Z2 and U1 symmetry

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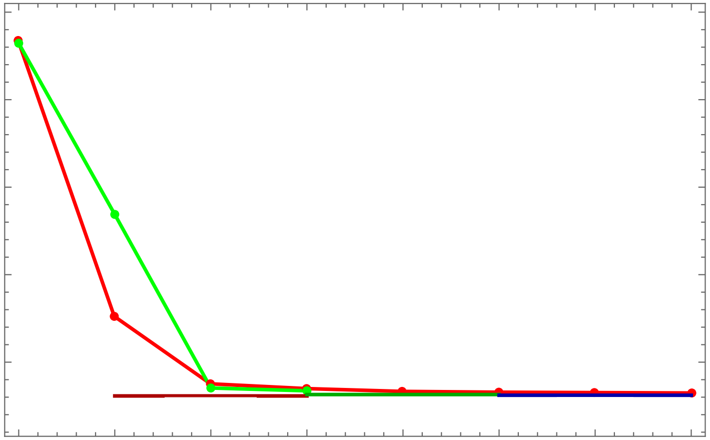
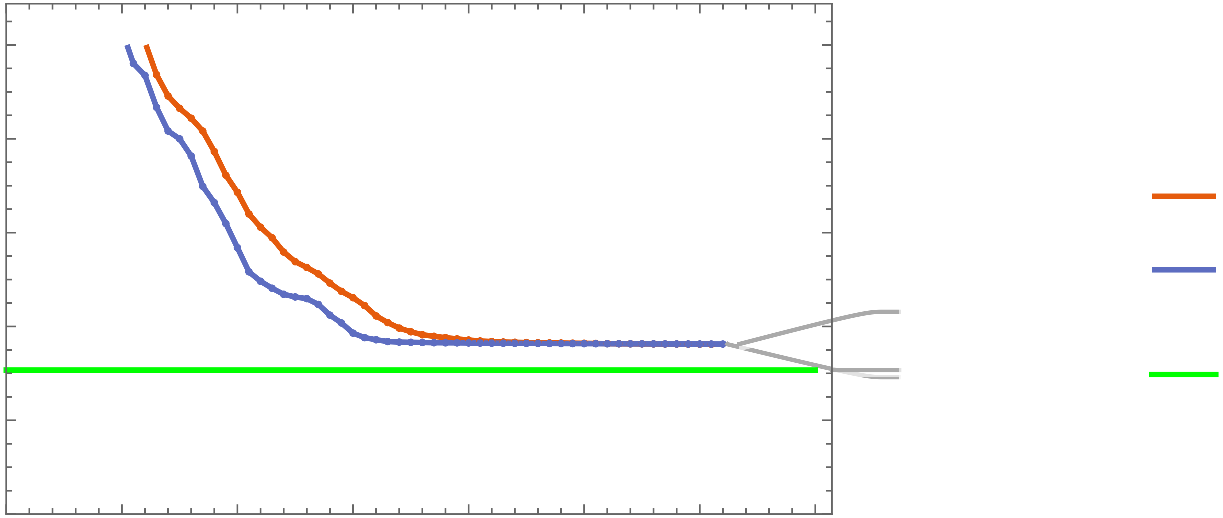
Improvement of Z2 program

- Change way of store a Z2 tensor
  - From all blocked matrix to tensor
  - Make permutation and reshape easier
- Big-Blocked matrix multiplication rather than fragmentary
  - example

Result

- enough low result for $D = 3$
  - E = -0.3241 v.s. -0.3238
- Correct D = 4 result
  - E = -0.36375 v.s. -0.36379





discuss

- Initialization is crucial
  - Down from up and right from left
- Z2 is only faster when $D \geq 6$
  - GPU multiplication is fast
- Explore U1

Tensor network states and algorithms in the presence of a global U(1) symmetry

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- Defination of U1 tensor → Canonical form
- Fuse and split → Permute and reshape → tensor contraction

U(1) representations

- unitary representation of the group U(1).

$$\hat{W}_\varphi : \mathbb{V} \to \mathbb{V}$$

$$\hat{W}_\varphi^\dagger \hat{W}_\varphi = \hat{W}_\varphi \hat{W}_\varphi^\dagger = \mathbb{I}, \quad \forall\, \varphi \in [0, 2\pi),$$

$$\hat{W}_{\varphi_1} \hat{W}_{\varphi_2} = \hat{W}_{\varphi_2} \hat{W}_{\varphi_1} = \hat{W}_{\varphi_1 + \varphi_2 |2\pi}, \quad \forall\, \varphi_1, \varphi_2 \in [0, 2\pi).$$

