Symmetries III: Outer multiplicity, X-Symbols

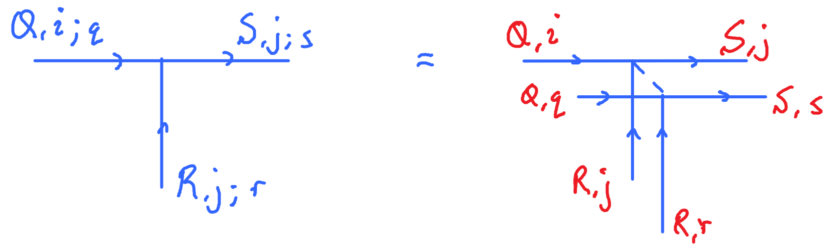
[Weichselbaum2020]

For representation theory of SU(N), see [Alex2011]

1. Motivation

'Symmetries II: non-Abelian' showed: in the presence of symmetries, A-tensors factorize:

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



Goal: reduce explicit reliance on Clebsch-Gordan tensors (CGT) as much as possible!

Why? CGT can become very large objects for groups of large rank, e.g. SU(N) with N > 3.
Hence, whenever possible, avoid computing and contracting them explicitly.

Multiplet dimensions

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

$$V^Q \equiv \mathrm{span}\{|Q,q\rangle\} \quad , \quad q = 1, \dots, \dim(V^Q) \equiv d_Q \equiv |Q| \tag{1}$$

'irrep' label or 'symmetry' label (Q); 'internal' label, distinguishes states in multiplet (q).

In general, internal label is a composite label, $q = (q_1, q_2, \dots, q_r)$ (2)

where r is the 'rank' of the group, i.e. the number of commuting generators, $\hat{S}_1, \dots, \hat{S}_r$

These span the 'Cartan subalgebra', can be diagonalized simultaneously:

$$\hat{S}_a |q\rangle = q_a |q\rangle \quad , \quad a = 1, \dots, r \tag{3}$$

Their eigenvalues can be used to label a basis for V^Q, as done in (1).

Multiplet dimension: $$|Q| = \prod_{a=1}^{r} q_a^{max} \sim \left(q^{max}_{average}\right)^r \tag{4}$$

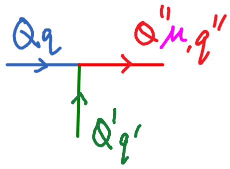
'Typical multiplet dimension' grows exponentially with r.

For SU(N), $r = N-1$, typical dimensions grow as $\sim 10^{N-1}$, 'large' for $N \gtrsim 4$ (5)

Hence: efficient numerics tries to avoid working 'inside' multiplets; rather treat them as closed units.

2. Outer multiplicity

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



$$V^{Q} \otimes V^{Q'} = \sum_{\oplus Q''} N^{QQ'}_{Q''} V^{Q''} = \sum_{\oplus Q''} \sum_{\mu=1}^{N^{QQ'}_{Q''}} V^{Q'';\mu} \qquad (6)$$

schematic notation — explicit notation

'Outer multiplicity' (OM) $N^{QQ'}_{Q''}$ is an integer specifying how often the irrep Q'' occurs in the decomposition of the direct product $V^{Q} \otimes V^{Q'}$.

For given Q'', 'outer multiplicity index' $\mu = 1, \dots, N^{QQ'}_{Q''}$ distinguishes different occurrences of that irrep. States in direct sum decomposition are labeled $|Q'', \mu; q\rangle$. (7)

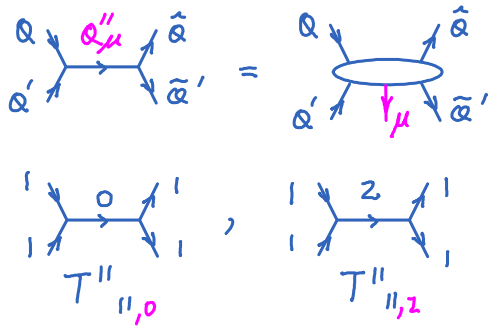
For SU(2), we have $$N^{SS'}_{S''} = \begin{cases} 1 & \text{for } |S-S'| \le S'' \le S+S' \\ 0 & \text{otherwise} \end{cases} \qquad (8)$$

For other groups, e.g. $SU(N \geq 3)$, the OM can be > 1. (9)

The extra OM-index brings additional complexity to tensor network codes. 'SU(3) is much harder than SU(2)'.

