# The Schmidt Decomposition

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# 1 Abstract

The Schmidt decomposition is a key tool in quantum information that breaks down a bipartite quantum state into a sum of orthogonal product states. This report explains the decomposition, its properties, and its role in dense coding and teleportation. We also explore its broader applications in quantum computing for analyzing entangled states and more complex computations in higher-dimensional order.

# 2 Introduction

### 2.1 Motivation

Our motivation stems from the Week 6 puzzle: "The dense coding protocol allows Alice to communicate 2 bits to Bob by sending one qubit. But can we optimize this further to enable Alice to send 3 bits with just one qubit?" While Professor Giulio provided an insightful conceptual explanation, we sought a more rigorous understanding. This led us to the concept of Schmidt decomposition, marking the beginning of our exploration.

# 2.2 Schmidt Decomposition Derivation

**Lemma 1** (Singular Value Decomposition). An  $m \times n$  complex matrix A can be factorized into the form  $A = U \sum V^{\dagger}$ , where V is the modal matrix of  $A^{\dagger}A$ , U is the modal matrix of  $AA^{\dagger}$ ,  $\sum$  is an  $m \times n$  rectangle diagonal matrix, of which the diagonal entry  $\sigma_i = \sum_{ii} = \sqrt{\lambda_i}$  ( $\sigma_i \in R_{\geq 0}$ ) and  $\lambda_{ii}$  is the corresponding eigenvalue of  $A^{\dagger}A$ .

**Lemma 2.** Lemma 2. can also be expressed as  $A = \sum_{i=0}^{n} \sigma_i u_i v_i^{\dagger}$ , where  $u_i$  and  $v_i$  are the  $i^{th}$  column of U and V, and n denotes min(m,n)

Proof. Let 
$$U = (u_1 \quad u_2 \quad \dots u_m), V = (v_1 \quad v_2 \quad \dots v_n), \text{ where } u_i = \begin{pmatrix} u_{0i} \\ u_{1i} \\ \vdots \\ u_{mi} \end{pmatrix} \text{ and } v_i = \begin{pmatrix} v_{0i} \\ v_{1i} \\ \vdots \\ v_{ni} \end{pmatrix} \text{ is }$$

the  $i^{th}$  column of U and V, and  $m \ge n$ , then

$$A = (u_1 \quad u_2 \quad \dots u_m) \begin{pmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \end{pmatrix} \begin{pmatrix} v_1^{\dagger} \\ v_2^{\dagger} \\ \vdots \\ v_n^{\dagger} \end{pmatrix} = \sum_{i=0}^n \sigma_i u_i v_i^{\dagger}$$

If  $m \leq n$ , then just take  $A^{\dagger}$ , and the situation is the same again.

**Theorem 1.** Let M and N be two Hilbert spaces of dimensions m and n respectively. For any vector  $|\Psi\rangle$  in the tensor space  $M\otimes N$ , there exist orthonormal basis  $\{|u_1\rangle,\ldots,|u_m\rangle\}\subset M$  and  $\{|v_1\rangle,\ldots,|v_n\rangle\}\subset N$ , such that

$$|\Psi\rangle = \sum_{k=0}^{\min(m,n)} \sigma_k |\alpha_k\rangle_M \otimes |\beta_k\rangle_N,$$

where  $\sigma_i$  are real, non-negative numbers.

*Proof.*  $|\Psi\rangle$  can be expressed by computational basis in  $M \otimes N$  as  $|\Psi\rangle = \sum_{i=0}^{m} \sum_{j=0}^{n} a_{ij} |i\rangle_{M} \otimes |j\rangle_{N}$ . Here, we define the coefficient matrix A as