- Irreducible representations $\mathbb{V} \cong \bigoplus_n \mathbb{V}_n$

$$\hat{n} \equiv \sum_n n \hat{P}_n, \quad \hat{P}_n \equiv \sum_{t_n=1}^{d_n} |n t_n\rangle\langle n t_n|$$

$$\hat{n}|n t_n\rangle = n|n t_n\rangle, \quad t_n = 1, \ldots, d_n$$

$$\hat{W}_\varphi = e^{-\mathrm{i}\hat{n}\varphi}.$$

Example 1. Consider a two-dimensional space $\mathbb{V}$ that decomposes as $\mathbb{V} \cong \mathbb{V}_0 \oplus \mathbb{V}_1$, where the irreps $n = 0$ and $n = 1$ are nondegenerate (i.e., $d_0 = d_1 = 1$). Then the orthogonal vectors $\{|n = 0, t_0 = 1\rangle, |n = 1, t_1 = 1\rangle\}$ form a basis of $\mathbb{V}$. In column vector notation,

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |n = 0, t_0 = 1\rangle, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |n = 1, t_1 = 1\rangle, \quad (26)$$

the particle number operator $\hat{n}$ and transformation $\hat{W}_\varphi$ read

$$\hat{n} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{W}_\varphi \equiv \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\varphi} \end{pmatrix}. \quad (27)$$

Example 2. Consider a four-dimensional space $\mathbb{V}$ that decomposes as $\mathbb{V} \cong \mathbb{V}_0 \oplus \mathbb{V}_1 \oplus \mathbb{V}_2$, where $d_0 = d_2 = 1$ and $d_1 = 2$, so that now irrep $n = 1$ is twofold degenerate. Let $\{|n = 1, t_1 = 1\rangle, |n = 1, t_1 = 2\rangle\}$ form a basis of $\mathbb{V}_1$. In column vector notation,

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \equiv |n = 0, t_0 = 1\rangle, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \equiv |n = 1, t_1 = 1\rangle, \tag{28}$$

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \equiv |n = 1, t_1 = 2\rangle, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \equiv |n = 2, t_2 = 1\rangle, \tag{29}$$

the particle number operator $\hat{n}$ and transformation $\hat{W}_\varphi$ read

$$\hat{n} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad \hat{W} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-\mathrm{i}\varphi} & 0 & 0 \\ 0 & 0 & e^{-\mathrm{i}\varphi} & 0 \\ 0 & 0 & 0 & e^{-\mathrm{i}2\varphi} \end{pmatrix}. \tag{30}$$

Symmetric states and operators

- Symmetric state/vector

$$\hat{W}_\varphi|\Psi\rangle = e^{-in\varphi}|\Psi\rangle, \quad \forall\,\varphi \in [0,2\pi)$$

$$\hat{n}|\Psi\rangle = n|\Psi\rangle, \quad |\Psi\rangle = \sum_{t_n=1}^{d_n}(\hat{\Psi}_n)_{t_n}|nt_n\rangle$$

- Symmetric operators/matrix

$$[\hat{T},\hat{n}] = 0$$

$$\hat{W}_\varphi \hat{T} \hat{W}_\varphi^\dagger = \hat{T},$$

$$\hat{T} = \bigoplus_n \hat{T}_n$$

Example 1 revisited. In example 1 above, symmetric vectors must be proportional to either $|n = 0, t_0 = 1\rangle$ or $|n = 1, t_1 = 1\rangle$. An invariant operator $\hat{T} = \hat{T}_0 \oplus \hat{T}_1$ is of the form

$$\hat{T} = \begin{pmatrix} \alpha_0 & 0 \\ 0 & \alpha_1 \end{pmatrix}, \quad \alpha_0, \alpha_1 \in \mathbb{C}. \tag{36}$$