OM also enters [even for SU(2)] when coupling more than two irreps:
Suppose four given irreps $Q, Q', \tilde{Q}, \tilde{Q}'$ can be coupled using M different choices for the intermediate irrep, Q''_μ, $\mu = 1, \dots, M$.
Then each choice yields a different four-leg tensor, $T^{QQ'}_{\tilde{Q}\tilde{Q}',\mu}$ distinguished by an OM index μ.

Example:

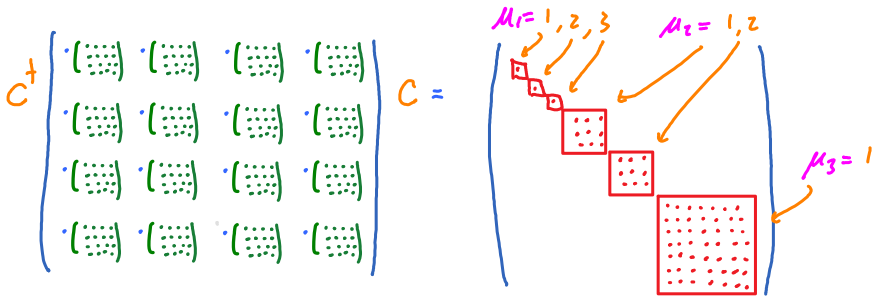


Clebsch-Gordan tensors (CGT)

Action of generators: $$\hat{C}^{\dagger}\left(\hat{S}^{a}_{1} \otimes \hat{\mathbb{1}}_{2} + \hat{\mathbb{1}}_{1} \otimes \hat{S}^{a}_{2}\right)\hat{C} = \sum_{\oplus S''} \hat{S}^{a} \qquad (10)$$

dimensions: $d_Q \times d_Q$ $\quad d_{Q'} \times d_{Q'}$ $\quad d_{Q''} \times d_{Q''}$

$\hat{C}$ transforms generators into block-diagonal form: (drawn for $N^{QQ'}_{Q''_1} = 3$, $N^{QQ'}_{Q''_2} = 2$, $N^{QQ'}_{Q''_3} = 1$)



(11)

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

$$|Q''\mu, q'' ; Q, Q'\rangle = \overbrace{\sum_{qq'} |Q', q'\rangle \otimes |Q, q\rangle \, \langle Q, q| \otimes \langle Q', q'|}^{\text{completeness in direct product space}} \; |Q''\mu, q''; Q, Q'\rangle \tag{12}$$

CGC = $\langle Q,q ; Q',q' | Q'', q''; Q Q' \rangle \equiv \left(C^{QQ'}{}_{Q''\mu}\right)^{qq'}{}_{q''}$

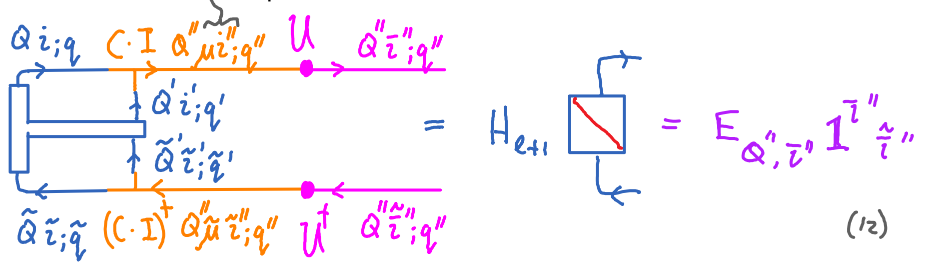
carries all info on which irreps contribute, and with which multiplicities

$$= \sum_{qq'} |Q', q'\rangle \otimes |Q, q\rangle \underbrace{\left(C^{QQ'}{}_{Q''\mu}\right)^{qq'}{}_{q''}}_{= C \text{ for short}} \tag{13}$$