$$A = \begin{pmatrix} a_{00} & a_{01} & \dots & a_{0,n-1} \\ a_{10} & a_{11} & \dots & a_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m-1,0} & a_{m-1,1} & \dots & a_{m-1,n-1} \end{pmatrix} = \sum_{k=0}^{\min(m,n)} \sigma_k \begin{pmatrix} u_{0k} \overline{v_{k0}} & u_{0i} \overline{v_{k1}} & \dots & u_{0k} \overline{v_{k_{n-1}}} \\ u_{1k} \overline{v_{k0}} & u_{1i} \overline{v_{k1}} & \dots & u_{1k} \overline{v_{k_{n-1}}} \\ \vdots & \vdots & \ddots & \vdots \\ u_{m-1,k} \overline{v_{k0}} & u_{m-1,k} \overline{v_{k1}} & \dots & u_{m-1,k} \overline{v_{k_{n-1}}} \end{pmatrix} \stackrel{|0\rangle_M}{\underset{\vdots}{|m\rangle_M}} (1)_{i}^{N}$$

By Lemma 2,  $A = \sum_{k=0}^{\min(m,n)} \sigma_k u_k v_k^{\dagger}$ , let  $|\alpha_i\rangle = \sum_{i=0}^m u_{ik} |i\rangle_M$ ,  $|\beta_j\rangle = \sum_{j=0}^n \overline{v_{kj}} |j\rangle_N$ , where  $u_{ki}$  is the  $i^{th}$  component of column vector  $u_k$ ,  $\overline{v_{kj}}$  is the  $j^{th}$  component of row vector  $v_k^{\dagger}$ .

$$|\Psi\rangle = \sum_{i=0}^{m} \sum_{j=0}^{n} \sum_{k=0}^{\min(m,n)} \sigma_k u_{ik} v_{kj} |i\rangle_M \otimes |j\rangle_N = \sum_{k=0}^{\min(m,n)} \sigma_k |\alpha_k\rangle_M \otimes |\beta_k\rangle_N \tag{2}$$

## 3 Puzzle Discussion

## 3.1 Dense Coding Puzzle

Here is the puzzle.

**Lemma 3.** There are at most n vectors orthogonal to each other in an n-dimensional Hilbert space.

### Solution:

By Lemma 3, in a  $2 \otimes 2$  tensor space, there are at most 4 states orthogonal to each other, so Alice can do at most 4 different operations in her space, which indicates that there are at most 2 bits being transferred.

Generally, let us assume that A is 2-dimensional and B is d-dimensional (d > 2). By Schmidt decomposition, the entangled states  $|\Psi\rangle$  in  $2 \otimes d$  tensor space can be expressed as

$$|\Psi\rangle = \sigma_1|a_1\rangle \otimes |b_1\rangle + \sigma_2|a_2\rangle \otimes |b_2\rangle$$

Here we can see that  $|\Psi\rangle$  is in a  $2\otimes 2$  subspace spanned by  $\{|a_1\rangle, |b_1\rangle, |a_2\rangle, |b_2\rangle\}$ . By implementing operations in only Alice's space, Bob's space remains unchanged, so  $|\Psi\rangle$  is still in the original  $2\otimes 2$  subspace. As a result, Alice can do at most 4 different operations in her space, which indicates that there are at most 2 bits being transferred.

# 3.2 Teleportation Puzzle

Imagine that Alice's qubit Q is entangled with another quantum system, call it R, and the two systems are in some state  $|\Psi\rangle_{RQ}$ . Then, Alice applies the teleportation protocol to system Q (i.e. she performs a Bell measurement on qubit Q and another qubit A, initially in the state  $|\Phi^+\rangle_{AB} = \frac{|0\rangle\otimes|0\rangle+|1\rangle\otimes|1\rangle}{\sqrt{2}}$  with a qubit B in Bob's laboratory, and communicates the outcome of her measurement to Bob). After receiving the information about Alice's measurement outcome, Bob performs the correction operations as in the teleportation protocol. What is the final state of systems B and R?

#### **Solution:**

The initial state of the composite system RQAB is  $|\Psi\rangle_{RQ} \otimes |\Phi^+\rangle_{AB}$ . By Schmidt decomposition,  $|\Psi\rangle_{RQ} = \sigma_1|r_1\rangle \otimes |q_1\rangle + \sigma_2|r_2\rangle \otimes |q_2\rangle$ , where  $\{|r_1\rangle, |r_2\rangle\}$ ,  $\{|q_1\rangle, |q_2\rangle\}$  are ONBs in the system R and Q.

