2.5 The Schmidt decomposition and purifications

Density operators and the partial trace are just the beginning of a wide array of tools useful for the study of composite quantum systems, which are at the heart of quantum computation and quantum information. Two additional tools of great value are the *Schmidt decomposition* and *purifications*. In this section we present both these tools, and try to give the flavor of their power.

Theorem 2.7: **(Schmidt decomposition)** Suppose $|\psi\rangle$ is a pure state of a composite system, AB. Then there exist orthonormal states $|i_A\rangle$ for system A, and orthonormal states $|i_B\rangle$ of system B such that

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle|i_B\rangle, \tag{2.202}$$

where λ_i are non-negative real numbers satisfying $\sum_i \lambda_i^2 = 1$ known as *Schmidt co-efficients*.

This result is very useful. As a taste of its power, consider the following consequence: let $|\psi\rangle$ be a pure state of a composite system, AB. Then by the Schmidt decomposition $\rho^A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$ and $\rho^B = \sum_i \lambda_i^2 |i_B\rangle\langle i_B|$, so the eigenvalues of ρ^A and ρ^B are identical, namely λ_i^2 for both density operators. Many important properties of quantum systems are completely determined by the eigenvalues of the reduced density operator of the system, so for a pure state of a composite system such properties will be the same for both systems. As an example, consider the state of two qubits, $(|00\rangle + |01\rangle + |11\rangle)/\sqrt{3}$. This has no obvious symmetry property, yet if you calculate $\operatorname{tr}\left((\rho^A)^2\right)$ and $\operatorname{tr}\left((\rho^B)^2\right)$ you will discover that they have the same value, $7/9$ in each case. This is but one small consequence of the Schmidt decomposition.

Proof

We give the proof for the case where systems A and B have state spaces of the same dimension, and leave the general case to Exercise 2.76. Let $|j\rangle$ and $|k\rangle$ be any fixed orthonormal bases for systems A and B, respectively. Then $|\psi\rangle$ can be written

$$|\psi\rangle = \sum_{jk} a_{jk}|j\rangle|k\rangle, \tag{2.203}$$

for some matrix a of complex numbers a_{jk}. By the singular value decomposition, $a = udv$, where d is a diagonal matrix with non-negative elements, and u and v are unitary matrices. Thus

$$|\psi\rangle = \sum_{ijk} u_{ji} d_{ii} v_{ik} |j\rangle|k\rangle. \tag{2.204}$$

Defining $|i_A\rangle \equiv \sum_j u_{ji}|j\rangle$, $|i_B\rangle \equiv \sum_k v_{ik}|k\rangle$, and $\lambda_i \equiv d_{ii}$, we see that this gives

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle|i_B\rangle. \tag{2.205}$$

It is easy to check that $|i_A\rangle$ forms an orthonormal set, from the unitarity of u and the orthonormality of $|j\rangle$, and similarly that the $|i_B\rangle$ form an orthonormal set. $\square$

Exercise 2.76: Extend the proof of the Schmidt decomposition to the case where A and B may have state spaces of different dimensionality.

Exercise 2.77: Suppose ABC is a three component quantum system. Show by example that there are quantum states $|\psi\rangle$ of such systems which can not be written in the form

$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle |i_C\rangle, \tag{2.206}$$

where λ_i are real numbers, and $|i_A\rangle, |i_B\rangle, |i_C\rangle$ are orthonormal bases of the respective systems.

The bases $|i_A\rangle$ and $|i_B\rangle$ are called the *Schmidt bases* for A and B, respectively, and the number of non-zero values λ_i is called the *Schmidt number* for the state $|\psi\rangle$. The Schmidt number is an important property of a composite quantum system, which in some sense quantifies the 'amount' of entanglement between systems A and B. To get some idea of why this is the case, consider the following obvious but important property: the Schmidt number is preserved under unitary transformations on system A or system B alone. To see this, notice that if $\sum_i \lambda_i |i_A\rangle |i_B\rangle$ is the Schmidt decomposition for $|\psi\rangle$ then $\sum_i \lambda_i (U|i_A\rangle)|i_B\rangle$ is the Schmidt decomposition for $U|\psi\rangle$, where U is a unitary operator acting on system A alone. Algebraic invariance properties of this type make the Schmidt number a very useful tool.