Rank-3 CGTs are sometimes called '3-j symbols', since they link 3 irreps.

Factorization of A-tensor (see Sym-II.15) must account for OM:

Recall iterative diagonalization, transform to energy eigenbasis via unitary transformation:

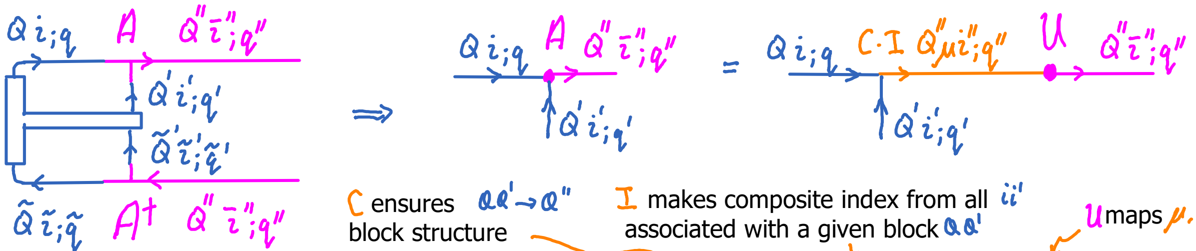


(12)

$\boxed{U_{Q''}}^{\mu, i''}{}_{\bar{i}''}$ $\quad \dim(\mu) \cdot \dim(i'') = \dim(\bar{i}'')$

output index has status of composite index, combining outer multiplicity μ with previous multiplicity i'' into new multiplicity $\bar{i}''$

Combined transformation from old energy eigenbasis to new energy eigenbasis:



(13)

C ensures $QQ' \to Q''$ block structure

I makes composite index from all ii' associated with a given block QQ'

U maps μ, i'' to $\bar{i}''$

$$A^{(Qi;q)(Q'i';q')}{}_{(Q''\bar{i}'';q'')} := \left[C^{QQ'}{}_{Q''\mu}\right]^{qq'}{}_{q''} \left[I^{QQ'}{}_{Q''}\right]^{ii'}{}_{i''} \left[U_{[Q'']}\right]^{\mu, i''}{}_{\bar{i}''} \tag{14}$$

identify factorized form: $A = \tilde{A}\,\tilde{C}$

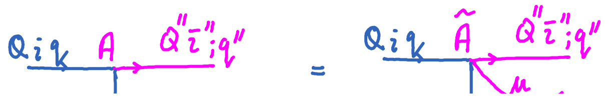
$$=: \left[\tilde{A}^{QQ'\mu}{}_{,Q''}\right]^{ii'}{}_{\bar{i}''} \left[C^{QQ'}{}_{Q''\mu}\right]^{qq'}{}_{q''} \tag{15}$$

or more general notation:

$$= \left[\tilde{A}^{QQ'\mu}{}_{,Q''}\right]^{ii'}{}_{\bar{i}''} \, w_\mu{}^\nu \left[C^{QQ'}{}_{Q''\nu}\right]^{qq'}{}_{q''} \tag{16}$$