Then, Alice will measure the composite system QA on the Bell basis  $\{\Phi_i, i=0,1,2,3\}$ . Using the steering formula, we can compute the vector

$$\begin{split} |v_{i}\rangle_{RB} &= (I_{R} \otimes \langle \Phi_{i}|_{QA} \otimes I_{B})(|\Psi\rangle_{RQ} \otimes |\Phi^{+}\rangle_{AB}) \\ &= (I_{R} \otimes (\langle \Phi^{+}|_{QA}(U_{i}^{\dagger} \otimes I_{A})) \otimes I_{B})(|\Psi\rangle_{RQ} \otimes |\Phi^{+}\rangle_{AB}) \\ &= (I_{R} \otimes \langle \Phi^{+}|_{QA} \otimes I_{B})(I_{R} \otimes (U_{i}^{\dagger} \otimes I_{A}) \otimes I_{B})(|\Psi\rangle_{RQ} \otimes |\Phi^{+}\rangle_{AB}) \\ &= (I_{R} \otimes \langle \Phi^{+}|_{QA} \otimes I_{B})((I_{R} \otimes U_{i}^{\dagger})|\Psi\rangle_{RQ} \otimes |\Phi^{+}\rangle_{AB}) \\ &= (I_{R} \otimes \langle \Phi^{+}|_{QA} \otimes I_{B})((I_{R} \otimes U_{i}^{\dagger})|\Psi\rangle_{RQ} \otimes |\Phi^{+}\rangle_{AB}) \\ &= (I_{R} \otimes (\frac{\langle 0|_{Q} \otimes \langle 0|_{A} + \langle 1|_{Q} \otimes \langle 1|_{A}}{\sqrt{2}}) \otimes I_{B})((I_{R} \otimes U_{i}^{\dagger})|\Psi\rangle_{RQ} \otimes (\frac{|0\rangle_{A} \otimes |0\rangle_{B} + |1\rangle_{A} \otimes |1\rangle_{B})) \\ &= \frac{1}{2}((I_{R} \otimes \langle 0|_{Q}U_{i}^{\dagger})|\Psi\rangle_{RQ} \otimes |0\rangle_{B} + (I_{R} \otimes \langle 1|_{Q}U_{i}^{\dagger})|\Psi\rangle_{RQ} \otimes |1\rangle_{B}) \\ &= \frac{1}{2}(\sigma_{1}|r_{1}\rangle \otimes \langle 0|U_{i}^{\dagger}|q_{1}\rangle \otimes |0\rangle_{B} + \sigma_{2}|r_{2}\rangle \otimes \langle 0|U_{i}^{\dagger}|q_{2}\rangle \otimes |0\rangle_{B} + \sigma_{1}|r_{1}\rangle \otimes \langle 1|U_{i}^{\dagger}|q_{1}\rangle \otimes |1\rangle_{B} \\ &+ \sigma_{2}|r_{2}\rangle \otimes \langle 1|U_{i}^{\dagger}|q_{2}\rangle \otimes |1\rangle_{B}) \\ &= \frac{1}{2}(\sigma_{1}|r_{1}\rangle \otimes (|0\rangle_{B}\langle 0|U_{i}^{\dagger}|q_{1}\rangle + |1\rangle_{B}\langle 1|U_{i}^{\dagger}|q_{1}\rangle) + \sigma_{2}|r_{2}\rangle \otimes (|0\rangle_{B}\langle 0|U_{i}^{\dagger}|q_{2}\rangle + |1\rangle_{B}\langle 1|U_{i}^{\dagger}|q_{2}\rangle) \\ &= \frac{1}{2}(\sigma_{1}|r_{1}\rangle_{R} \otimes U_{i}^{\dagger}|q_{1}\rangle_{B} + \sigma_{2}|r_{2}\rangle_{R} \otimes U_{i}^{\dagger}|q_{2}\rangle_{B}) \\ &= \frac{1}{2}(I_{R} \otimes U_{i}^{\dagger})(\sigma_{1}|r_{1}\rangle_{R} \otimes |q_{1}\rangle_{B} + \sigma_{2}|r_{2}\rangle_{R} \otimes |q_{2}\rangle_{B}) \\ &= \frac{1}{2}(I_{R} \otimes U_{i}^{\dagger})(\Psi)_{RB} \end{split}$$

We are done.