Example 2 revisited. In example 2 above, a symmetric vector $|\Psi\rangle$ must be of the form

$$|\Psi\rangle = \begin{pmatrix} \alpha_0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |\Psi\rangle = \begin{pmatrix} 0 \\ \alpha_1 \\ \beta_1 \\ 0 \end{pmatrix}, \quad \text{or} \quad |\Psi\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \alpha_2 \end{pmatrix}, \tag{37}$$

where $\alpha_0, \alpha_1, \beta_1, \alpha_2 \in \mathbb{C}$. An invariant operator $\hat{T} = \hat{T}_0 \oplus \hat{T}_1 \oplus \hat{T}_2$ is of the form

$$\hat{T} = \begin{pmatrix} \alpha_0 & 0 & 0 & 0 \\ 0 & \alpha_1 & \beta_1 & 0 \\ 0 & \gamma_1 & \delta_1 & 0 \\ 0 & 0 & 0 & \alpha_2 \end{pmatrix}, \tag{38}$$

where $\hat{T}_1$ corresponds to the 2×2 central block and $\alpha_0, \alpha_1, \beta_1, \gamma_1, \delta_1, \alpha_2 \in \mathbb{C}$.

Tensor product of two representation

$$\mathbb{V}^{(A)} \cong \bigoplus_{n_A} \mathbb{V}^{(A)}_{n_A}, \quad \mathbb{V}^{(B)} \cong \bigoplus_{n_B} \mathbb{V}^{(B)}_{n_B}$$

- Tensor product $\mathbb{V}^{(AB)} \cong \mathbb{V}^{(A)} \otimes \mathbb{V}^{(B)}$

$$\hat{n}^{(AB)} \equiv \hat{n}^{(A)} \otimes \mathbb{I} + \mathbb{I} \otimes \hat{n}^{(B)} \qquad \hat{W}^{(AB)}_{\varphi} \equiv e^{-\mathrm{i}\hat{n}^{(AB)}\varphi}$$

$$\mathbb{V}^{(AB)} \cong \bigoplus_{n_{AB}} \mathbb{V}^{(AB)}_{n_{AB}}$$

$$\mathbb{V}^{(AB)}_{n_{AB}} \cong \bigoplus_{n_A, n_B|_{n_A+n_B=n_{AB}}} \mathbb{V}^{(A)}_{n_A} \otimes \mathbb{V}^{(B)}_{n_B}$$

Fuse and split

$$|n_A t_{n_A}; n_B t_{n_B}\rangle \equiv |n_A t_{n_A}\rangle \otimes |n_B t_{n_B}\rangle$$

$$|n_{AB} t_{n_{AB}}\rangle = \sum_{n_A t_{n_A} n_B t_{n_B}} \Upsilon^{\text{fuse}}_{n_A t_{n_A}, n_B t_{n_B} \to n_{AB} t_{n_{AB}}} \times \left|n_A t_{n_A}; n_B t_{n_B}\right\rangle.$$

$$\left|n_A t_{n_A}; n_B t_{n_B}\right\rangle = \sum_{n_{AB} t_{n_{AB}}} \Upsilon^{\text{split}}_{n_{AB} t_{n_{AB}} \to n_A t_{n_A}, n_B t_{n_B}} \times \left|n_{AB} t_{n_{AB}}\right\rangle,$$

$$\Upsilon^{\text{split}}_{n_{AB} t_{n_{AB}} \to n_A t_{n_A}, n_B t_{n_B}} = \Upsilon^{\text{fuse}}_{n_A t_{n_A}, n_B t_{n_B} \to n_{AB} t_{n_{AB}}}$$

Example 3. Consider the case where both $\mathbb{V}^{(A)}$ and $\mathbb{V}^{(B)}$ correspond to the space of example 1, that is, $\mathbb{V}^{(A)} \cong \mathbb{V}_0^{(A)} \oplus \mathbb{V}_1^{(A)}$ and $\mathbb{V}^{(B)} \cong \mathbb{V}_0^{(B)} \oplus \mathbb{V}_1^{(B)}$, where $\mathbb{V}_0^{(A)}$, $\mathbb{V}_1^{(A)}$, $\mathbb{V}_0^{(B)}$, and $\mathbb{V}_1^{(B)}$ all have dimension 1. Then $\mathbb{V}^{(AB)}$ corresponds to the space in example 2, namely

$$\begin{aligned} \mathbb{V}^{(AB)} &\cong \mathbb{V}^{(A)} \otimes \mathbb{V}^{(B)} \\ &\cong (\mathbb{V}_0^{(A)} \oplus \mathbb{V}_1^{(A)}) \otimes (\mathbb{V}_0^{(B)} \oplus \mathbb{V}_1^{(B)}) \\ &\cong \mathbb{V}_0^{(AB)} \oplus \mathbb{V}_1^{(AB)} \oplus \mathbb{V}_2^{(AB)}, \end{aligned} \tag{49}$$

