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Tutorial 11 (Quantum numbers and conservation laws in tensor networks)
In Exercise 9.1 we have introduced the concept of a symmetry operator, P. In physics one typically denotes the eigenvalues of P as *quantum numbers*, and it is desirable to work with “symmetric” quantum states (i.e., eigenvectors of P). In case a state ψ is represented as tensor network, like a MPS, it can be possible to enforce such a symmetry on the level of the individual tensors.

To better understand how this works, let us interpret the qubit basis state $|0\rangle$ as “empty state” and $|1\rangle$ as “occupied state” with one particle. For a systems of (possible several) qubits, the overall quantum number is the total particle number. This also applies to a superposition like $\frac{1}{\sqrt{2}}(|101\rangle + |011\rangle)$, as long as each basis state has the same quantum number, 2 in this case.

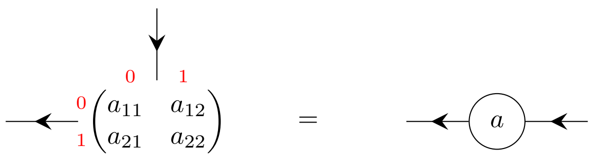
We now define an “annihilation operator” a and its adjoint (conjugate transpose) $a^\dagger$ denoted “creation operator”, which satisfy

$$\begin{aligned} a^\dagger |0\rangle &= |1\rangle\,, \\ a\,|1\rangle &= |0\rangle\,, \\ a^\dagger a\,|1\rangle &= |1\rangle\,. \end{aligned}$$

Application to any other basis state not specified here gives zero. Intuitively, $a^\dagger$ “creates” and a “annihilates” a particle, and $a^\dagger a$ counts the particle number.

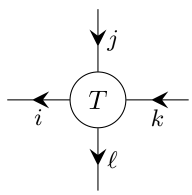
(a) Write down the matrix representation of a and label the columns and rows. Can you notice any relationship between these indices and the particle number?

Graphically, we keep track of the “inflow” and “outflow” of quantum numbers by augmenting tensor legs with arrows, and associating a quantum number with each possible value of an index:



For example, a non-zero entry a_{12} changes the quantum number by -1, from 1 to 0.

(b) Consider the following tensor T of degree 4. How could one impose particle number conservation?



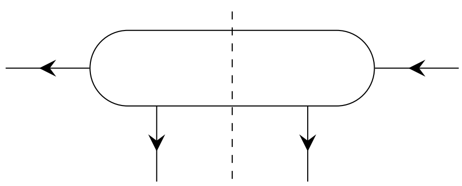
(c) Given a block matrix

$$M = \begin{pmatrix} A & C \\ B & D \end{pmatrix},$$

find a decomposition of M in terms of the SVD of A, B, C and D. Assume now that M is block diagonal and write down the SVD of M.

(d) How could one efficiently compute the SVD of a matrix which is known to conserve a quantum number?

(e) You are given the tensor from the diagram below and are asked to split it via SVD. Knowing that the quantum number represented by the arrows is conserved and making use of part (d), briefly explain an algorithm that is able to do this efficiently.



Solution

(a) If we assume we have the following basis vectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We can write down the corresponding matrix representation of the three operators as

$$a^\dagger = \begin{array}{c c} & \begin{array}{cc} 0 & 1 \end{array} \\ \begin{array}{c} 0 \\ 1 \end{array} & \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{array} \quad , \quad a = \begin{array}{c c} & \begin{array}{cc} 0 & 1 \end{array} \\ \begin{array}{c} 0 \\ 1 \end{array} & \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{array} \quad , \quad a^\dagger a = \begin{array}{c c} & \begin{array}{cc} 0 & 1 \end{array} \\ \begin{array}{c} 0 \\ 1 \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \end{array}.$$

We can see that the column index for the non-zero element is equal to the initial particle number and its row index is the number of remaining particles after the operator application.

(b) We can generalise the concept that an index corresponds to the particle number to higher order tensors. In this case the incoming legs are indexed by j and k. Thus the number of incoming particles is $j+k$. By an analogous argument the number of outgoing particles is given by $i+\ell$. Particle conservation implies

$$j + k = i + \ell.$$

Therefore any tensor element $T_{ijk\ell}$, for which this condition is not fulfilled has to be zero. This can be enshured by including a kronecker delta:

$$T_{ijk\ell} = T_{ijk\ell}\, \delta_{i+\ell, j+k}.$$

(c) For $J \in \{A, B, C, D\}$ we write denote the SVD as

$$J = U_J S_J V_J^\dagger.$$

Therefore

$$\begin{aligned} M &= \begin{pmatrix} U_A S_A V_A^\dagger & U_C S_C V_C^\dagger \\ U_B S_B V_B^\dagger & U_D S_D V_D^\dagger \end{pmatrix} \\ &= \begin{pmatrix} U_A S_A & 0 & U_C S_C & 0 \\ 0 & U_B S_B & 0 & U_D S_D \end{pmatrix} \begin{pmatrix} V_A^\dagger & 0 \\ V_B^\dagger & 0 \\ 0 & V_C^\dagger \\ 0 & V_D^\dagger \end{pmatrix} \qquad = \mathcal{U}\mathcal{S}\mathcal{V}. \\ &= \begin{pmatrix} U_A & 0 & U_C & 0 \\ 0 & U_B & 0 & U_D \end{pmatrix} \operatorname{diag}(S_A, S_B, S_C, S_D) \begin{pmatrix} V_A^\dagger & 0 \\ V_B^\dagger & 0 \\ 0 & V_C^\dagger \\ 0 & V_D^\dagger \end{pmatrix} \end{aligned}$$

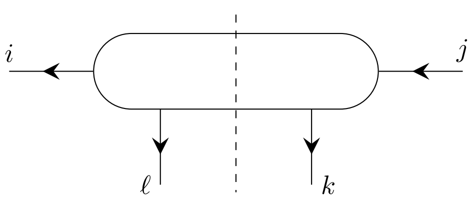
While $\mathcal{S}$ is indeed diagonal, $\mathcal{U}$ is not generally unitary. Therefore this decomposition is not an SVD. However, if we assume M to be block diagonal, i.e., $B = 0$ and $C = 0$, we find that

$$\begin{aligned} M &= \begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix} \\ &= \begin{pmatrix} U_A & 0 \\ 0 & U_D \end{pmatrix} \begin{pmatrix} S_A & 0 \\ 0 & S_D \end{pmatrix} \begin{pmatrix} V_A^\dagger & 0 \\ 0 & V_D^\dagger \end{pmatrix}. \end{aligned}$$

This decomposition is an SVD.

(d) If we know that a matrix M conserves a quantum number, sucvh as particle numbers, we also know that it is very sparse (remember the kronecker delta). By moving rows and columns, we can bring M into a block diagonal form. Then we just have to compute the SVD for each block, which are significantly smaller than M. By permuting rows and columns back, we obtain the SVD of the original M.

(e) First we denote each leg with an index:

$T_j^{ik\ell} =$ 

Note that we can rewrite the conservation condition as

$$T_i^{ik\ell}\,\delta_{i+k+\ell,j} = T_j^{ik\ell}\,\delta_{i+\ell,j-k}.$$

Therefore we reshape T into a matrix

$$T_j^{ik\ell} \longrightarrow M_{(ij),(k\ell)} = M_{(i\ell),(jk)}\,\delta_{i+\ell,j-k}.$$

Now we can proceed the same as in part (d).