The probability that Alice get outcome i is  $p_A(i) = |||v_i\rangle||^2 = \frac{1}{4}$ , and the state of the composite system RB is  $|\psi_i\rangle = \frac{|v_i\rangle}{|||v_i\rangle||} = (I_R \otimes U_i^{\dagger})|\Psi\rangle_{RB}$ .

After Bob performs the gate  $U_i$  to his qubit, then the state in the composite system RB is the same as the entangled state  $|\Psi\rangle_{RQ}$ .

# 4 Analyzing Entangled States

The Schmidt decomposition can also be applied in determining a bipartite quantum state is entangled or separable. For any pure state  $|\psi\rangle_{AB}$  of a composite system AB, the Schmidt decomposition takes the form:

$$|\psi\rangle_{AB} = \sum_{i=1}^{r} \sigma_i |a_i\rangle \otimes |b_i\rangle$$

where  $\{|a_i\rangle\}$  and  $\{|b_i\rangle\}$  form orthonormal bases for subsystems A and B respectively,  $\sigma_i > 0$ , and  $\sum_i \sigma_i^2 = 1$ , and r is the Schmidt rank.

# 4.1 Entanglement Detection

**Theorem 2.**  $|\psi\rangle$  is separable if and only if its Schmidt rank r=1. If the state  $|\psi\rangle$  is entangled, its Schmidt rank r>1 and its number of non-zero Schmidt coefficients measuring its entanglement dimensionality.

*Proof.* We prove both directions of the equivalence:

If  $|\psi\rangle$  is separable, it can be written as  $|\psi\rangle_{AB} = |\phi\rangle_A \otimes |\chi\rangle_B$ . This has Schmidt form with r=1. If r=1: the decomposition reduces to  $|\psi\rangle_{AB} = \sigma_1 |\phi\rangle_A \otimes |\chi\rangle_B$  with  $\sigma_1 = 1$ , which is a product state.

Example: Consider the Bell state  $|\Phi^{+}\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle)$ . Its Schmidt decomposition implies that the Schmidt coefficients for  $|\Phi^{+}\rangle$  are  $\sigma_{1} = \sigma_{2} = 1/\sqrt{2}$ , and the Schmidt rank is r = 2.

In conclusion, for the state with  $r \geq 2$ , because it cannot be decomposed into fewer than r product terms, it is r-dimensionally entangled.

# 5 Higher order Schmidt decomposition

From the above section, we learn that the Schmidt decomposition allows any bipartite pure state  $|\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  to be written as  $|\phi\rangle = \sum_{i=1}^r \sigma_i |a_i\rangle \otimes |b_i\rangle$ . However, for multipartite systems (e.g.,  $|\phi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$ ), can we also define a generalized Schmidt decomposition for them?

## 5.1 Difficulties for higher order Schmidt decomposition

Consider there is a n-partite system, each system distributes d-dimensional space. Then, their pure state  $|\phi\rangle$  is in a  $d^n$ -dimensional space, and depends on  $2d^n$  real parameters. (including real part and imaginary part)

The n-partite systems with d-dimensional subsystems can be shown as:

$$|\phi\rangle = \sum_{i=1}^{d} \sigma_i |\gamma_i^1\rangle_d \otimes |\gamma_i^2\rangle_d \otimes \dots \otimes |\gamma_i^n\rangle_d, \tag{3}$$

where  $\{\gamma_i^j\}_{i=0}^{d-1}$  is the orthonormal basis in  $j^{th}$  subsystem. For each  $\{\gamma_i^j\}_{i=0}^{d-1}$ , there are d vectors with size  $d \times 1$ , and there are n subspaces, so in total there are  $2nd^2$  real parameters. (including real part and imaginary part) The tensor of orthogonal basis  $\{\{\gamma_i^j\}_{i=0}^{d-1}\}_{j=1}^n$  is insufficient to fully constrain the state into a Schmidt-like decomposed form when n > 2. Thus, a generalized

Schmidt decomposition does not always exist for arbitrary pure states in n-partite systems (n > 2) with d-dimensional subsystems. This result shows the unlikeliness of solving the high-order Schmidt decomposition in general.