where

$$\mathbb{V}_0^{(AB)} \cong \mathbb{V}_0^{(A)} \otimes \mathbb{V}_0^{(B)}, \tag{50}$$

$$\mathbb{V}_1^{(AB)} \cong (\mathbb{V}_0^{(A)} \otimes \mathbb{V}_1^{(B)}) \oplus (\mathbb{V}_1^{(A)} \otimes \mathbb{V}_0^{(B)}), \tag{51}$$

$$\mathbb{V}_2^{(AB)} \cong \mathbb{V}_1^{(A)} \otimes \mathbb{V}_1^{(B)}. \tag{52}$$

The coupled basis $\{|n_{AB} t_{n_{AB}}\rangle\}$ reads

$$\Upsilon^{\text{fuse}}_{01,01\to01} = \Upsilon^{\text{fuse}}_{01,11\to11} = \Upsilon^{\text{fuse}}_{11,01\to12} = \Upsilon^{\text{fuse}}_{11,11\to21} = 1$$

$$\begin{aligned} |n_{AB} = 0, t_0 = 1\rangle &= |n_A = 0, t_0 = 1\rangle \otimes |n_B = 0, t_0 = 1\rangle, \\ |n_{AB} = 1, t_1 = 1\rangle &= |n_A = 0, t_0 = 1\rangle \otimes |n_B = 1, t_1 = 1\rangle, \\ |n_{AB} = 1, t_1 = 2\rangle &= |n_A = 1, t_1 = 1\rangle \otimes |n_B = 0, t_0 = 1\rangle, \\ |n_{AB} = 2, t_2 = 1\rangle &= |n_A = 1, t_1 = 1\rangle \otimes |n_B = 1, t_1 = 1\rangle, \end{aligned} \tag{53}$$

U1 tensor

Let us consider the action of U(1) on the space

$$\mathbb{V}^{[i_1]} \otimes \mathbb{V}^{[i_2]} \otimes \cdots \otimes \mathbb{V}^{[i_k]}$$

given by

$$\hat{X}_{\varphi}^{(1)} \otimes \hat{X}_{\varphi}^{(2)} \otimes \cdots \otimes \hat{X}_{\varphi}^{(k)},$$

where

$$\hat{X}_{\varphi}^{(l)} = \left\{ \begin{array}{lll} \hat{W}_{\varphi}^{(l)*} & \text{if} & i_l \in I, \\ \hat{W}_{\varphi}^{(l)} & \text{if} & i_l \in O. \end{array} \right\}$$

U(1) invariant tensor

$$\sum_{i_1, i_2, \ldots, i_k} \left(\hat{X}_{\varphi}^{(1)}\right)_{i_1' i_1} \left(\hat{X}_{\varphi}^{(2)}\right)_{i_2' i_2} \cdots \left(\hat{X}_{\varphi}^{(k)}\right)_{i_k' i_k} \hat{T}_{i_1 i_2 \cdots i_k} = \hat{T}_{i_1' i_2' \cdots i_k'}$$

Example 4. A U(1)-invariant vector $|\Psi\rangle$—that is, a vector with $\hat{n}|\Psi\rangle = 0$ and components $(\hat{\Psi}_{n=0})_{t_0}$ in the subspace $\mathbb{V}_{n=0}$ which corresponds to vanishing particle number $n = 0$ [cf. Eq. (32)]—fulfills

$$(\hat{\Psi}_{n=0})_{t_0'} = \sum_{t_0} (\hat{W}_\varphi)_{t_0' t_0} (\hat{\Psi}_{n=0})_{t_0}, \quad \forall\, \varphi \in [0,2\pi), \tag{73}$$

in accordance with Eq. (31), as shown in Fig. 9(a).