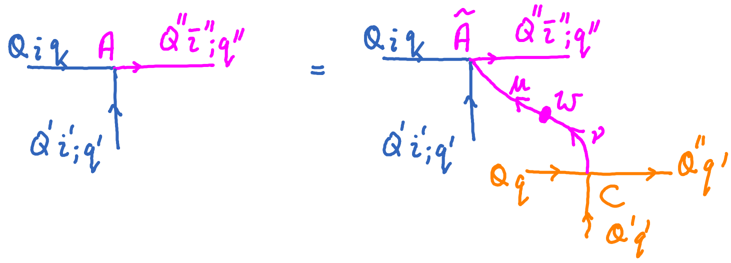
[$w_\mu{}^\nu$ connects A^μs with different OM labels to associated C_ν s]

A-matrix factorizes, into product of reduced A-matrix and CGT !! $\quad A = \left(\tilde{A}^\mu \, w_\mu{}^\nu\right) C_\nu = \tilde{\tilde{A}}^\nu C_\nu$



A 'does not know' about OM.

But its factorization does!



A 'does not know' about OM.

But its factorization does!

This structure can be exploited

to reduce numerical costs:

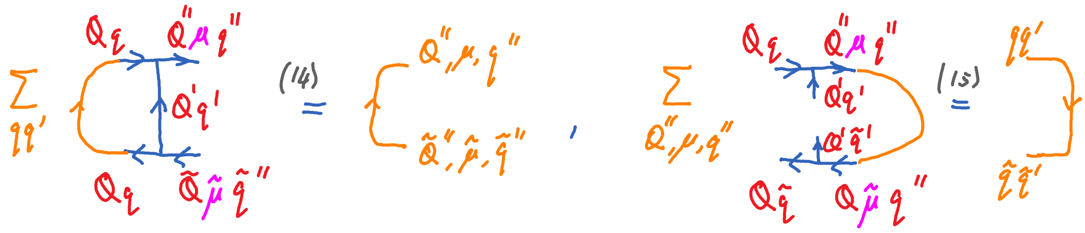
Associate w with $\tilde{A}$ rather than with C

3. Arrow inversion

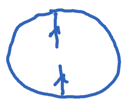
CGTs can always be chosen real. According to (13), they represent a unitary transformation.
Hence, for fixed Q, Q', they satisfy:

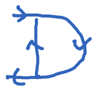
$$\sum_{qq'} \left(C^{\dagger\,\tilde Q'',\tilde\mu}{}_{Q'Q}\right)^{\tilde q''}{}_{q'q} \left(C^{QQ'}{}_{Q'',\mu}\right)^{qq'}{}_{q''} = \mathbb{1}^{\tilde Q''}{}_{Q''}\, \mathbb{1}^{\tilde\mu}{}_{\mu}\, \mathbb{1}^{\tilde q''}{}_{q''} \tag{14}$$

$$\sum_{Q'',\mu,q''} \left(C^{QQ'}{}_{Q'',\mu}\right)^{\tilde q\tilde q'}{}_{q''} \left(C^{Q'',\mu}{}_{Q'Q}\right)^{q''}{}_{q'q} = \mathbb{1}^{\tilde q}{}_{q}\, \mathbb{1}^{\tilde q'}{}_{q'} \tag{15}$$



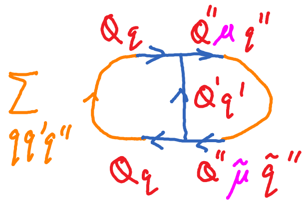
(16)

Note: $\sum_q (15)\big|_{\tilde q = q} = \mathbb{1}^{\tilde q'}{}_{q'}\, |Q|$  $=$  $\cdot\, |Q|$ (17)