# 5.2 Review on Bipartite Schmidt Decomposition

For a pure state  $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ , the Schmidt decomposition is:

$$|\psi\rangle = \sum_{i=1}^{r} \sigma_i |u_i\rangle_A \otimes |v_i\rangle_B$$

where  $\sigma_i > 0$  are Schmidt coefficients, and  $\{|u_i\rangle\}, \{|v_i\rangle\}$  are orthonormal bases.

**Lemma 4.** For Schmidt decomposition in  $\mathcal{H}_A \otimes \mathcal{H}_B$ , if there are some Schmidt coefficients  $\sigma_{m_1} = \sigma_{m_2} = \dots \sigma_{m_k} = \sigma$ , then the corresponding Schmidt vector in  $\mathcal{H}_A$  and  $\mathcal{H}_B$  can be a linear combination of  $\{|u_{m_1}\rangle, |u_{m_2}\rangle, \dots, |u_{m_k}\rangle\}$  and  $\{|v_{m_1}\rangle, |v_{m_2}\rangle, \dots, |v_{m_k}\rangle\}$ . We stimulate the linear transformation by applying an orthonormal gate  $Q = (|\alpha_1\rangle |\alpha_2\rangle \dots |\alpha_k\rangle)$  and  $Q' = \bar{Q}$  on these two set of eigenvectors, where  $\{|\alpha_i\rangle\}_{i=1}^k$  is an ONB of dimension k.

*Proof.* According to Lemma.2, after operation, new SVD will be  $A = (U \sum Q)(Q^{\dagger}V^{\dagger}) = (U\sigma IQ)(Q'^TV^{\dagger}) = \sigma(UQ)(Q'^TV^{\dagger})$ , so new Schmidt vectors will be:

$$|\tilde{u}_i\rangle = \sum_{j=1}^k Q_{ij}|u_j\rangle, \ |\tilde{v}_i\rangle = \sum_{j=1}^k Q'_{ij}|v_j\rangle.$$

The state  $|\phi\rangle$  is unchanged because:

$$\sum_{i=1}^{k} |\tilde{u}_{i}\rangle \otimes |\tilde{v}_{i}\rangle = \sum_{j,l} (\sum_{i} Q_{ij} Q'_{il}) |u_{j}\rangle \otimes |v_{l}\rangle = \sum_{j,l} \langle \alpha_{j} |\alpha_{l}\rangle |u_{j}\rangle \otimes |v_{l}\rangle = \sum_{j,l} \delta_{jl} |u_{j}\rangle \otimes |v_{l}\rangle = \sum_{j} |u_{j}\rangle \otimes |v_{j}\rangle.$$

If all  $\sigma_i$  are distinct, the bases are unique up to global phases.

If some  $\sigma_i$  are equal, then the corresponding Schmidt vectors can be unitarily transformed as follows.

Suppose  $\sigma_{m_1} = \sigma_{m_2} = \ldots = \sigma_{m_k} = \sigma_{(m)}$  (a degenerate subset). Then, the state can be written as:

$$|\phi\rangle = \sigma_{(m)} \sum_{i=1}^{k} |u_i\rangle \otimes |v_i\rangle + \{\text{other terms}\}$$

The sum  $\sum_{i=1}^{k} |u_i\rangle \otimes |v_i\rangle$  is invariant under joint unitary transform of  $\{|u_i\rangle\}$  and  $\{|v_i\rangle\}$ , because the coefficient  $\sigma_{(m)}$  are identical.

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### 5.3 Tripartite/Multipartite Generalization

We now consider a tripartite state situation.

