constraint, $A'^\dagger A' = I$. This gives

$$X^{ji} = A^s_{i'i} \sqrt{\frac{2i'+1}{2i+1}} \tag{142}$$

where $j = (i'\bar{s})$. The reverse of this is

$$A^s_{i'i} = X_{ji} \sqrt{\frac{2i+1}{2i'+1}} \tag{143}$$

11.2 Single matrix, truncating basis 1

Here we consider the decomposition of an A-matrix into

$$A^s = X = UDV^s \tag{144}$$

where we treat X as a $m \times dm$ matrix. For the subspace expansion technique, A^s is expanded on the left-hand side to be m' states, so that X is $m' \times dm$, then we have V^s as $d \times m' \times m$, and U, D are $m' \times m'$.

In writing A^s as a scalar operator, we need to get the coupling coefficients correct because the same index on the right of A^s can appear in more than one s sector. The matrix elements of A^s are

$$\langle\, i'\iota' \,|\, A^{[s]}_\sigma \,|\, i\iota \,\rangle = C^{i\,s\,i'}_{\iota\sigma\iota'} \langle\, i' \,\|\, \boldsymbol{A}^{[s]} \,\|\, i \,\rangle \tag{145}$$

Converting this into a scalar by coupling spins i, s to spin i', gives

$$\langle\, i' \,|\, A^{[0]}_0 \,|\, i'(is) \,\rangle = C^{i'\,0\,i'}_{\iota'\,0\,\iota'} C^{i\,s\,i'}_{\iota\sigma\iota'} \langle\, i' \,\|\, \boldsymbol{A}^{[0]} \,\|\, i'(is) \,\rangle \tag{146}$$

The coupling coefficient for mapping (i, s) into i' coincides with that of the original reduced matrix element, which is convenient. The extra term is $C^{i'\,0\,i'}_{\iota'\,0\,\iota'}$ which is identically 1, from Eq. (6). Hence we have

$$\langle\, i' \,\|\, \boldsymbol{A}^{[0]} \,\|\, i'(is) \,\rangle = \langle\, i' \,\|\, \boldsymbol{A}^{[s]} \,\|\, i \,\rangle \tag{147}$$

11.3 Direct SVD of two MPS

For two-site algorithms that act on the A-matrices directly, we need to combine the two sites into one (which is a simple multiplication of the A-matrices using Eq. (40)), and then decompose this back into two A-matrices with a singular value decomposition. To do this decomposition, we multiply both sites of Eq. (40) by

$$(-1)^{j+j'+k} \sqrt{(2r+1)(2k+1)} \begin{Bmatrix} j' & k_1 & r \\ k_2 & j & k \end{Bmatrix} \tag{148}$$

and sum over k. Using the orthogonality constraint Eq. (16) this gives

$$\begin{aligned} &\langle\, j' \,\|\, \boldsymbol{S}^{[k_1]} \,\|\, r \,\rangle \langle\, r \,\|\, \boldsymbol{T}^{[k_2]} \,\|\, j \,\rangle \\ &\quad = (-1)^{j+j'+k} \textstyle\sum_k \sqrt{(2r+1)(2k+1)} \begin{Bmatrix} j' & k_1 & r \\ k_2 & j & k \end{Bmatrix} \\ &\quad \times \langle\, j' \,\|\, \left[\boldsymbol{S}^{[k_1]} \times \boldsymbol{T}^{[k_2]}\right]^{[k]} \,\|\, j \,\rangle \end{aligned} \tag{149}$$

which is pleasingly symmetric with Eq. (40).

12 Delta Shifts

When inserting sites into a MPS we want to manipulate the quantum number of the target state. This operation corresponds to inserting an operator that transforms as k (ie. the quantum number of the inserted sites) which we need to apply to all tensors to the left, and then project onto the desired new target state for the full system.

In the case where the $SU(2)$ quantum number strictly *increases*, this has a simplified form, because then the basis size is unchanged; each state j simply shifts $j \to j + \Delta$. Clearly we cannot do this if $j + \Delta$ is negative, but the common case will be, eg, fixed magnetization per site, in which case $\Delta \geq 0$. We refer to this as a Δ-*shift*, it corresponds to the application of a *unit tensor operator* [**?**].