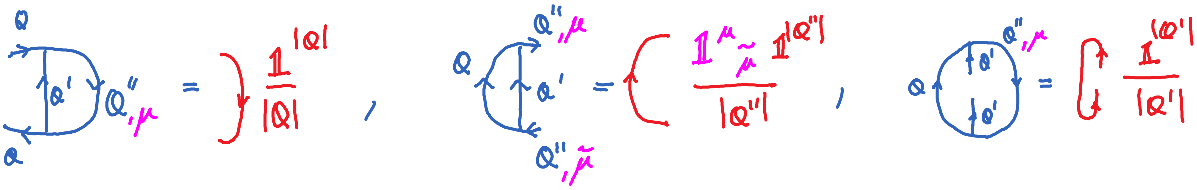
$\sum_{q'} (15)\big|_{\tilde q' = q'} = \mathbb{1}^{\tilde q}{}_{q}\, |Q'|$  $=$  $\cdot\, |Q'|$ (18)

Weichselbaum2019 uses a different normalization, such that, for fixed Q,Q',Q'',
'full contraction of all indices except OM index' yields:

$$\mathrm{Tr}\left[C^{\dagger\,Q'',\tilde\mu} C_{Q'',\mu}\right] \equiv \sum_{qq'q''} \left(C^{\dagger\,\tilde Q'',\tilde\mu}{}_{Q'Q}\right)^{\tilde q''}{}_{q'q} \left(C^{QQ'}{}_{Q'',\mu}\right)^{qq'}{}_{q''} = \mathbb{1}^{\tilde\mu}{}_{\mu} \tag{19}$$

 $= \mathbb{1}^{\tilde\mu}{}_{\mu}$ (20)

Then, 'opening' any leg yields unit matrix divided by dimension of that leg:

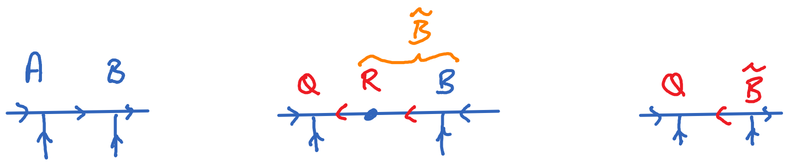


(21)

Prefactor on r.h.s. follows from requirement that trace over open leg reproduces (20).

Inverting arrows

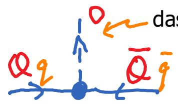
Recall general procedure:



(22)

How does one invert arrows in CGT-sector?

dashes indicate trivial irrep

Define $\quad (U^{Q\bar{Q}}{}_0)^{q\bar{q}} = \sqrt{|Q|}\,(C^{Q\bar{Q}}{}_0)^{q\bar{q}} = \sqrt{|Q|}$  (23)

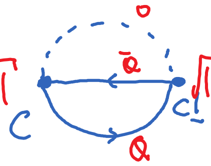
coupling irrep Q and its conjugate irrep $\bar{Q}$ to the trivial, one-dimensional irrep 0 .

dimensions: $\quad |Q| = |\bar{Q}| , \qquad |0| = 1$ (24)

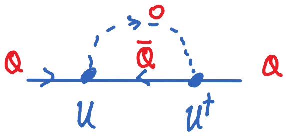
Then U is unitary: $\quad U^{Q\bar{Q}}{}_0\, U^{\dagger 0}{}_{\bar{Q}Q} = \mathbb{1}^{|Q|}$, (25a) $\qquad U^{\dagger 0}{}_{\bar{Q}Q}\, U^{Q\bar{Q}}{}_0 = \mathbb{1}^{|\bar{Q}|}$ (25b)

shorthand for $(\mathbb{1}^{|Q|})^{q'}{}_q$

Graphical argument shows why: consider

$\mathrm{Tr}\; U^{Q\bar{Q}}{}_0\, U^{\dagger 0}{}_{\bar{Q}Q} = \sqrt{|Q|}$  $\sqrt{|Q|} \overset{(20)}{=} |Q|$ (24)

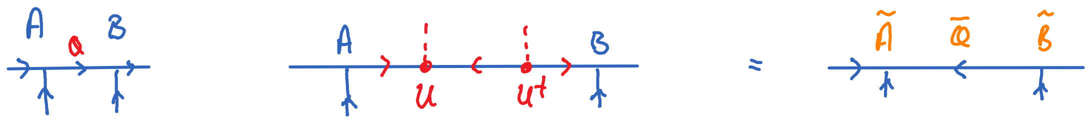
now open Q-leg:

