Uniqueness of Purification

Formal statement

Let ρ(A) be a density operator on a finite-dimensional Hilbert space mathcal H(A). Suppose

$$|\psi\rangle_{AR} \in \mathcal{H}_A \otimes \mathcal{H}_R$$

and

$$|\phi\rangle_{AS} \in \mathcal{H}_A \otimes \mathcal{H}_S$$

are two purifications of the same state ρ(A). This means

$$\mathrm{Tr}_R(|\psi\rangle\langle\psi|_{AR}) = \rho_A = \mathrm{Tr}_S(|\phi\rangle\langle\phi|_{AS}).$$

Then the two purifications differ only by an isometry acting on the purifying system. More precisely, there exists a partial isometry

$$V : \mathcal{H}_R \to \mathcal{H}_S$$

whose initial space is the support of the reduced state of R and whose final space is the support of the reduced state of S, such that

$$|\phi\rangle_{AS} = (I_A \otimes V)|\psi\rangle_{AR}.$$

If dim mathcal H(S)≥ dim mathcal H(R), and the unused dimensions are included appropriately, V can be extended to an isometry from all of mathcal H(R) into mathcal H(S). If mathcal H(R) and mathcal H(S) have the same dimension, then the isometry can be extended to a unitary operator on the purifying system.

This is the precise version of the common statement: any two purifications of the same density operator are the same up to a reversible change of coordinates on the reference system.

Why the support condition is necessary

The phrase “differ by an isometry on the purifying system” is correct, but it hides a small technical detail. The two purifying systems may have different dimensions. For example, a rank-two qubit state may be purified using a two-dimensional reference system, but it may also be purified using a larger three-dimensional or ten-dimensional reference system with some unused dimensions. A full isometry from a larger Hilbert space into a smaller one may not exist. What always exists is an isometry between the subspaces that actually participate in the purification.

The participating subspace is the support of the reduced density operator of the purifying system. If a reference dimension is never occupied by the purification, it is irrelevant. The uniqueness theorem says that the occupied part of one reference system can be isometrically identified with the occupied part of the other reference system.

In the most common quantum-information setting, one chooses purifying systems of the same dimension. Then the theorem becomes especially simple:

$$|\phi\rangle_{AR} = (I_A \otimes U_R)|\psi\rangle_{AR}$$

for some unitary U_R on the reference system.

Proof by Schmidt decomposition

We prove the theorem in finite dimensions. Since $|\psi\rangle_{AR}$ is a purification of ρ_A, it is a pure bipartite state across the cut A:R. Therefore it has a Schmidt decomposition. Because tracing out R gives ρ_A, the Schmidt probabilities must be the nonzero eigenvalues of ρ_A, and the A-side Schmidt vectors must be eigenvectors of ρ_A, up to unitary rotations inside degenerate eigenspaces.

Let the spectral decomposition of ρ_A be

$$\rho_A = \sum_{i=1}^{r} \lambda_i |i\rangle\langle i|_A,$$

where

$$\lambda_i > 0, \qquad \sum_{i=1}^{r} \lambda_i = 1,$$

and r=rank(ρ_{A}). For simplicity of notation, first assume the eigenbasis \$|i\rangle_{A}$\ has been chosen once and for all, including a particular orthonormal basis inside each degenerate eigenspace.

Since $|\psi\rangle_{AR}$ purifies ρ_{A}, it can be written as

$$|\psi\rangle_{AR} = \sum_{i=1}^{r} \sqrt{\lambda_i}\, |i\rangle_A |r_i\rangle_R,$$

where \$|r_i\rangle_{R}$\$_{i=1}^{r}$ is an orthonormal set in mathcal H_{R}. Similarly, since $|\varphi\rangle_{AS}$ also purifies ρ_{A}, it can be written as

$$|\phi\rangle_{AS} = \sum_{i=1}^{r} \sqrt{\lambda_i}\, |i\rangle_A |s_i\rangle_S,$$

where \$|s_i\rangle_{S}$\$_{i=1}^{r}$ is an orthonormal set in mathcal H_{S}.

