Schmidt Decomposition

Q1: What is Schmidt decomposition?
A1: It tells you that any *pure* state of a bipartite quantum system (consisting system A and system B) can be expressed by a *single* sum of bi-orthogonal basis.

$$|\psi\rangle = \sum_j \lambda_j |a_j\rangle |b_j\rangle$$

where $\sum_j \lambda_j^2 = 1$, $\langle a_j | a_k \rangle = \langle b_j | b_k \rangle = \delta_{jk}$ and the number of terms is, in general, equal to the size of the smaller system. (For example, if one of them is a two state system, then there is at most two terms, even if it is coupled to an infinite system such as a harmonic oscillator.)

*by convention, λ_j is defined to be real.

Q2: Why Schmidt decomposition?
A: The entanglement between the pure state of A and B can be readily read off from the Schmidt (expansion) coefficients λ_j.

Q3: How does it work?

A3: To show this, we consider the density matrix $\rho = |\psi\rangle\langle\psi|$ and also the reduced density matrix $\rho_A = tr_B \rho$ and $\rho_B = tr_B \rho$. However, I need to invoke a *very* useful property of the trace operator tr (also works for partial trace operator $tr_{A,B}$).

For any outer product $|p\rangle\langle q|$ (which may be considered as a square matrix), to do the trace is just the same as a sum over the diagonal elements in some (complete) basis.

$$tr|p\rangle\langle q| = \sum_j \langle e_j | p \rangle \langle q | e_j \rangle = \sum_j \langle q | e_j \rangle \langle e_j | p \rangle = \langle q | p \rangle$$

In other words, taking the trace in the bra-ket notation is the same as taking the inner product between them.

Now, we consider the Schmidt-decomposed density matrix in Q1,

$$\rho_A = tr_B |\psi\rangle\langle\psi| = \sum_{j,k} \lambda_j \lambda_k |a_j\rangle\langle a_k| \otimes tr_B |b_j\rangle\langle b_k|$$
$$= \sum_j \lambda_j^2 |a_j\rangle\langle a_j|$$

where we used $\langle b_j | b_k \rangle = \delta_{jk}$. Similarly, $\rho_B = \sum_j \lambda_j |b_j\rangle\langle b_j|$. Therefore, ρ_A and ρ_B have the same eigenvalue spectrum. This explains why the number of Schmidt coefficients is determined by the smaller system.

We are now ready to see how the Schmidt decomposition can be used to determine entanglement between systems A and B. Recall that the entropy is defined as

$$E = -tr\rho_A \ln \rho_A = -tr\rho_B \ln \rho_B$$

By diagonalize the density matrices, we have

$$E = -\sum_j \lambda_j^2 \ln \lambda_j^2$$

Note that $E = 0$ (no entanglement) iff $\lambda_j = \{1, 0, 0, ...\}$.

Q4: Now, let us prove the statement in A1? Namely, any pure bipartite state can be decomposed into the Schmidt form.
A4: The most general expression describing two systems in a pure state can be expressed as

$$|\psi\rangle = \sum_{j,k} c_{jk} |\tilde{a}_j\rangle |\tilde{b}_k\rangle$$

where $\langle \tilde{a}_j | \tilde{a}_k \rangle = \langle \tilde{b}_j | \tilde{b}_k \rangle = \delta_{jk}$. Note that the state is a *double* sum and the reduced density matrix is in general not diagonalized $\rho_A = \sum_{j,k,l} c_{jk} c_{lk}^* |a_j\rangle\langle a_l|$.

It is general and perhaps too general to be useful. Recall that we can use any two complete bases $|\tilde{a}_j\rangle |\tilde{b}_k\rangle$ to expand the full state. Why don't we choose the basis that can diagonalize the reduced density matrix? (In fact, our final purpose is to find two such bases) Once, we choose such a basis for system A, it is non-trivial to say another basis for system B can also diagonalize the corresponding reduced density matrix. Perhaps, it is better to illustrate with mathematics:

Step 1: Expanding $\left|\tilde{a}_j\right\rangle = \sum_k \left\langle a_k \middle| \tilde{a}_j \right\rangle \left|a_k\right\rangle \;\Rightarrow\; \left|\psi\right\rangle = \sum_{j,k} \tilde{\lambda}_{jk} \left|a_j\right\rangle \left|\tilde{b}_k\right\rangle$. Note that by definition $\left|a_j\right\rangle$ is a basis which makes $\rho_A = \sum_j \lambda_j^2 \left|a_j\right\rangle\left\langle a_j\right|$ diagonal.

