Schmidt Decomposition

Quantum Foundations · Module 4 — Entanglement

Node 4.3

Position in Knowledge Graph

System: Quantum Foundations **Structural Domain:** Entanglement **Node:** 4.3

The Schmidt decomposition is the canonical form of a bipartite pure state. It says that any $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, no matter how complicated its expression in a generic product basis, can be brought into a diagonal sum

$$|\Psi\rangle = \sum_i \lambda_i |i_A\rangle \otimes |i_B\rangle$$

by suitable local choices of orthonormal bases. Structurally, this is the singular value decomposition (SVD) wearing physics notation. Operationally, it is the single most useful tool for analysing the entanglement of bipartite pure states: every entanglement quantity that depends only on local degrees of freedom is a function of the **Schmidt coefficients** $\{\lambda_i\}$.

Formal Statement

Theorem (Schmidt decomposition). Let $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ be a pure bipartite state, with $\dim \mathcal{H}_A = d_A$ and $\dim \mathcal{H}_B = d_B$. Then there exist:

- orthonormal vectors $\{|i_A\rangle\}_{i=1}^r \subset \mathcal{H}_A$,
- orthonormal vectors $\{|i_B\rangle\}_{i=1}^r \subset \mathcal{H}_B$,
- strictly positive real numbers $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0$,

such that

$$|\Psi\rangle = \sum_{i=1}^r \lambda_i \, |i_A\rangle \otimes |i_B\rangle, \qquad \sum_{i=1}^r \lambda_i^2 = 1.$$

The integer $r \leq \min(d_A, d_B)$ is the **Schmidt rank** of $|\Psi\rangle$. The numbers λ_i are the **Schmidt coefficients**, and the sets $\{|i_A\rangle\}, \{|i_B\rangle\}$ are the **Schmidt bases** for the respective sides.

The decomposition is unique up to:

- reordering of equal-magnitude Schmidt coefficients,
- relative phases between paired $(|i_A\rangle, |i_B\rangle)$ compensating each other.

Corollary. $|\Psi\rangle$ is a product state $\iff$ Schmidt rank $r = 1$. In that case the single Schmidt coefficient is $\lambda_1 = 1$.

Corollary. A bipartite pure state is **maximally entangled** when all Schmidt coefficients are equal: $\lambda_i = 1/\sqrt{r}$ for $i = 1, \ldots, r$, with $r = \min(d_A, d_B)$.

Intuition

A generic bipartite pure state, written in a product basis $\{|i\rangle_A \otimes |j\rangle_B\}$, has a coefficient matrix C_{ij} with no particular structure — it can have many nonzero entries, and there is no obvious way to read off "how entangled" the state is from its coefficients.

The Schmidt decomposition is the statement that you can always *rotate the bases on each side independently* — that is, perform local unitaries $U_A \otimes U_B$ — to bring C into diagonal form. The number of nonzero diagonal entries (the rank of C) is then a basis-invariant feature of the state, called the Schmidt rank, and the diagonal entries themselves capture everything there is to say about local entanglement structure.

The diagonal form is exactly the SVD of the coefficient matrix $C = U\Lambda V^\dagger$, with U and V the local unitary changes of basis on A and B, and Λ the diagonal matrix of singular values.

The key intuition: **entanglement is a property of how a bipartite state distributes its amplitude across product directions**, and the Schmidt decomposition is the canonical view in which that distribution is laid out cleanly. A state with one nonzero Schmidt coefficient is a product. A state with all Schmidt coefficients equal is maximally entangled. Everything in between interpolates monotonically.