The effect is the same as tensor product with an $m = 1$ identity operator, with only one non-zero matrix element $\langle\, \Delta \,\|\, \boldsymbol{M}^{[0]} \,\|\, \Delta \,\rangle$. In the tensor product we want to take only the basis states in the heightest weight, $D(j) \otimes D(\Delta) \to D(j + \Delta)$. This is equation Eq. (108) with Eq. (42) restricted to a single j', j. The phase factor from Eq. (108) vanishes leaving a matrix element

$$
\begin{aligned}
&\langle\, j' + \Delta \,\|\, \boldsymbol{M}^{[0]} \otimes \boldsymbol{A}^{[k]} \,\|\, j + \Delta \,\rangle \\
&= \langle\, \Delta \,\|\, \boldsymbol{M}^{[0]} \,\|\, \Delta \,\rangle \langle\, j' \,\|\, \boldsymbol{A}^{[k]} \,\|\, j \,\rangle \begin{bmatrix} \Delta & j & j+\Delta \\ 0 & k & k \\ \Delta & j' & j'+\Delta \end{bmatrix}
\end{aligned}
\tag{150}
$$

Making use of the zero to reduce this to a $6j$ coefficient, the coupling coefficient is (need to verify this!)

$$
\begin{aligned}
\begin{bmatrix} \Delta & j & j+\Delta \\ 0 & k & k \\ \Delta & j' & j'+\Delta \end{bmatrix} &= (-1)^{(j+\Delta)+k+\Delta+j'} \sqrt{(2j+2\Delta+1)(2j'+1)} \\
&\quad \times \begin{Bmatrix} j & j' & k \\ j'+\Delta & j+\Delta & \Delta \end{Bmatrix}
\end{aligned}
\tag{151}
$$

Unfortunately, this approach does not work: the effect of applying an $m = 1$ identity operator and projecting onto some target $j + \Delta$ state is not equivalent to applying the Δ shift to each A-matrix. Consider the left-most A-matrix, where the left basis is one-dimensional and represents the target state. Without restricting the right basis, the product coefficient is

$$
\begin{bmatrix} \Delta & j & j+a \\ 0 & k & k \\ \Delta & j' & j'+\Delta \end{bmatrix}
\tag{152}
$$

where a is the quantum number in the right basis. The restrictions on the possible values of a arise from the need to satisfy the triangle constraints for the first row and third column. This gives $|j - \Delta| \leq a \leq j + \Delta$ and $|j' + \Delta - k| \leq a \leq j' + \Delta + k$. Thus, in general, more than one a will satisfy these constraints. We can understand this by viewing the Δ-shift as a two-step operation; firstly we apply the $m = 1$ operator, which gives up to $2\Delta + 1$ target states; at this point the A-matrices will preserve whatever normalization constraints they had previously. Follow this by a projection onto a single target state. As for any form of projection, this does not preserve the normalization.

The question remains: can we get away with a Δ-shift followed by a reorthogonalization of the basis? Or do we need, as suggested above, to include all states? How can we have an (approximately) translationally invariant state if we need to include all states, as this would magnify the basis size for higher quantum numbers?

13 Translation MPO

In this section, we deduce the MPO representation for the translation operator that shifts sites to the left or right.

13.1 Right translation

Here we define a right translation, that is an operator that acts on a wavefunction so that the site originally labelled site 0 becomes site 1 after the shift. In the notation of Eq. (104), this has the form

$$\langle\, s'; j' \,\|\, \boldsymbol{T_R}^{[k]} \,\|\, s; j \,\rangle = \delta_{s'j'}\delta_{sj}\epsilon_{sks'}\frac{2k+1}{2s+1} \tag{153}$$

where k takes on all values that satisfy the triangle condition $\epsilon_{sks'} = 1$.