Now define a linear map V on the occupied part of mathcal H_{R} by

$$V|r_i\rangle_R = |s_i\rangle_S$$

for every i=1,...,r, and extend it linearly. Because both \$|r_i\rangle_{R}$\ and \$|s_i\rangle_{S}$\ are orthonormal sets, this map preserves inner products on the span of the $|r_i\rangle_{R}$'s. Therefore V is an isometry from

$$\mathrm{span}\{|r_1\rangle_R, \ldots, |r_r\rangle_R\}$$

onto

$$\mathrm{span}\{|s_1\rangle_S, \ldots, |s_r\rangle_S\}.$$

Applying $I_{A}\otimes$ V to $|\psi\rangle_{AR}$, we obtain

$$\begin{aligned}(I_A \otimes V)|\psi\rangle_{AR} &= \sum_{i=1}^{r} \sqrt{\lambda_i}\,|i\rangle_A V|r_i\rangle_R \\ &= \sum_{i=1}^{r} \sqrt{\lambda_i}\,|i\rangle_A|s_i\rangle_S \\ &= |\phi\rangle_{AS}.\end{aligned}$$

Thus the two purifications differ only by an isometry acting on the purifying system.

The assumption that we chose the same eigenbasis of $\rho_{(A)}$ is harmless. If $\rho_{(A)}$ has degenerate eigenspaces, different Schmidt decompositions may use different bases inside those degenerate subspaces. But those basis changes can be absorbed into a corresponding unitary mixing of the reference vectors inside the same degenerate sector. The conclusion remains the same: all freedom in the purification can be pushed to the purifying system.

This proves the theorem.

Operational meaning

The purification theorem says that every mixed state can be seen as part of a larger pure state. The uniqueness of purification says that this larger pure state is essentially unique, provided we do not care how the inaccessible reference system is labelled.

This is a powerful idea. Suppose an observer only has access to system A. The state they see is $\rho_{(A)}$. There may be many possible purifications of $\rho_{(A)}$, for example

$$|\psi\rangle_{AR}$$

or

$$|\phi\rangle_{AS}.$$

At first this looks like a serious ambiguity. Are these different physical explanations of the same mixed state? The uniqueness theorem says that, from the viewpoint of A, the ambiguity is only in the reference system. The same local state $\rho_{(A)}$ fixes the entanglement spectrum, the Schmidt coefficients, and the support dimension. What remains unfixed is only how the purifying degrees of freedom are named, rotated, embedded, or represented.

The mental image is this. A purification is like a perfect record system that explains the mixedness of A. The uniqueness theorem says that two perfect record systems for the same $\rho_{(A)}$ contain the same information, up to a change of coordinates on the record system. If one purification stores the label i as $|r_i\rangle_{(R)}$, and another stores the same label as $|s_i\rangle_{(S)}$, then an isometry maps one encoding of the record into the other.

Thus, the reference system has gauge freedom. It is not part of the observed system. We may rotate it, relabel it, or embed it in a larger space without changing anything measurable on A.

Example 1: two Bell-state purifications of the maximally mixed qubit

Let

$$\rho_A = \frac{I}{2}.$$

One purification is

$$|\Phi^+\rangle_{AR} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}.$$

Another purification is

$$|\Phi^-\rangle_{AR} = \frac{|00\rangle - |11\rangle}{\sqrt{2}}.$$

Both reduce to I/2 on system A. The two purifications differ only by a unitary on the reference qubit:

$$|\Phi^-\rangle_{AR} = (I_A \otimes Z_R)|\Phi^+\rangle_{AR},$$

because

$$Z|0\rangle = |0\rangle, \qquad Z|1\rangle = -|1\rangle.$$

Operationally, the relative sign between |00⟩ and |11⟩ is invisible if we only inspect A. The sign lives in the phase convention of the purifying system.