Exercise 2.78: Prove that a state $|\psi\rangle$ of a composite system AB is a product state if and only if it has Schmidt number 1. Prove that $|\psi\rangle$ is a product state if and only if ρ^A (and thus ρ^B) are pure states.

A second, related technique for quantum computation and quantum information is *purification*. Suppose we are given a state ρ^A of a quantum system A. It is possible to introduce another system, which we denote R, and *define* a *pure state* $|AR\rangle$ for the joint system AR such that $\rho^A = \mathrm{tr}_R(|AR\rangle\langle AR|)$. That is, the pure state $|AR\rangle$ reduces to ρ^A when we look at system A alone. This is a purely mathematical procedure, known as *purification*, which allows us to associate pure states with mixed states. For this reason we call system R a *reference* system: it is a fictitious system, without a direct physical significance.

To prove that purification can be done for *any* state, we explain how to construct a system R and purification $|AR\rangle$ for ρ^A. Suppose ρ^A has orthonormal decomposition $\rho^A = \sum_i p_i |i^A\rangle\langle i^A|$. To purify ρ^A we introduce a system R which has the same state space as system A, with orthonormal basis states $|i^R\rangle$, and define a pure state for the combined system

$$|AR\rangle \equiv \sum_i \sqrt{p_i} |i^A\rangle |i^R\rangle. \tag{2.207}$$

We now calculate the reduced density operator for system A corresponding to the state $|AR\rangle$:

$$\mathrm{tr}_R(|AR\rangle\langle AR|) = \sum_{ij} \sqrt{p_i p_j} |i^A\rangle\langle j^A| \, \mathrm{tr}(|i^R\rangle\langle j^R|) \tag{2.208}$$

$$= \sum_{ij} \sqrt{p_i p_j} |i^A\rangle\langle j^A| \, \delta_{ij} \tag{2.209}$$

$$= \sum_i p_i |i^A\rangle\langle i^A| \tag{2.210}$$

$$= \rho^A. \tag{2.211}$$

Thus $|AR\rangle$ is a purification of ρ^A.

Notice the close relationship of the Schmidt decomposition to purification: the procedure used to purify a mixed state of system A is to define a pure state whose Schmidt basis for system A is just the basis in which the mixed state is diagonal, with the Schmidt coefficients being the square root of the eigenvalues of the density operator being purified.

In this section we've explained two tools for studying composite quantum systems, the Schmidt decomposition and purifications. These tools will be indispensable to the study of quantum computation and quantum information, especially quantum information, which is the subject of Part III of this book.

Exercise 2.79: Consider a composite system consisting of two qubits. Find the Schmidt decompositions of the states

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}; \quad \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2}; \text{ and } \quad \frac{|00\rangle + |01\rangle + |10\rangle}{\sqrt{3}}. \tag{2.212}$$

Exercise 2.80: Suppose $|\psi\rangle$ and $|\varphi\rangle$ are two pure states of a composite quantum system with components A and B, with identical Schmidt coefficients. Show that there are unitary transformations U on system A and V on system B such that $|\psi\rangle = (U \otimes V)|\varphi\rangle$.

Exercise 2.81: (Freedom in purifications) Let $|AR_1\rangle$ and $|AR_2\rangle$ be two purifications of a state ρ^A to a composite system AR. Prove that there exists a unitary transformation U_R acting on system R such that $|AR_1\rangle = (I_A \otimes U_R)|AR_2\rangle$.

Exercise 2.82: Suppose $\{p_i, |\psi_i\rangle\}$ is an ensemble of states generating a density matrix $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ for a quantum system A. Introduce a system R with orthonormal basis $|i\rangle$.

(1) Show that $\sum_i \sqrt{p_i}|\psi_i\rangle|i\rangle$ is a purification of ρ.

(2) Suppose we measure R in the basis $|i\rangle$, obtaining outcome i. With what probability do we obtain the result i, and what is the corresponding state of system A?

(3) Let $|AR\rangle$ be *any* purification of ρ to the system AR. Show that there exists an orthonormal basis $|i\rangle$ in which R can be measured such that the corresponding post-measurement state for system A is $|\psi_i\rangle$ with probability p_i.

2.6 EPR and the Bell inequality

Anybody who is not shocked by quantum theory has not understood it.
– Niels Bohr