Structural Role

The Schmidt decomposition organizes essentially every other concept in pure-state entanglement theory:

- **Schmidt rank as entanglement classifier.** Schmidt rank 1 = product = separable. Schmidt rank > 1 = entangled. The maximum possible Schmidt rank is $\min(d_A, d_B)$, achieved by maximally entangled states.
- **Reduced density operators are Schmidt-diagonal.** Tracing out B gives $\rho_A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$, with eigenvalues equal to the squared Schmidt coefficients. The reduced state on A is automatically diagonal in the Schmidt basis. The same holds for ρ_B.
- **Entanglement entropy (Node 4.5).** $S(\rho_A) = -\sum_i \lambda_i^2 \log \lambda_i^2$. This is the canonical entanglement measure for pure states, and it is *symmetric* in A and B: $S(\rho_A) = S(\rho_B)$, since both reduced states share the same Schmidt spectrum.
- **Local unitary equivalence.** Two pure bipartite states are related by a local unitary $U_A \otimes U_B$ if and only if they have the same Schmidt coefficients. The Schmidt spectrum is a complete invariant for the local unitary orbit of pure bipartite states.
- **Purification (Node 5.2).** Every mixed state ρ_A on $\mathcal{H}_A$ is the reduced state of a pure state on $\mathcal{H}_A \otimes \mathcal{H}_B$ (its "purification"). Schmidt decomposition makes this construction immediate: take $|\Psi\rangle = \sum_i \sqrt{p_i}|i\rangle_A \otimes |i\rangle_B$ where $\rho_A = \sum_i p_i |i\rangle\langle i|$.

Mathematical Development

Proof via SVD

Choose any orthonormal product basis $\{|i\rangle_A \otimes |j\rangle_B\}$ of $\mathcal{H}_A \otimes \mathcal{H}_B$. Write

$$|\Psi\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} C_{ij}\, |i\rangle_A \otimes |j\rangle_B.$$

The coefficients C_{ij} form a complex $d_A \times d_B$ matrix C. Apply the singular value decomposition:

$$C = U\Sigma V^\dagger,$$

where $U \in U(d_A)$, $V \in U(d_B)$, and Σ is a $d_A \times d_B$ "diagonal" matrix with non-negative real entries σ_i on the diagonal (zero elsewhere). The number of nonzero σ_i is $r := \operatorname{rank} C$.

Substitute back:

$$|\Psi\rangle = \sum_{i,j} \sum_k U_{ik} \sigma_k (V^\dagger)_{kj} \, |i\rangle_A \otimes |j\rangle_B = \sum_{k=1}^{r} \sigma_k \left(\sum_i U_{ik} |i\rangle_A \right) \otimes \left(\sum_j V^*_{jk} |j\rangle_B \right).$$

Define

$$|k_A\rangle := \sum_i U_{ik} |i\rangle_A, \qquad |k_B\rangle := \sum_j V^*_{jk} |j\rangle_B, \qquad \lambda_k := \sigma_k.$$

Then

$$|\Psi\rangle = \sum_{k=1}^{r} \lambda_k \, |k_A\rangle \otimes |k_B\rangle.$$

Since U and V are unitary, $\{|k_A\rangle\}_k$ and $\{|k_B\rangle\}_k$ are orthonormal. Normalization $\langle \Psi | \Psi \rangle = 1$ is equivalent to $\sum_k \lambda_k^2 = 1$ (sum of squared singular values = Frobenius norm squared = 1). ∎

Schmidt rank is basis-independent

The Schmidt rank is the rank of any matrix representation of the coefficients, which is invariant under left and right unitary multiplication. So replacing the original product basis by any other orthonormal product basis leaves the Schmidt rank unchanged. This is the structural reason Schmidt rank is a meaningful entanglement classifier.

Reduced density operators

Trace out B from $|\Psi\rangle\langle\Psi|$:

$$\rho_A = \operatorname{Tr}_B \left(\sum_{i,j} \lambda_i \lambda_j |i_A\rangle\langle j_A| \otimes |i_B\rangle\langle j_B| \right) = \sum_{i,j} \lambda_i \lambda_j \, |i_A\rangle\langle j_A| \, \langle j_B | i_B \rangle = \sum_i \lambda_i^2 \, |i_A\rangle\langle i_A|,$$

using orthonormality of $\{|i_B\rangle\}$. The reduced state is diagonal in the Schmidt basis with eigenvalues λ_i^2. By the same calculation $\rho_B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|$, so

$$\operatorname{spec}(\rho_A) = \operatorname{spec}(\rho_B) \quad \text{(up to padding with zeros).}$$

This is a structural fact peculiar to *pure* bipartite states: the two marginals have identical nonzero spectra. It fails badly for tripartite or mixed states.