To prove this, we construct the full matrix elements,

$$\langle\, s'q'; j'm' \,|\, {T_R}^{[k]}_r \,|\, sq; jm \,\rangle = \delta_{s'j'}\delta_{sj}\epsilon_{sks'}\; C^{s\,k\,s'}_{q\,r\,q'}\; C^{j\;\,k\,j'}_{m\,r\,m'}\frac{2k+1}{2s+1} \tag{154}$$

To obtain the physical matrix elements we sum over k, r, and make use of the orthogonality of columns of the Clebsch-Gordan coefficients,

$$C^{s\,k\,s'}_{q\,r\,q'}\; C^{j\;\,k\,j'}_{m\,r\,m'} = (-1)^{s-q}\sqrt{\frac{2s+1}{2k+1}}C^{s\;\;s'\;\;k}_{q\,-q'\,-r}(-1)^{j-m}\sqrt{\frac{2j+1}{2k+1}}C^{j\;\;\,j'\;\;\,k}_{m\,-m'\,-r} \tag{155}$$

Thus

$$\sum_{k,r}\delta_{s'j'}\delta_{sj}\epsilon_{sks'}(-1)^{2s-q-m}C^{s\;\;s'\;\;k}_{q\,-q'\,-r}C^{j\;\;\,j'\;\;\,k}_{m\,-m'\,-r} = (-1)^{2s-q-m}\delta_{s'j'}\delta_{sj}\delta_{q'm'}\delta_{qm} \tag{156}$$

The phase factor out the front vanishes: s and q are either both integer or both odd-half-integer, so $s-q$ is always integer, and $2(s-q)$ is always even. And finally,

$$\langle\, s'q'; j'm' \,|\, {T_R}^{[k]}_r \,|\, sq; jm \,\rangle = \delta_{s'j'}\delta_{sj}\epsilon_{sks'}\;\delta_{q'm'}\delta_{qm} \tag{157}$$

as expected.

13.2 Left translation

Here we define a left translation, that is an operator that acts on a wavefunction so that the site originally labelled site 1 becomes site 0 after the shift. In the notation of Eq. (104), this has the form

$$\langle\, s'; j' \,\|\, \boldsymbol{T_L}^{[k]} \,\|\, s; j \,\rangle = \delta_{s'j}\delta_{sj'}\epsilon_{sks'}\frac{2k+1}{2s+1} \tag{158}$$

The full matrix elements are

$$\langle\, s'q'; j'-m' \,|\, {T_R}^{[k]}_r \,|\, sq; j-m \,\rangle = \delta_{s'j}\delta_{sj'}\epsilon_{sks'}\;\frac{2k+1}{2s+1}C^{s\,k\,s'}_{q\,r\,q'}\;C^{s'\;\;\,k\,s}_{-m\,r\,-m'} \tag{159}$$

Using the symmetries of the Clebsch-Gordan coefficients,

$$\begin{aligned}\langle\, s'q'; j'm' \,|\, {T_R}^{[k]}_r \,|\, sq; jm \,\rangle &= \delta_{s'j}\delta_{sj'}\epsilon_{sks'}\;\frac{2k+1}{2s+1}(-1)^{s-q}\sqrt{\frac{2s+1}{2k+1}}C^{s\;\;s'\;\;k}_{q\,-q'\,-r}\;(-1)^{s'+m}\sqrt{\frac{2s+1}{2k+1}}(-1)^{s+s'-k}C^{s\;\;\;s'\;\;\;k}_{m'\,-m\,-r} &(160)\\ &= \delta_{s'j}\delta_{sj'}\epsilon_{sks'}(-1)^{k-q+m}C^{s\;\;s'\;\;k}_{q\,-q'\,-r}C^{s\;\;\;s'\;\;\;k}_{m'\,-m\,-r} &(161)\end{aligned}$$

Summing over k, r, and using the orthogonality of columns,

$$= \delta_{s'j}\delta_{sj'}\epsilon_{sks'}\delta_{q,m'}\delta_{q',m}(-1)^{k-m'+m} \tag{162}$$

14 Partial transpose

(incomplete)

For the calculation of exponents of operators, we need the partial transpose operation. Writing the matrix elements of M as

$$\langle\, a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, a \,\rangle \tag{163}$$

where the a', a indices have a tensor decomposition,

$$\begin{aligned} \|a'\rangle &= \|j_1\rangle\|j_2\rangle \\ \|a\rangle &= \|i_1\rangle\|i_2\rangle \end{aligned} \tag{164}$$

this gives the reduced matrix elements

$$\langle\, (i_1 i_2) a' \,\|\, \boldsymbol{M}^{[k]} \,\|\, (j_1 j_2) a \,\rangle\ , \tag{165}$$

which has reduced matrix elements

$$C^{i_1\ i_2\ a'}_{m_1 m_2 \alpha'} C^{j_1\ j_2\ a}_{n_1 n_2 \alpha} C^{a\ k\ a'}_{\alpha\, q\, \alpha'} \langle\, (i_1, n_1; i_2, n_2) a', \alpha' \,|\, M^{[k]}_q \,|\, (j_1, n_1; j_2, n_2) a, \alpha \,\rangle \tag{166}$$

