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Exercise 12.1 (Schmidt decomposition and entanglement entropy)
As in tutorial 12, let $|\psi\rangle$ be a pure state of a composite system, AB. The Schmidt decomposition of this state is denoted by $|\psi\rangle = \sum_{i=1}^{k} \sigma_i |i_\mathsf{A}\rangle |i_\mathsf{B}\rangle$.

(a) Verify that

$$\langle\psi|\psi\rangle = \sum_{i=1}^{k} \sigma_i^2.$$

In general, the *von Neumann entropy* of a density matrix ρ is defined as

$$\mathcal{S}(\rho) = -\operatorname{tr}[\rho \log(\rho)],$$

with the logarithm interpreted as matrix function, and the convention $0\log(0) = \lim_{x\to 0} x\log(x) = 0$.

In tutorial 12 we found the reduced density matrices of the subsystems, defined as $\rho_1 = \operatorname{tr}_2[|\psi\rangle\langle\psi|]$ and $\rho_2 = \operatorname{tr}_1[|\psi\rangle\langle\psi|]$. We observed that ρ_1 and ρ_2 have the same eigenvalues $(\sigma_i^2)_{i=1,\dots,k}$. The *entanglement entropy* between the two subsystems is then given by

$$\mathcal{S}_\mathsf{ent} = \mathcal{S}(\rho_1) = \mathcal{S}(\rho_2) = -\sum_{i=1}^{k} \sigma_i^2 \log(\sigma_i^2).$$

(You should convince yourself that $\mathcal{S}(\rho_1)$ and $\mathcal{S}(\rho_2)$ are indeed equal to the sum on the right.) Intuitively, the entanglement entropy measures how strongly the subsystems are intertwined.

(b) Which sets of singular values $(\sigma_i)_{i=1,\dots,k}$ minimize and maximize the entanglement entropy, respectively, under the normalization condition $\sum_{i=1}^{k} \sigma_i^2 = 1$? ($k$ should be regarded as fixed.)
Hints: The smallest possible entanglement entropy is zero. Regarding maximization, you can take the normalization condition via a Lagrange multiplier into account.

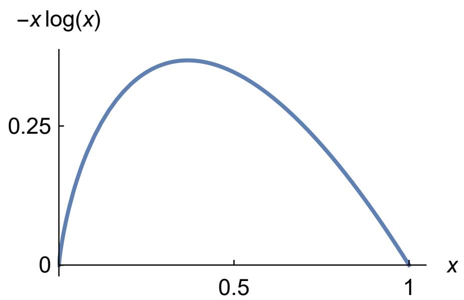
(c) Show that $\mathcal{S}_\mathsf{ent} = 0$ (completely unentangled case) implies that $|\psi\rangle$ can be written as tensor product of a state from subsystem A and one from subsystem B.

Solution

(a) Inserting the Schmidt decomposition of $|\psi\rangle$ directly leads to:

$$\langle\psi|\psi\rangle = \sum_{i,j=1}^{k} \sigma_i \sigma_j \underbrace{\langle i_A|j_A\rangle}_{\delta_{ij}} \underbrace{\langle i_B|j_B\rangle}_{\delta_{ij}} = \sum_i \sigma_i^2.$$

(b) We know that singular values are (in general) real and non-negative. Moreover, due to the normalization condition, $\sigma_i^2 \in [0,1]$ for all i. The following figure visualizes $-x\log(x)$, which is non-negative for any $x \in [0,1]$, and equal to 0 precisely if $x = 0$ or $x = 1$.



By identifying x with σ_i^2, one concludes that the entanglement entropy is non-negative. $\mathcal{S}_\mathsf{ent} = 0$ is reached by setting the first singular values to 1 and the others to 0 (which satisfies the normalization condition).

Regarding maximization of the entanglement entropy, we take the normalization constraint by a Lagrange multiplier $\lambda \in \mathbb{R}$ into account, and abbreviate $\sigma_i^2 = x_i$ for convenience:

$$\mathcal{L}(x_1, \dots, x_k, \lambda) = -\sum_{i=1}^{k} x_i \log(x_i) - \lambda \left(\sum_{i=1}^{k} x_i - 1 \right).$$

Finding an extremum of $\mathcal{L}$ by differentiation w.r.t. x_i, and using that $\log'(x) = \frac{1}{x}$ for $x > 0$, gives

$$0 \stackrel{!}{=} \frac{\partial \mathcal{L}}{\partial x_i} = -\log(x_i) - 1 - \lambda \quad \rightsquigarrow \quad x_i = e^{-1-\lambda}.$$

In particular, all x_i take the same value; combined with the normalization condition, one arrives at $x_i = \frac{1}{k}$ for all $i = 1, \dots, k$. This assignment indeed maximizes $\mathcal{L}$ since $-x \log(x)$ is concave. The corresponding singular values are $\sigma_i = \frac{1}{\sqrt{k}}$ for $i = 1, \dots, k$, and

$$\max_{\sigma_1, \dots, \sigma_k} \mathcal{S}_{\mathsf{ent}} = -\log(1/k) = \log(k).$$

(c) As already mentioned, $\mathcal{S}_{\mathsf{ent}} = 0$ is reached by setting the first singular values to 1 and the others to 0, and this is actually the only case in which $\mathcal{S}_{\mathsf{ent}} = 0$ since $-x \log(x) = 0$ implies $x = 0$ or $x = 1$. In terms of the Schmidt decomposition $|\psi\rangle = \sum_{i=1}^{k} \sigma_i |i_{\mathsf{A}}\rangle |i_{\mathsf{B}}\rangle$, only the first term remains, i.e.,

$$|\psi\rangle = |1_A\rangle |1_B\rangle$$

is a tensor product of two basis states.