Local unitary equivalence

If $|\Psi\rangle$ and $|\Psi'\rangle$ have the same Schmidt coefficients, they differ by a local unitary: pick U_A sending the Schmidt basis of $|\Psi\rangle$ on A to that of $|\Psi'\rangle$, and similarly U_B. Then $(U_A \otimes U_B)|\Psi\rangle = |\Psi'\rangle$. Conversely, local unitaries preserve Schmidt coefficients, since $U_A \otimes U_B$ acts on the coefficient matrix as $C \mapsto U_A C U_B^T$, and SVD is invariant under left/right unitary multiplication.

The maximally entangled state

A state of the form

$$|\Phi\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle_A \otimes |i\rangle_B, \qquad d = \min(d_A, d_B),$$

has all Schmidt coefficients equal to $1/\sqrt{d}$, Schmidt rank d, and reduced state $\rho_A = I_d/d$ (maximally mixed). It is the unique (up to local unitaries) state with this property and is the canonical "Bell pair" generalization to dimension d.

Worked Example

Schmidt decomposition of the Bell states

The four Bell states on two qubits:

$$|\Phi^{\pm}\rangle = \tfrac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \qquad |\Psi^{\pm}\rangle = \tfrac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle).$$

For $|\Phi^+\rangle$ the coefficient matrix in the computational product basis is $C = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, already diagonal with singular values $(1/\sqrt{2}, 1/\sqrt{2})$. The Schmidt decomposition is the same as the original expression: Schmidt rank 2, equal Schmidt coefficients $1/\sqrt{2}$, maximally entangled. The reduced state on either side is $\rho_A = \rho_B = I/2$.

For $|\Phi^-\rangle$, $C = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The SVD is $C = U\Sigma V^\dagger$ with $U = I$, $\Sigma = \frac{1}{\sqrt{2}}I$, $V^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. The Schmidt bases are: $|1_A\rangle = |0\rangle, |2_A\rangle = |1\rangle$, $|1_B\rangle = |0\rangle, |2_B\rangle = -|1\rangle$. The decomposition becomes

$$|\Phi^-\rangle = \tfrac{1}{\sqrt{2}}\big(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes (-|1\rangle_B)\big),$$

with both Schmidt coefficients $1/\sqrt{2}$. The minus sign has been absorbed into the local basis on B — it disappears from the *coefficients*, illustrating that the Schmidt spectrum is local-unitary invariant.

For $|\Psi^+\rangle$ the coefficient matrix is $C = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, the Pauli X matrix scaled by $1/\sqrt{2}$. Its SVD has singular values $(1/\sqrt{2}, 1/\sqrt{2})$. Schmidt rank 2, equal coefficients, maximally entangled.

Conclusion. All four Bell states are maximally entangled with identical Schmidt spectra $(1/\sqrt{2}, 1/\sqrt{2})$. They differ only by local unitaries on Bob's side: $|\Psi^+\rangle = (I \otimes X)|\Phi^+\rangle$, $|\Psi^-\rangle = (I \otimes XZ)|\Phi^+\rangle$, $|\Phi^-\rangle = (I \otimes Z)|\Phi^+\rangle$. The Schmidt decomposition cannot distinguish them, because as far as local entanglement structure goes they are the same state.

A non-maximally entangled example

Consider $|\Psi\rangle = \sqrt{0.9}\,|00\rangle + \sqrt{0.1}\,|11\rangle$. The coefficient matrix is $\mathrm{diag}(\sqrt{0.9}, \sqrt{0.1})$, already in Schmidt form with coefficients $(\sqrt{0.9}, \sqrt{0.1})$. The reduced state is $\rho_A = 0.9|0\rangle\langle 0| + 0.1|1\rangle\langle 1|$, a strongly biased mixture. Entanglement entropy:

$$S(\rho_A) = -0.9 \log_2 0.9 - 0.1 \log_2 0.1 \approx 0.469 \text{ bits}.$$

Compare with the Bell state's 1 bit. The state is "less entangled" in the precise sense that its Schmidt spectrum is more concentrated.