Now we want to do a partial transpose, to write

$$\langle\, (i_1 j_1) a_1 \,\|\, \boldsymbol{M}^{\boldsymbol{PT}[k]} \,\|\, (i_2 j_2) a_2 \,\rangle \tag{167}$$

which has reduced matrix elements

$$C^{i_1\ j_1\ a_1}_{n_1 m_1 \alpha_1} C^{i_2\ j_2\ a_2}_{n_2 m_2 \alpha_2} C^{a_2\, k\, a_1}_{\alpha_2\, q\, \alpha_1} \langle\, (i_1, n_1; j_1, m_1) a_1, \alpha_1 \,\|\, {M^{PT}}^{[k]}_q \,\|\, (i_2, n_2; j_2, m_2) a_2, \alpha_2 \,\rangle \tag{168}$$

Starting from Eq. (167), we write the reduced matrix element as

$$\begin{aligned} &\langle\, (i_1 j_1) a_1 \,\|\, \boldsymbol{M}^{\boldsymbol{PT}[k]} \,\|\, (i_2 j_2) a_2 \,\rangle \\ &\quad = \frac{1}{2a_1+1} \sum_{\alpha_1 q \alpha_2} C^{a_2\, k\, a_1}_{\alpha_2\, q\, \alpha_1} \langle\, a_1, \alpha_1 \,\|\, {M^{PT}}^{[k]}_q \,\|\, a_2, \alpha_2 \,\rangle \\ &\quad = \frac{1}{2a_1+1} \sum_{\alpha_1 q \alpha_2} \sum_{m_1 m_2 n_1 n_2} C^{i_1\ j_1\ a_1}_{n_1 m_1 \alpha_1} C^{i_2\ j_2\ a_2}_{n_2 m_2 \alpha_2} C^{a_2\, k\, a_1}_{\alpha_2\, q\, \alpha_1} \\ &\quad\quad \times \langle\, (i_1, n_1; j_1, m_1) a_1, \alpha_1 \,\|\, {M^{PT}}^{[k]}_q \,\|\, (i_2, n_2; j_2, m_2) a_2, \alpha_2 \,\rangle \end{aligned} \tag{169}$$

15 Swap gates

(incomplete)

In this section we deduce the matrix elements of an MPO that effect the swap gate between two sites. The swap gate is a scalar operator that acts on two sites, and has the matrix elements

$$\mathrm{Swap}\|j_1\rangle\|j_2\rangle = \|j_2\rangle\|j_1\rangle\ , \tag{170}$$

or, more explicitly, the full matrix elements are

$$\langle\, j'(j'_1 j'_2 \alpha'_1 \alpha'_2) \,\|\, \mathrm{Swap} \,\|\, j(j_1 j_2 \alpha_1 \alpha_2) \,\rangle = \delta_{j' j} \delta_{j'_1 j_2} \delta_{j'_2 j_1} \delta_{\alpha'_1 \alpha_2} \delta_{\alpha'_2 \alpha_1}\ . \tag{171}$$

The commutation of indices j'_1, j'_2 brings in a phase factor, Eq. (22),

$$\langle\, j'(j'_2 j'_1 \alpha'_2 \alpha'_1) \,\|\, \mathrm{Swap} \,\|\, j(j_1 j_2 \alpha_1 \alpha_2) \,\rangle = (-1)^{j_1+j_2-0} \delta_{j' j} \delta_{j'_1 j_1} \delta_{j'_2 j_2} \delta_{\alpha'_1 \alpha_1} \delta_{\alpha'_2 \alpha_2}\ . \tag{172}$$

The right hand side is just the identity operation with a phase factor.

16 TODO

Expectation Values. The formulas are already covered, just make the notation explicit.