Example 5. A U(1)-invariant matrix $\hat{T}$ (35) fulfills

$$\hat{T}_{a'b'} = \sum_{a,b} (\hat{W}_\varphi)_{a'a} (\hat{W}^*_\varphi)_{b'b} \hat{T}_{ab} \tag{74}$$

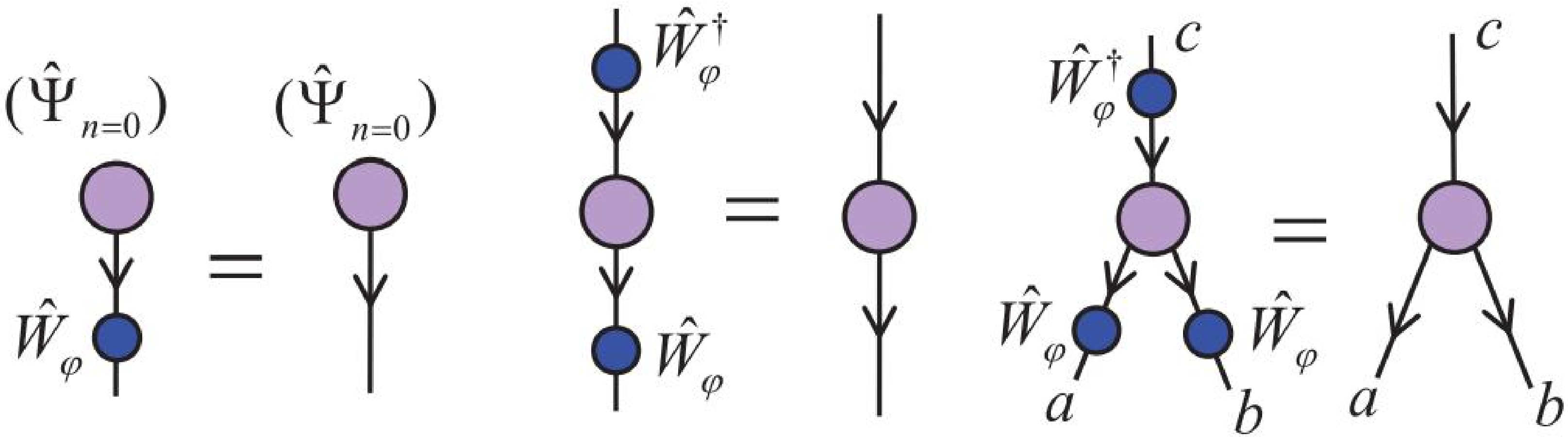
$$= \sum_{a,b} (\hat{W}_\varphi)_{a'a} \hat{T}_{ab} (\hat{W}^\dagger_\varphi)_{bb'}, \quad \forall\, \varphi \in [0,2\pi), \tag{75}$$

Example 6. Tensor $\hat{T}$ in Eq. (16), with components $\hat{T}_{abc}$, where a and b are outgoing indices and c is an incoming index, is U(1) invariant if

$$\hat{T}_{a'b'c'} = \sum_{a,b,c} \left(\hat{W}_{\varphi}^{(1)}\right)_{a'a} \left(\hat{W}_{\varphi}^{(2)}\right)_{b'b} \left(\hat{W}_{\varphi}^{(3)*}\right)_{c'c} \hat{T}_{abc} \tag{76}$$

$$= \sum_{a,b,c} \left(\hat{W}_{\varphi}^{(1)}\right)_{a'a} \left(\hat{W}_{\varphi}^{(2)}\right)_{b'b} \hat{T}_{abc} \left(\hat{W}_{\varphi}^{(3)\dagger}\right)_{cc'} \tag{77}$$

for all $\varphi \in [0, 2\pi)$ [see Fig. 9(c)].



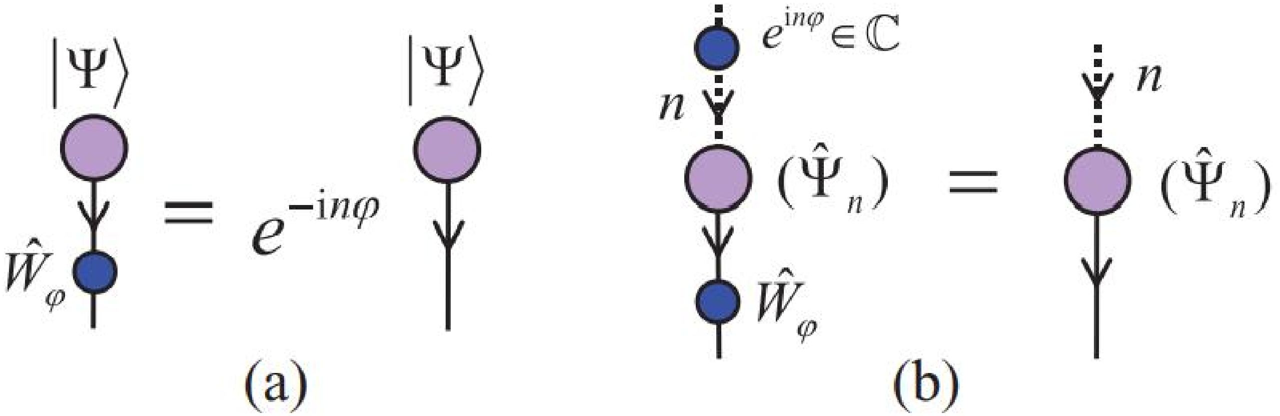
$(\hat{\Psi}_{n=0})$
$\hat{W}_\varphi$
=
$(\hat{\Psi}_{n=0})$
$\hat{W}_\varphi^\dagger$
$\hat{W}_\varphi$
=
c
$\hat{W}_\varphi^\dagger$
$\hat{W}_\varphi$
$\hat{W}_\varphi$
a
b
=
c
a
b

