The Schmidt Decomposition

For any pure state $|\psi\rangle$ of a composite system AB, there exist orthonormal bases $\{|i_A\rangle\}$, $\{|i_B\rangle\}$ for subsystems A and B, respectively, such that

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle|i_B\rangle$$

where $\{\lambda_i\}$ are non-negative real numbers such that $\sum_i \lambda^2 = 1$.

Proof. Let

$$|\psi\rangle = \sum_{j,k} c_{jk}|a_j\rangle|b_k\rangle$$

in some basis for the joint system. Assume wlog $C = [c_{j,k}]$ is square. By SVD there exist unitary U, V, and a diagonal non-negative D such that $C = UDV$. Then

$$\begin{aligned} |\psi\rangle &= \sum_{j,k,i} u_{j,i} d_{i,i} v_{i,k} |a_j\rangle|b_k\rangle \\ &= \sum_i \underbrace{d_{i,i}}_{\lambda_i} \underbrace{\left(\sum_j u_{j,i}|a_j\rangle\right)}_{|i_A\rangle} \otimes \underbrace{\left(\sum_k v_{i,k}|b_k\rangle\right)}_{|i_B\rangle} . \end{aligned}$$

A corollary

The densities for subsystems A and B corresponding to a pure state

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle$$

have the form

$$\rho_A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$$

and

$$\rho_B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|,$$

namely, the same matrix form in the Schmidt basis.

Purification

Given a system A in state

$$\rho^A = \sum_{i=1}^{n} p_i |a_i\rangle\langle a_i|$$

where $\{|a_i\rangle\}$ is an orthonormal basis.

Imagine an n-dimensional system B with an arbitrary orthonormal basis $\{|b_i\rangle;\ i = 1, \ldots, n\}$ and consider the state

$$|\psi_{AB}\rangle = \sum_i \sqrt{p_i} |a_i\rangle |b_i\rangle$$

for the joint system AB. It is easy to verify that

$$\rho^A = \mathrm{tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|).$$

So, the mixed state ρ^A can be seen as the reduced state of a pure state $|\psi_{AB}\rangle$ in a larger system.