$U^{Q\bar{Q}}{}_0\, U^{\dagger 0}{}_{\bar{Q}Q} =$  $\overset{(24)/(21)}{=} |Q|\,\dfrac{\mathbb{1}^{|Q|}}{|Q|} = \mathbb{1}^{|Q|}$ $\qquad = (25a)$ ✓

Similarly, opening $\bar{Q}$ leg leads to (25b). Compact graphical notation: drop dashed loop

 (25)

hence arrows can be inverted by inserting $\; UU^\dagger = \mathbb{1} \;$ or $\; U^\dagger U = \mathbb{1}$ (26)



$$A\,B = (A\,U)(U^\dagger B) = \tilde{A}\,\tilde{B} \tag{27}$$

U is sometimes called '1-j symbol', since it involves only a single irrep and its conjugate.

U can be computed by finding the ground state of a pseudo-Hamiltonian acting on V^Q

built from generators of the symmetry

$$\hat{H}_Q = \sum_{\alpha=1}^{r} \hat{J}_\alpha^\dagger \hat{J}_\alpha + \hat{J}_\alpha \hat{J}_\alpha^\dagger \tag{28}$$

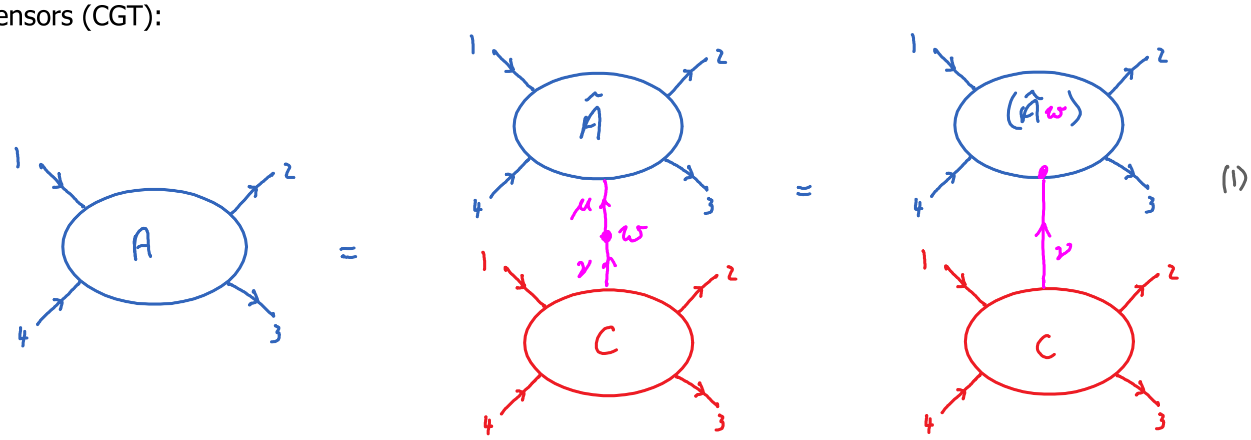
The state satisfying $\; \hat{H}_Q |0\rangle = 0 \;$ is the trivial multiplet (since annihilated by all generators).