Given a pure state  $|\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ , it follows a triple Schmidt decomposition if it can be written in:

$$|\phi\rangle = \sum_{\mu=1}^{r} \sigma_{\mu} |u_{\mu}\rangle_{A} \otimes |v_{\mu}\rangle_{B} \otimes |w_{\mu}\rangle_{C}$$

where  $\{|u_{\mu}\rangle\},\{|v_{\mu}\rangle\}$  and  $\{|w_{\mu}\rangle\}$  are three orthonormal bases in  $\mathcal{H}_A,\mathcal{H}_B,\,\mathcal{H}_C$  respectively.

We take the bipartite form with partitioning A and BC:

$$|\phi\rangle = \sum_{\mu} \sigma_{\mu} |\gamma_{\mu}\rangle_A \otimes |\omega_{\mu}\rangle_{BC},$$

where  $\{|\gamma_{\mu}\rangle\}$  is orthonormal basis in  $\mathcal{H}_{\mathcal{A}}$ ,  $\{|\omega_{\mu}\rangle\}$  is orthonormal basis in  $\mathcal{H}_{\mathcal{B}}\otimes\mathcal{H}_{\mathcal{C}}$ , and  $|\omega_{\mu}\rangle$  can be expressed by computational basis  $\{|b\rangle\}$  in  $\mathcal{H}_{\mathcal{B}}$  and  $\{|c\rangle\}$  in  $\mathcal{H}_{\mathcal{C}}$ :

$$\forall \mu, \ |\omega_{\mu}\rangle = \sum_{b} \sum_{c} [\Omega_{\mu}]_{bc} |b\rangle_{B} \otimes |c\rangle_{C}$$

and  $\Omega_{\mu}$  are coefficient matrices of  $|\omega_{\mu}\rangle$ .

If all  $\sigma_{\mu}$  are distinct, the decomposition is unique (up to global phases).

*Proof.* If all  $\sigma_{\mu}$  are distinct, then the eigenvalues of  $A^{\dagger}A$  and  $AA^{\dagger}$  are distinct, then their corresponding eigenvectors are unique because, with no equal eigenvalues, the linear combination of eigenvectors no longer satisfies the condition  $Uv = \lambda v$ , so the decomposition is unique and one  $\sigma_{\mu}$  corresponds to one  $|\gamma_{\mu}\rangle_{A} \otimes |\omega_{\mu}\rangle_{BC}$ .

Then the following conditions should be satisfied:

1. Each  $\omega_{\mu}$  is a product state in  $\mathcal{H}_{\mathcal{B}} \otimes \mathcal{H}_{\mathcal{C}}$ , so the corresponding  $\Omega_{\mu}$  is of rank 1.

*Proof.* We prove this by contraposition and contradiction. If there exists at least one  $|\omega_{\mu}\rangle$  that is entangled, then  $\sum_{\mu} \sigma_{\mu} |\gamma_{\mu}\rangle_{A} \otimes |\omega_{\mu}\rangle_{BC} \neq \sum_{\mu=1}^{r} \sigma_{\mu} |u_{\mu}\rangle_{A} \otimes |v_{\mu}\rangle_{B} \otimes |w_{\mu}\rangle_{C}$ . Here we assume that

$$\sum_{\mu} \sigma_{\mu} |\gamma_{\mu}\rangle_{A} \otimes |\omega_{\mu}\rangle_{BC} = \sum_{\mu=1}^{r} \sigma_{\mu} |u_{\mu}\rangle_{A} \otimes |v_{\mu}\rangle_{B} \otimes |w_{\mu}\rangle_{C}$$
(4)

First, since the decomposition is unique, then  $|\gamma_{\mu}\rangle = |u_{\mu}\rangle$ . We multiply  $\langle u_{\mu}|$  on both sides of Eq.4 and get

$$\sigma_{\mu}|\omega_{\mu}\rangle_{BC} = \sigma_{\mu}|v_{\mu}\rangle_{B} \otimes |w_{\mu}\rangle_{C},$$

which contradicts the condition that at least one entangled  $\omega_{\mu}$ .

2. To ensure orthogonality,  $\langle \omega_{\mu} | \omega_{\nu} \rangle = 0$ . Since  $\langle \omega_{\mu} | \omega_{\nu} \rangle = \text{Tr}(\Omega_{\mu}^{\dagger} \Omega_{\nu})$  (Eq.1), we have  $\Omega_{\mu}^{\dagger} \Omega_{\nu} = 0$  for  $\mu \neq \nu$ .