A non-trivial example requiring the SVD

$$|\Psi\rangle = \tfrac{1}{2}|00\rangle + \tfrac{1}{2}|01\rangle + \tfrac{1}{2}|10\rangle - \tfrac{1}{2}|11\rangle.$$

The coefficient matrix is $C = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} = \frac{1}{\sqrt{2}}H$, where H is the Hadamard. The SVD: H is unitary (in fact $H^\dagger H = I$), so the singular values of $H/\sqrt{2}$ are both $1/\sqrt{2}$. The Schmidt decomposition has rank 2 with coefficients $(1/\sqrt{2}, 1/\sqrt{2})$ — this state is also maximally entangled, despite looking quite different from the Bell states. The Schmidt bases on each side are the eigenvectors of $C^\dagger C$ and $CC^\dagger$; for this example they turn out to be $\{|+\rangle, |-\rangle\}$ up to phases. Explicitly:

$$|\Psi\rangle = \tfrac{1}{\sqrt{2}}\big(|+\rangle_A|+\rangle_B + |-\rangle_A|-\rangle_B\big),$$

a Bell state in the Hadamard basis.

Cross-Links

- **Linear Algebra:** The singular value decomposition. Schmidt decomposition = SVD with the matrix indices interpreted as bipartite labels.
- **Statistics:** Low-rank matrix factorization, principal component analysis. The Schmidt rank is the algebraic rank of the bipartite coefficient matrix; PCA picks out the same singular structure for data matrices.
- **Module 4.5 (Entanglement measures):** Entanglement entropy and all related monotones for pure states are functions of the Schmidt coefficients alone.
- **Module 5.2 (Reduced density operators):** Tracing out one subsystem of a pure bipartite state always yields a state diagonal in the Schmidt basis with Schmidt-squared eigenvalues. Purification reverses this construction.
- **Module 7.4 (Quantum teleportation):** The teleportation protocol exploits the Schmidt structure of Bell states — every qubit state can be moved across by local Bell-basis operations.

Structural Compression

Invariant: Every bipartite pure state has a unique-up-to-rotation list of Schmidt coefficients $\{\lambda_i\}$, which is its complete local-unitary invariant.

Mechanism: SVD of the coefficient matrix C_{ij} of $|\Psi\rangle$ in any product basis. The singular values are the Schmidt coefficients; the left/right singular vectors define the Schmidt bases on A and B.

Cross-System Echo: The same algebraic operation appears as PCA in statistics, low-rank approximation in numerical analysis, and latent factor models in machine learning. In quantum mechanics it acquires a structural interpretation as the canonical form of bipartite entanglement: the singular spectrum *is* the entanglement spectrum.

Exercises

1. Compute the Schmidt decomposition of $|\Psi\rangle = \frac{1}{\sqrt{3}}|00\rangle + \frac{1}{\sqrt{3}}|01\rangle + \frac{1}{\sqrt{3}}|10\rangle$. What is its Schmidt rank?
2. Show that for a pure bipartite state, the Schmidt rank equals the rank of ρ_A (and equally of ρ_B).
3. Verify that all four Bell states have the same Schmidt spectrum $(1/\sqrt{2}, 1/\sqrt{2})$, and find local unitaries connecting them to $|\Phi^+\rangle$.
4. Prove that a pure bipartite state $|\Psi\rangle$ is a product state if and only if its reduced density operator ρ_A is pure.

5. Given a mixed state $\rho_A = \sum_i p_i |i\rangle\langle i|$ on $\mathcal{H}_A$, construct an explicit purification $|\Psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ with $\rho_A = \mathrm{Tr}_B\, |\Psi\rangle\langle\Psi|$. What is the minimum dimension of $\mathcal{H}_B$?
6. For $|\Psi\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$, show that the maximum value of the entanglement entropy $S(\rho_A)$ is $\log d$, achieved exactly by maximally entangled states.
7. Argue, structurally, why the Schmidt decomposition cannot be straightforwardly generalized to tripartite pure states. (Hint: try to diagonalize a three-index tensor by local unitaries and see what goes wrong.)

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Concepts: eigenvalue-decomposition, tensor-product, entanglement
Prerequisites: 4.1, 1.6
Enables: 4.5, 5.2

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