Let $\; |0\rangle = |Q_q\rangle\, u^q , \quad \langle 0| = \langle \bar{Q}\bar{q}|\, u^{\bar{q}}$, then $\; (U^{Q\bar{Q}}{}_0)^{q\bar{q}} = u^q (u^{\bar{q}})^*$ (29)

since this maps $\; V^Q \otimes V^{\bar{Q}} \to V^0 : \quad |0\rangle\langle 0| = |Q_q\rangle\, u^q (u^{\bar{q}})^* \langle \bar{Q}\bar{q}| = |Q_q\rangle\, (U^{Q\bar{Q}}{}_0)^{q\bar{q}} \langle \bar{Q}_{\bar{q}}|$ (30)

4. Pairwise contractions and X-symbols

Consider a four-leg tensor, factorized into reduced matrix element tensors (RMT) and Clebsch-Gordan tensors (CGT):

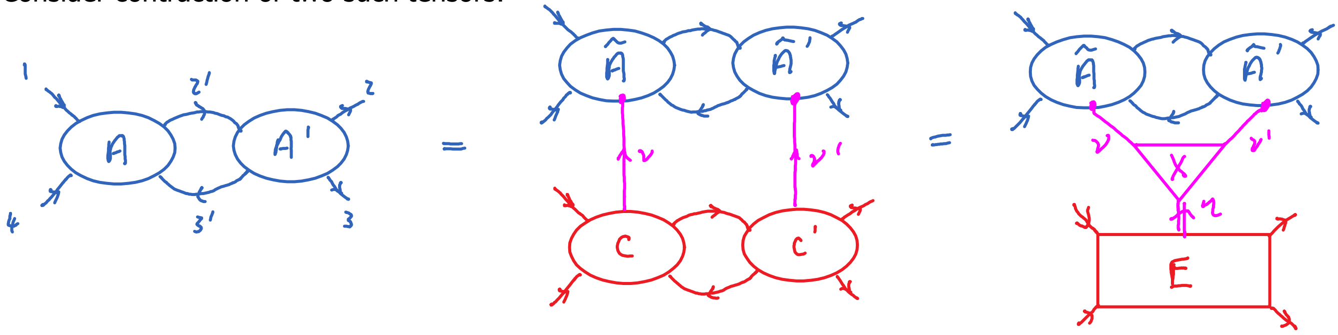


The OM-matrix w can always be contracted onto the RMT, as indicated on the right.

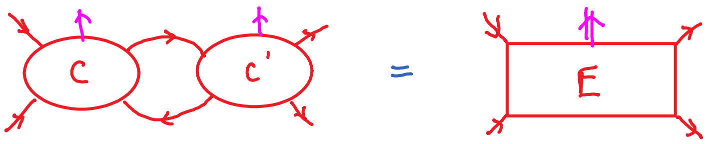
$\tilde{A}$ is in active memory (has to be stored, updated, etc.), whereas

C is 'known' (stored in library on hard disk).

Consider contraction of two such tensors:

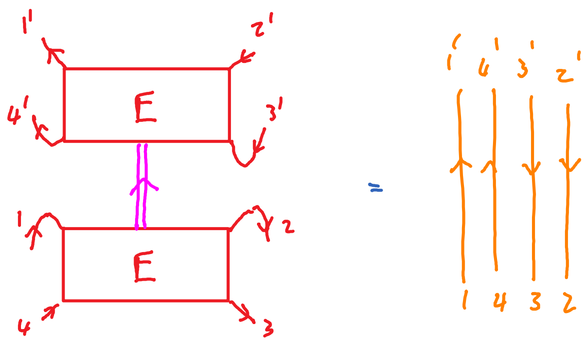


Since CGTs are fully determined by group theory, we know contraction of $C\,C'$ must yield another CGT, E.