Example 2: changing the reference basis

Again take

$$\rho_A = \frac{I}{2}.$$

The Bell purification can be written as

$$|\Phi^+\rangle_{AR} = \frac{|0\rangle_A|0\rangle_R + |1\rangle_A|1\rangle_R}{\sqrt{2}}.$$

Now define the reference basis

$$|+\rangle_R = \frac{|0\rangle_R + |1\rangle_R}{\sqrt{2}}, \qquad |-\rangle_R = \frac{|0\rangle_R - |1\rangle_R}{\sqrt{2}}.$$

A different purification may use |+⟩₍R₎ and |-⟩₍R₎ as the reference labels:

$$|\chi\rangle_{AR} = \frac{|0\rangle_A|+\rangle_R + |1\rangle_A|-\rangle_R}{\sqrt{2}}.$$

This is also a purification of I/2. It differs from |Φ⁺⟩ by the Hadamard unitary on the reference:

$$|\chi\rangle_{AR} = (I_A \otimes H_R)|\Phi^+\rangle_{AR}.$$

Here the purification has not changed the local physics of A. It has only changed the coordinate system in which the reference stores its perfectly correlated label.

Example 3: a nonmaximally mixed qubit

Consider

$$\rho_A = 0.9|0\rangle\langle 0| + 0.1|1\rangle\langle 1|.$$

A natural purification is

$$|\psi\rangle_{AR} = \sqrt{0.9}|0\rangle_A|0\rangle_R + \sqrt{0.1}|1\rangle_A|1\rangle_R.$$

Another purification is

$$|\phi\rangle_{AS} = \sqrt{0.9}|0\rangle_A|\alpha\rangle_S + \sqrt{0.1}|1\rangle_A|\beta\rangle_S,$$

where $|\alpha\rangle_{(S)}$ and $|\beta\rangle_{(S)}$ are any two orthonormal states of S. The uniqueness theorem says that there is an isometry V satisfying

$$V|0\rangle_R = |\alpha\rangle_S, \qquad V|1\rangle_R = |\beta\rangle_S.$$

Therefore

$$|\phi\rangle_{AS} = (I_A \otimes V)|\psi\rangle_{AR}.$$

This example shows that the unequal Schmidt weights 0.9 and 0.1 are not arbitrary. They are fixed by $\rho_{(A)}$. What can change is the way the reference system encodes the two labels.

Example 4: larger purifying systems and unused dimensions

Let

$$\rho_A = \frac{I}{2}.$$

A minimal purification uses a two-dimensional reference:

$$|\psi\rangle_{AR} = \frac{|0\rangle_A|0\rangle_R + |1\rangle_A|1\rangle_R}{\sqrt{2}}.$$

But we may also purify the same state using a qutrit reference S:

$$|\phi\rangle_{AS} = \frac{|0\rangle_A|0\rangle_S + |1\rangle_A|2\rangle_S}{\sqrt{2}}.$$

The state |1⟩₍S₎ of the qutrit is unused. The isometry from R to S can be defined by

$$V|0\rangle_R = |0\rangle_S, \qquad V|1\rangle_R = |2\rangle_S.$$

Then

$$|\phi\rangle_{AS} = (I_A \otimes V)|\psi\rangle_{AR}.$$

This example explains why the theorem is naturally stated using isometries rather than only unitaries. A unitary maps a Hilbert space to another Hilbert space of the same dimension. An isometry can embed a smaller reference into a larger one.

Example 5: ensemble decompositions as measurements on the reference

The maximally mixed qubit has many ensemble decompositions:

$$\frac{I}{2} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

and also

$$\frac{I}{2} = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -|.$$

These two decompositions can be generated from the same purification by measuring the reference in different bases. Start with

$$|\Phi^+\rangle_{AR} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}.$$

If the reference is measured in the computational basis, system A is conditionally prepared in $|0\rangle$ or $|1\rangle$. If the reference is measured in the X-basis, system A is conditionally prepared in $|+\rangle$ or $|-\rangle$, up to known phase conventions depending on the Bell state used.

