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Tutorial 12 (Schmidt decomposition and purifications[1])

(a) Prove the following theorem:

Theorem (**Schmidt decomposition**) Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_\mathsf{A}\rangle_{i=1,\dots,k}$ for system A, and orthonormal states $|i_\mathsf{B}\rangle_{i=1,\dots,k}$ for system B such that

$$|\psi\rangle = \sum_{i=1}^{k} \lambda_i \, |i_\mathsf{A}\rangle \, |i_\mathsf{B}\rangle \,,$$

where λ_i are non-negative real numbers satisfying $\sum_{i=1}^{k} \lambda_i^2 = 1$ known as *Schmidt coefficients*.

(b) Show that, as consequence of the Schmidt decomposition, the deduced density matrices for subsystems A and B have the same eigenvalues if the composite system is in a pure state $|\psi\rangle$.

(c) Given a density operator ρ^A on a quantum system A, construct a pure state $|\psi\rangle$ on an extended quantum system AR such that $\rho^\mathsf{A} = \mathrm{tr}_\mathsf{R}[|\psi\rangle\langle\psi|]$. This procedure is known as *purification*.

Solution

(a) The Schmidt decomposition is basically an application of the *singular value decomposition* of matrices (see also the linear algebra cheat sheet):

Theorem (**Singular value decomposition**) Let $A \in \mathbb{C}^{m\times n}$ be a complex matrix, then there exist unitary matrices $U \in \mathbb{C}^{m\times m}$ and $V \in \mathbb{C}^{n\times n}$ as well as non-negative real numbers $\sigma_1, \dots, \sigma_k$, $k = \min(m, n)$, with $\sigma_1 \geq \dots \geq \sigma_k \geq 0$ (denoted singular values) such that

$$A = U S V^\dagger,$$

where S is the $m \times n$ "diagonal" matrix with diagonal entries $(\sigma_i)_{i=1,\dots,k}$ and zeros otherwise.

Remarks:

- The singular value decomposition also works for real (instead of complex) matrices, in which case U and V are likewise real.
- The singular value decomposition exists for any matrix A, i.e., there are no requirements on A.
- When denoting the column vectors of U by $|u_i\rangle_{i=1,\dots,m}$ such that $U = \big(u_1|u_2|\cdots|u_m\big)$, and the column vectors of V by $|v_i\rangle_{i=1,\dots,n}$ such that $V = \big(v_1|v_2|\cdots|v_n\big)$, then $A = USV^\dagger$ can be written as

$$A = \sum_{i=1}^{k} \sigma_i \, |u_i\rangle \langle v_i| \,.$$

To derive the Schmidt decomposition, let $|a_j\rangle_{j=1,\dots,m}$ and $|b_\ell\rangle_{\ell=1,\dots,n}$ be orthonormal bases for systems A and B, respectively. Then $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_{j=1}^{m} \sum_{\ell=1}^{n} c_{j\ell} \, |a_j\rangle \, |b_\ell\rangle$$

for some complex matrix $C = (c_{j\ell}) \in \mathbb{C}^{m\times n}$. By the singular value decomposition, $C = USV^\dagger$ with U, V, S as described above and the diagonal entries of S the singular values (σ_i). Thus

$$|\psi\rangle = \sum_{i,j,\ell} u_{ji} \, \sigma_i \, v_{\ell i}^* \, |a_j\rangle \, |b_\ell\rangle \,.$$

Defining $|i_\mathsf{A}\rangle = \sum_{j=1}^{m} u_{ji} \, |a_j\rangle$, $|i_\mathsf{B}\rangle = \sum_{\ell=1}^{n} v_{\ell i}^* \, |b_\ell\rangle$ and $\lambda_i = \sigma_i$ for $i = 1, \dots, k$ results in

$$|\psi\rangle = \sum_{i=1}^{k} \lambda_i \, |i_\mathsf{A}\rangle \, |i_\mathsf{B}\rangle \,.$$

Since U and V are unitary and $|a_j\rangle$, $|b_\ell\rangle$ orthonormal bases, the states $|i_\mathsf{A}\rangle$ and $|i_\mathsf{B}\rangle$ are likewise orthonormal. The property $\sum_{i=1}^{k} \lambda_i^2 = 1$ expresses the normalization of $|\psi\rangle$.

[1] M. A. Nielsen, I. L. Chuang: *Quantum Computation and Quantum Information*. Cambridge University Press (2010), Section 2.5

(b) Inserting the Schmidt decomposition into $\rho = |\psi\rangle\langle\psi|$ gives

$$\rho = \sum_{i,j=1}^{k} \lambda_i \, \lambda_j \, |i_{\mathsf{A}}\rangle \, |i_{\mathsf{B}}\rangle \, \langle j_{\mathsf{A}}| \, \langle j_{\mathsf{B}}| \, .$$

The reduced density matrices are then

$$\rho^{\mathsf{A}} = \mathrm{tr}_{\mathsf{B}}[\rho] = \sum_{i,j=1}^{k} \lambda_i \, \lambda_j \, |i_{\mathsf{A}}\rangle \, \langle j_{\mathsf{A}}| \, \underbrace{\langle j_{\mathsf{B}}|i_{\mathsf{B}}\rangle}_{\delta_{ij}} = \sum_{i=1}^{k} \lambda_i^2 \, |i_{\mathsf{A}}\rangle \, \langle i_{\mathsf{A}}| \, ,$$

and analogously

$$\rho^{\mathsf{B}} = \mathrm{tr}_{\mathsf{A}}[\rho] = \sum_{i=1}^{k} \lambda_i^2 \, |i_{\mathsf{B}}\rangle \, \langle i_{\mathsf{B}}| \, .$$

Since $|i_{\mathsf{A}}\rangle$ and $|i_{\mathsf{B}}\rangle$ are orthonormal, we have found the spectral decompositions of ρ^{A} and ρ^{B} with eigenvalues λ_i^2 in both cases.

(c) By the spectral decomposition of ρ^{A}, there exist orthonormal eigenvectors $|\varphi_i\rangle_{i=1,\dots,k}$ and corresponding non-negative eigenvalues p_i such that $\rho^{\mathsf{A}} = \sum_{i=1}^{k} p_i \, |\varphi_i\rangle \, \langle\varphi_i|$, where k denotes the dimension of A. Introduce a system R with the same dimension k and orthonormal basis states $|\chi_i\rangle_{i=1,\dots,k}$, and define the following state on the combined system:

$$|\psi\rangle = \sum_{i=1}^{k} \sqrt{p_i} \, |\varphi_i\rangle \, |\chi_i\rangle \, .$$

As in the calculation in part (b), one obtains

$$\mathrm{tr}_{\mathsf{R}}[|\psi\rangle \, \langle\psi|] = \sum_{i=1}^{k} p_i \, |\varphi_i\rangle \, \langle\varphi_i| = \rho^{\mathsf{A}},$$

as required.