U(1)-covariant and invariant

- U(1)-covariant

$$\sum_{t_n} (\hat{W}_\varphi)_{t_n' t_n} (\hat{\Psi}_n)_{t_n} = e^{-in\varphi} (\hat{\Psi}_n)_{t_n'},$$

$$\hat{T}_{i_1 i_2 \cdots i_k i} \equiv \hat{Q}_{i_1 i_2 \cdots i_k}, \qquad |i| = 1$$



Canonical form for U(1)-invariant tensors

- write a tensor $\hat{T}$ in a particle number basis

$$\hat{T}_{i_1 i_2 \cdots i_k} \equiv \left(\hat{T}_{n_1 n_2 \cdots n_k}\right)_{t_{n_1} t_{n_2} \cdots t_{n_k}}$$

$$N_{\text{in}} \equiv \sum_{n_l \in I} n_l, \quad N_{\text{out}} \equiv \sum_{n_l \in O} n_l$$

$$\hat{T} = \bigoplus_{n_1, n_2, \ldots, n_k} \hat{T}_{n_1 n_2 \cdots n_k} \delta_{N_{\text{in}}, N_{\text{out}}}$$

$$\hat{T}_{i_1 i_2 \cdots i_k} \equiv \left(\hat{T}_{n_1 n_2 \cdots n_k}\right)_{t_{n_1} t_{n_2} \cdots t_{n_k}} \delta_{N_{\text{in}}, N_{\text{out}}}$$

Permutation

- Exchange both particle numbers and tensor

$$\hat{T}_{abc} = \left(\hat{T}_{n_A n_B n_C}\right)_{t_{n_A} t_{n_B} t_{n_C}} \delta_{n_A+n_B,n_C}$$

$$(\hat{T}')_{acb} = \left(\hat{T}'_{n_A n_C n_B}\right)_{t_{n_A} t_{n_C} t_{n_B}} \delta_{n_A+n_B,n_C}$$

$$\left(\hat{T}'_{n_A n_C n_B}\right)_{t_{n_A} t_{n_C} t_{n_B}} = \left(\hat{T}_{n_A n_B n_C}\right)_{t_{n_A} t_{n_B} t_{n_C}}$$

reshape

- Use fuse and split

$$(\hat{T}')_{ad} = \left(\hat{T}'_{n_A n_D}\right)_{t_{n_A} t_{n_D}} \delta_{n_A, n_D}$$

$$\left(\hat{T}'_{n_A n_D}\right)_{t_{n_A} t_{n_D}} = \sum_{n_B, t_{n_B}, n_C, t_{n_C}} \left(\hat{T}_{n_A n_B n_C}\right)_{t_{n_A} t_{n_B} t_{n_C}} \times \Upsilon^{\text{fuse}}_{n_B t_{n_B}, n_C t_{n_C} \to n_D t_{n_D}},$$

Multiplication

$$\hat{R} = \bigoplus_n \hat{R}_n, \quad \hat{S} = \bigoplus_n \hat{S}_n$$

$$\hat{T} = \bigoplus_n \hat{T}_n$$

- each block $\hat{T}_n$ is obtained by multiplying the corresponding blocks $\hat{R}_n$ and $\hat{S}_n$,

$$\hat{T}_n = \hat{R}_n \cdot \hat{S}_n$$

Detail discuss about programing

- Direction or $\pm$ particle number ?
- Distribution of particle number and dimensions