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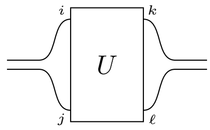
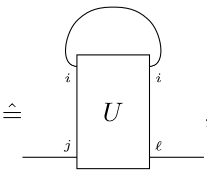
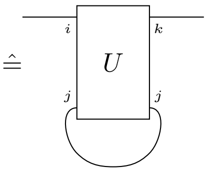
Exercise 5.1 (Partial trace)
Let $U \in \mathbb{C}^{m\times n\times m\times n}$ be a tensor of degree 4, which we can interpret as $mn \times mn$ matrix by combining the first two and last two dimensions:



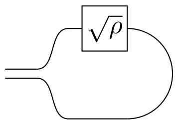
The *partial trace* is defined by "tracing out" (contracting) the subsystem corresponding to the upper two or lower two legs of U:

$$(\mathrm{tr}_1[U])_{j\ell} = \sum_{i=1}^{m} U_{ij,i\ell} \mathrel{\hat{=}}$$  , $$(\mathrm{tr}_2[U])_{ik} = \sum_{j=1}^{n} U_{ij,kj} \mathrel{\hat{=}}$$ 

Note that the partial trace yields a matrix: $\mathrm{tr}_1[U] \in \mathbb{C}^{n\times n}$, $\mathrm{tr}_2[U] \in \mathbb{C}^{m\times m}$.

(a) Show graphically that $\mathrm{tr}_1[A \otimes B] = \mathrm{tr}[A]\, B$ and $\mathrm{tr}_2[A \otimes B] = \mathrm{tr}[B]\, A$ for any square matrices A and B.

(b) Let $\rho \in \mathbb{C}^{n\times n}$ be a Hermitian, positive semidefinite matrix, such that its eigenvalues are non-negative and $\sqrt{\rho}$ is well defined. Let $\psi \in \mathbb{C}^{n^2}$ be the vectorization of $\sqrt{\rho}$:

$$\psi \quad =$$ 

Show that $\mathrm{tr}_2[\psi \circ \psi^*] = \rho$.

Hint: $\psi \circ \psi^*$ plays the role of the above U interpreted as matrix. $\sqrt{\rho}$ inherits the Hermitian property from ρ.

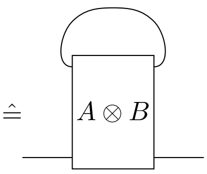
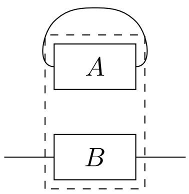
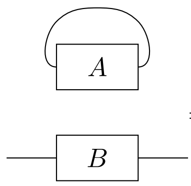
Remark: In terms of quantum mechanics, ρ is a "density matrix" and ψ denoted "purification" of ρ. The outer product $\psi \circ \psi^*$ is written in bra-ket notation as $|\psi\rangle \langle\psi|$.

(c) Conversely, let $\psi \in \mathbb{C}^{n^2}$ be an arbitrary vector. Show that $\mathrm{tr}_2[\psi\circ\psi^*]$ is Hermitian and positive semidefinite.

Hint: Revisit the proof of the SVD from the lecture to verify that $AA^\dagger$ is positive semidefinite for any matrix A.

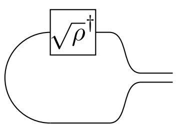
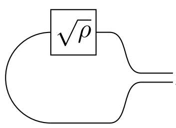
Solution

(a) For two square matrices A and B we can write

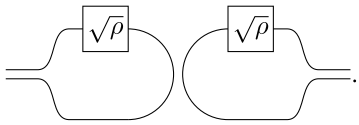
$$\mathrm{tr}_1[A \otimes B] \mathrel{\hat{=}}$$  $=$  $=$  $$\mathrel{\hat{=}} \mathrm{tr}[A]\, B.$$

An analogous proof shows that $\mathrm{tr}_2[A \otimes B] = \mathrm{tr}[B] A$.

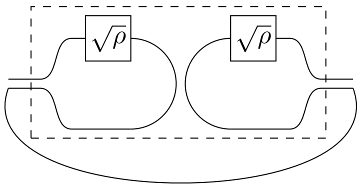
(b) Since ρ is hermitian, we find that

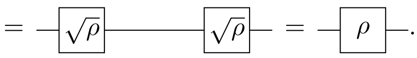
$$\psi^* =$$  $=$  .

Using the graphical depiction of both ψ and ψ^* we write

$\psi \circ \psi^* =$ 

Therefore

$\mathrm{tr}_2 [\psi \circ \psi^*] =$ 



(c) These properties can be shown without the graphical representation.

- *Hermitian*:
$$\mathrm{tr}_2 [\psi \circ \psi^*] = \sum_j \psi_{ij}\psi^*_{kj} = \psi\psi^\dagger = \left(\psi\psi^\dagger\right)^\dagger = \left(\mathrm{tr}_2 [\psi \circ \psi^*]\right)^\dagger .$$
The first equality uses the definition of the parital trace and the third equality uses that for any square matrix A
$$\left(AA^\dagger\right)^\dagger = \left(A^\dagger\right)^\dagger A^\dagger = AA^\dagger .$$

- *Positive semidefinite:*
$$\langle v| \, \mathrm{tr}_2 [\psi \circ \psi^*] \, |v\rangle = \langle v| \, \psi\psi^\dagger \, |v\rangle = \langle \psi^\dagger v | \psi^\dagger v\rangle = || \, |\psi^\dagger v\rangle \, ||^2 \geq 0$$
for all $v \in \mathbb{C}^d$.