Step 2: Do a trick: grouping, $\left|\psi\right\rangle = \sum_j \left|a_j\right\rangle \left|\beta_j\right\rangle$, where $\left|\beta_j\right\rangle \equiv \sum_k \tilde{\lambda}_{jk} \left|\tilde{b}_k\right\rangle$. With first look, it is not yet trivial that $\left\langle \beta_j \middle| \beta_k \right\rangle \propto \delta_{jk}$.

Step 3: Now we take the trace over system B and have $\rho_A = \sum_{j,k} \left|a_j\right\rangle\left\langle a_k\right| \otimes tr_B \left|\beta_j\right\rangle\left\langle \beta_k\right|$ $= \sum_{j,k} \left\langle \beta_k \middle| \beta_j \right\rangle \left|a_j\right\rangle\left\langle a_k\right|$. However, when we compare this with the one in step 1, we must conclude that $\left\langle \beta_j \middle| \beta_k \right\rangle = \lambda_j^2 \delta_{jk}$. Let us normalize the state and write $\left|\beta_j\right\rangle = \lambda_j^2 \left|b_j\right\rangle$.

This finishes our proof of the statement in A1.

Q5: Given an arbitrary pure state describing two systems, how do I perform the Schmidt decomposition *operationally*?
A5: First, you need to find the reduced density matrix either ρ_A or ρ_B. Then find their eigenvalues λ_j^2 and eigenvectors $\left|a_j\right\rangle$ or $\left|b_j\right\rangle$. The Schmidt form is

$$\left|\psi\right\rangle = \sum_j \lambda_j \left|a_j\right\rangle \left|b_j\right\rangle$$

The entanglement is determined by the eigenvalues only $E = -\sum_j \lambda_j^2 \ln \lambda_j^2$.

Q6: What is the simplest physical example?
A6: Consider a two level system being coupled to any arbitrary system. The reduced density matrix can always be expanded by the set $\left\{\sigma_0, \sigma_x, \sigma_y, \sigma_z\right\}$ with $\sigma_0 \equiv I$. What we need to know is that $\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$ and $tr\sigma_j = 0$. Thus,

$$\rho = \sum_j s_j \sigma_j$$

where $s_j = \frac{1}{2} tr\left(\rho_A \sigma_j\right) = \frac{1}{2}\left\langle \sigma_j \right\rangle$ (why? Since $\left\langle \sigma_j \right\rangle = \sum_k \lambda_k^2 \left\langle a_k \middle| \sigma_j \middle| a_k \right\rangle$) With $s_0 = 1/2$, we can write

$$\rho = \frac{1}{2}\left(1 + \vec{r}\cdot\vec{\sigma}\right)$$

where the vector norm is defined as $\vec{r} = \left\langle \sigma_x \right\rangle \hat{x} + \left\langle \sigma_y \right\rangle \hat{y} + \left\langle \sigma_z \right\rangle \hat{z}$. To find the eigenvalues of it. One can choose a coordinate such that

$$\rho' = \frac{1}{2}\left(1 + r\sigma_z\right)$$

This is diagonal. As $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, finally, $\lambda_{1,2} = \sqrt{\left(1 \pm r\right)/2}$. It is unentangled when $r = 1$ and maximally entangled when $r = 0$.

One may therefore interpret the norm r of the polarization vector as a measure of the amount of information between the two systems.

Q7: Consider the most general bipartite pure state $\left|\psi\right\rangle = a\left|00\right\rangle + b\left|01\right\rangle + c\left|10\right\rangle + d\left|11\right\rangle$, where $\left|a\right|^2 + \left|b\right|^2 + \left|c\right|^2 + \left|d\right|^2 = 1$. Find the conditions when the state is entangled? When is it maximally entangled?

A7. This is left as an exercise.