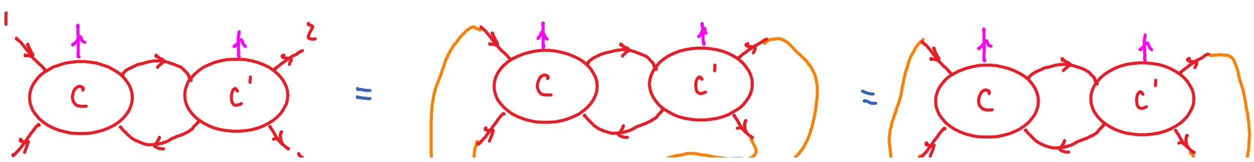


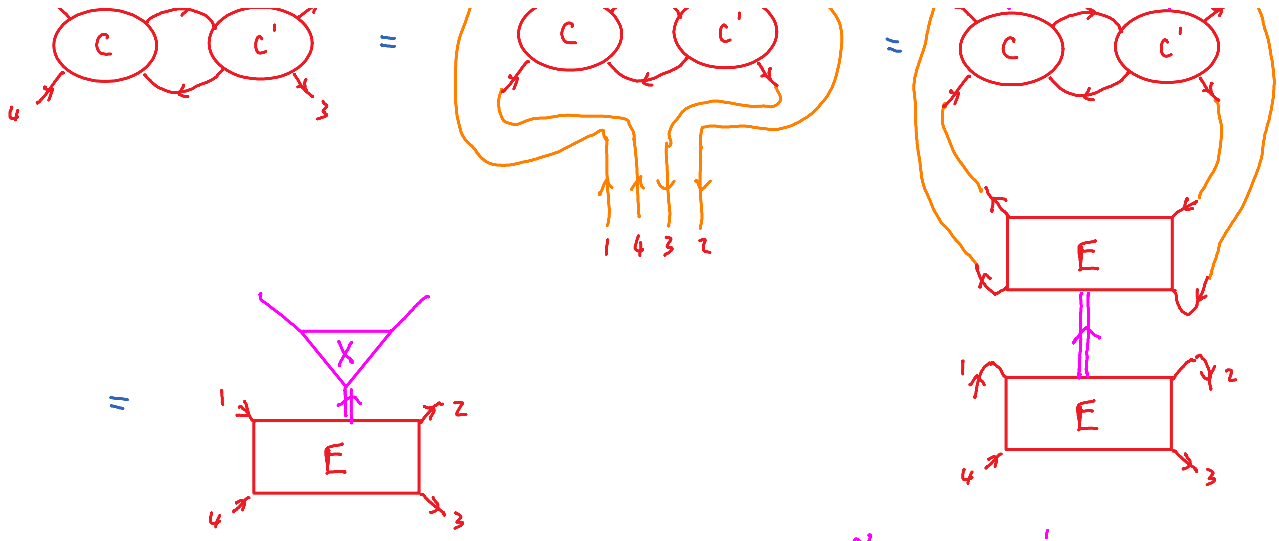
Resolve identity on space of all open legs:

$E^\dagger E = \mathbb{1}$:

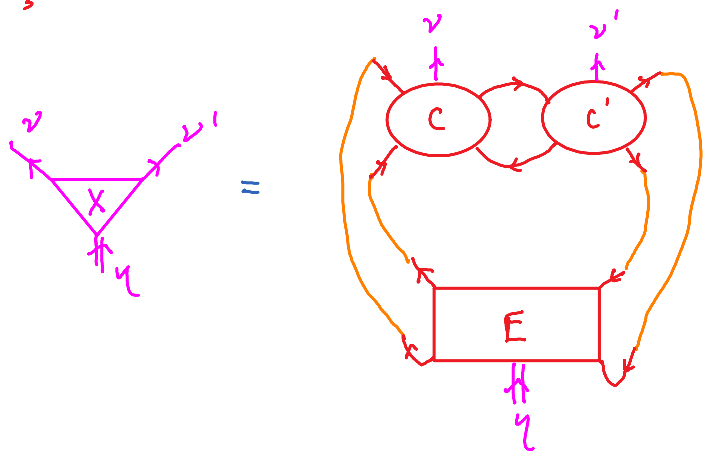


Then we obtain:





with X-symbol defined by:



Manipulations with A's happen in active memory, those with Cs, Es, Xs are done only once, then stored on hard disk for to be contracted in active memory. This brings huge reduction in numerical costs, since Cs, Es can be huge objects, whereas Xs are small.