If there are k coefficients  $\sigma_{\mu_1} = \sigma_{\mu_2} = \ldots = \sigma_{\mu_k} = \sigma$  are equal, then it is more complicated, and the following conditions should be satisfied:

1. Each  $\Omega_{\mu_i}$  can be expressed as a linear combination of rank 1 matrix  $\{\Omega'_j\}_{j=1}^m$  and  $\Omega'^{\dagger}_{\mu}\Omega'_{\nu}=0$  for  $\mu \neq \nu$  and  $m = \max_{\mu_i} (\operatorname{rank}(\Omega_{\mu_i}))$ .

*Proof.* Let  $U \in U(k)$  be a unitary matrix acting on the degenerate subspace of  $\{|\gamma_{\mu_i}\rangle\}$ . The corresponding  $\{|\omega_{\mu_i}\rangle\}$  transform as:

$$|\tilde{\omega}_{j}\rangle = \sum_{i=1}^{k} \overline{U_{ji}} |\omega_{\mu_{i}}\rangle, j = 1, \dots, k,$$

this won't change the property of Schmidt decomposition.

If  $|\tilde{\omega}_j\rangle$  are product states, then by transformation we can directly replace  $|\omega_{\mu}\rangle$  with  $|\tilde{\omega}_{\mu}\rangle$  and

$$\begin{split} |\phi\rangle &= \sum_{\mu \in \{\mu_1, \mu_2, \dots, \mu_m\}} \sigma_{\mu} |\gamma_{\mu}\rangle_A \otimes |\tilde{\omega}_{\mu}\rangle_{BC} + \{\text{other terms}\} \\ &= \sum_{\mu \in \{\mu_1, \mu_2, \dots, \mu_m\}} \sigma_{\mu} |u_{\mu}\rangle_A \otimes |v_{\mu}\rangle_B \otimes |w_{\mu}\rangle_C + \{\text{other terms}\} \end{split}$$

Otherwise, if we cannot find any unitary gate to transform  $\{|\omega_{\mu}\rangle\}$  into a set of product states  $\{|\tilde{\omega}_{j}\rangle\}$ , then there is no solution.

$$\tilde{\Omega}_j = \sum_{i=1}^k \overline{U_{ji}} \Omega_{\mu_i}.$$

The new matrices  $\tilde{\Omega}_j$  are linear combinations of the original  $\Omega_{\mu_i}$ 

2. Each  $\Omega_{\mu_i}$  is of rank not exceeding k, and the  $\Omega_{\mu_i}$  must be linearly independent in matrix space because all  $|\omega_{\mu}\rangle$  are orthogonal to each other.

**Lemma 5** (subadditive of rank).  $rank(A+B) \leq rank(A) + rank(B)$ 

*Proof.* We can prove this by contradiction. If  $\{\Omega_j\}_{j=1}^k$  are of rank bigger than k, then by Lemma5, it is impossible to transform  $\{\Omega_j\}_{j=1}^k$  into k rank 1 matrix with only a linear combination of size k.

To generalize the Schmidt decomposition to N-partite systems, we can recursively split the full system into two subsets and treat each subset as a new system, until it is a bipartite or tripartite system, and then follow the steps above.

The problem is done.

## 6 Conclusion

This study explored the Schmidt decomposition's derivation, its applications in quantum puzzles like dense coding and teleportation, and entanglement analysis. While effective for bipartite systems, we also analyze its limitations in multipartite generalizations. The results provide a clear boundary for the applicability of Schmidt decomposition techniques in quantum computation.

# 7 Reference

- 1. Nielsen, M. A. and Chuang, I. L. Quantum Computation and Quantum Information, 10th Anniversary Edition. Cambridge University Press (2010).
- 2. Peres, A., 1995, Phys. Lett. A 202, 16.
- 3. Strang, G. (2016). Introduction to linear algebra (5th ed.). Wellesley-Cambridge Press.