This is closely related to the Hughston-Jozsa-Wootters theorem, which classifies all ensemble decompositions of a given density operator. The uniqueness of purification is the pure-state backbone behind that classification.

Why the theorem is useful

The uniqueness of purification appears repeatedly in quantum information because it allows us to replace an unknown purification by a convenient one. If a proof only concerns system A, then it cannot depend on the particular basis chosen for the reference. Any two choices are related by an isometry on the reference, and the reference is not directly observed.

This idea is central in Uhlmann's theorem. The fidelity between two mixed states can be characterized by maximizing the overlap between their purifications. The reason this maximization is well behaved is exactly that all purifications of a fixed state are related by reference-system isometries or unitaries. Thus one may fix one purification and optimize only over a unitary or isometry on the purifying system.

It also appears in channel theory. Stinespring dilation says that a quantum channel can be represented by a unitary interaction with an environment followed by discarding that environment. The uniqueness part of Stinespring's theorem has the same flavor: minimal dilations of the same channel are unique up to a unitary on the environment. Purification uniqueness is the corresponding statement for states.

Common mistakes

A common mistake is to say that two purifications are equal. They are usually not equal as vectors in the larger Hilbert space. They become equivalent only after we allow an isometry or unitary on the purifying system.

A second mistake is to demand a unitary when the purifying systems have different dimensions. If one purification uses a two-dimensional reference and another uses a three-dimensional reference, a unitary between the full spaces does not exist. The correct map is an isometry from the smaller occupied reference space into the larger one, or more generally a partial isometry between the occupied support subspaces.

A third mistake is to think that freedom on the reference system changes $\rho_{(A)}$. It does not. If

$$|\phi\rangle_{AR} = (I_A \otimes U_R)|\psi\rangle_{AR},$$

then

$$\mathrm{Tr}_R(|\phi\rangle\langle\phi|) = \mathrm{Tr}_R(|\psi\rangle\langle\psi|).$$

The unitary on R disappears under the partial trace.

Final mental image

A purification explains the mixedness of A by imagining that A is entangled with a reference system. The uniqueness theorem says that the explanation is unique up to how the reference system stores its labels. The eigenvalues of $\rho_{(A)}$ fix the Schmidt weights. The support of $\rho_{(A)}$ fixes how many reference labels are needed. But the names, basis vectors, phases, and embeddings of those reference labels are arbitrary.

So the theorem can be remembered in one sentence:

$$\text{same mixed state on } A \quad \Longrightarrow \quad \text{same purification up to reference-system isomet}$$

This is why purification is not merely a representation trick. It is a stable representation trick. Once we purify $\rho_{(A)}$, we are free to choose the most convenient reference system, because every other valid choice differs only by an operation on the part we will trace out.

References

Nielsen, Michael A., and Isaac L. Chuang. Quantum Computation and Quantum Information. Cambridge University Press, 10th anniversary edition, 2010. See the discussion of Schmidt decomposition, purification, and the freedom in purifying systems.

Preskill, John. Lecture Notes for Physics 229: Quantum Information and Computation. See the chapters on entanglement and quantum information theory, where purification and Schmidt decompositions are used as standard tools.

Watrous, John. The Theory of Quantum Information. Cambridge University Press, 2018. See the early chapters on density operators, Schmidt decompositions, purifications, and isometric freedom of purifying spaces.

Wilde, Mark M. Quantum Information Theory. Cambridge University Press, 2nd edition, 2017. See the treatment of purifications, fidelity, and Uhlmann’s theorem.

Uhlmann, Armin. “The ‘transition probability’ in the state space of a -algebra.” Reports on Mathematical Physics 9, no. 2 (1976): 273–279.

Hughston, Lane P., Richard Jozsa, and William K. Wootters. “A complete classification of quantum ensembles having a given density matrix.” Physics Letters A 183 (1993): 14–18.

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