

# Chapter 2

## Quantum Theory

### 2.1 Quantum States

In quantum mechanics, any physical system is completely described by a state vector  $|\Psi\rangle$  in a Hilbert space  $\mathcal{H}$ . A system with a two-dimensional Hilbert space is also called a *qubit* (quantum bit). If not otherwise stated, we consider a Hilbert space with an arbitrary but finite dimension. For two parties, Alice ( $A$ ) and Bob ( $B$ ), with Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$  the total Hilbert space is a tensor product of the subsystem spaces:  $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ .

Any system which is described by a single state vector is said to be in a *pure state*. However, in a realistic experimental setup the physical state of the considered system is not completely known. If the system is in the pure state  $|\psi_i\rangle$  with probability  $p_i$ , the physical state of the system can be described using the *density operator*

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|. \quad (2.1)$$

The state of such a system is called *mixed state*. In the following, whenever we talk about quantum states, we usually mean mixed states.

In order to have a meaningful physical interpretation, any density operator has the following two properties:

- $\rho$  has trace equal to one:

$$\text{Tr}[\rho] = 1, \quad (2.2)$$

- $\rho$  is a positive operator:

$$\langle \psi | \rho | \psi \rangle \geq 0 \quad (2.3)$$

for any vector  $|\psi\rangle$ .

Note that the second property also implies that  $\rho$  is Hermitian:  $\rho^\dagger = \rho$ . These two conditions are essential for the definition of quantum measurements and operations, which is presented in the following.

## 2.2 Quantum Measurements and Operations

Quantum measurement is one of the most important concepts in quantum theory. Most physicists are familiar with the *projective measurement*: for a spin- $\frac{1}{2}$  particle in the state

$$|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle, \quad (2.4)$$

the probability to measure “spin up” or “spin down” is given by  $p(\uparrow) = |a|^2$  or  $p(\downarrow) = |b|^2 = 1 - p(\uparrow)$ . Moreover, the measurement postulate of quantum mechanics tells us that the quantum state after the measurement is either  $|\uparrow\rangle$  or  $|\downarrow\rangle$ , depending on the outcome of the measurement.

In quantum information theory, a more general definition is considered. A general quantum measurement is described by a collection  $\{E_i\}$  of *measurement operators* that satisfy the completeness equation:

$$\sum_i E_i^\dagger E_i = \mathbb{1}, \quad (2.5)$$

where  $\mathbb{1}$  is the identity operator. Given a density operator  $\rho$  and the set of measurement operators  $\{E_i\}$ , the probability that the result  $i$  occurs is given by

$$p_i = \text{Tr}[E_i^\dagger E_i \rho]. \quad (2.6)$$

After the measurement with outcome  $i$ , the state of the system is described by the density operator

$$\rho_i = \frac{1}{p_i} (E_i \rho E_i^\dagger). \quad (2.7)$$

The set of operators

$$M_i = E_i^\dagger E_i \quad (2.8)$$

is also called positive operator-valued measure (POVM). Due to the completeness Eq. (2.5), the POVM elements  $M_i$  sum up to the identity operator:  $\sum_i M_i = \mathbb{1}$ . Moreover, due to Eq. (2.6) the probabilities  $p_i$  can also be obtained from the POVM elements  $M_i$ :  $p_i = \text{Tr}[M_i \rho]$ . The positivity of the density operator  $\rho$  in Eq. (2.3) implies that all probabilities are nonnegative:  $p_i \geq 0$ . The completeness Eq. (2.5) together with Eq. (2.2) implies that the probabilities sum up to one:  $\sum_i p_i = 1$ .

For a projective measurement, the operators  $E_i$  are orthogonal projectors:  $E_i E_j = \delta_{ij} E_i$ . *Von Neumann measurement* is a special type of a projective measurement, where the measurement operators  $E_i$  are orthogonal projectors with rank one. Such a measurement was considered below Eq. (2.4), there the measurement operators are

$E_{\uparrow} = |\uparrow\rangle\langle\uparrow|$  and  $E_{\downarrow} = |\downarrow\rangle\langle\downarrow|$ . In general, the measurement operators do not have to be projectors, they only need to satisfy the completeness Eq. (2.5).

For composite systems consisting of two subsystems, Alice and Bob, it is possible to perform *local measurements* on one of the subsystems. If a local measurement is done on Alice's subsystem, the subsystem of Bob remains unchanged. In this case, the measurement operators have the form  $E_i = E_i^A \otimes \mathbb{1}^B$ , with the identity operator  $\mathbb{1}^B$  on Bob's Hilbert space. Similarly, measurement operators corresponding to local measurement on Bob's subsystem have the form  $E_i = \mathbb{1}^A \otimes E_i^B$ .

Finally, we also mention the concept of *quantum operations*, which is closely related to quantum measurements. Any set of measurement operators  $\{E_i\}$  can also be called a quantum operation. The corresponding operators  $E_i$  are then called *Kraus operators*. The action of a quantum operation  $\{E_i\}$  on a density operator  $\rho$  is given by

$$\Lambda(\rho) = \sum_i E_i \rho E_i^\dagger. \quad (2.9)$$

For composite systems, *local quantum operations* can be defined in the same way as it was done for local measurements. The importance of quantum operations lies in the fact that they describe the most general change of a quantum state possible in experiments. Quantum operations also play an important role in the study of noisy systems: noise is usually modeled as a quantum operation.

## 2.3 Reduced Density Operator

Sometimes one is only interested in one of the subsystems of a composite quantum system. This situation is captured by the concept of the *reduced density operator*. If the total system is described by the density operator  $\rho^{AB}$ , then the system of  $A$  is described by the reduced density operator

$$\rho^A = \text{Tr}_B[\rho^{AB}], \quad (2.10)$$

where  $\text{Tr}_B$  is called *partial trace* over the subsystem  $B$ . The partial trace is defined by

$$\text{Tr}_B[|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|] = |a_1\rangle\langle a_2| \text{Tr}[|b_1\rangle\langle b_2|], \quad (2.11)$$

where  $|a_1\rangle$  and  $|a_2\rangle$  are any two vectors in  $\mathcal{H}_A$ , and  $|b_1\rangle$  and  $|b_2\rangle$  are any two vectors in  $\mathcal{H}_B$ . The trace on the right hand side is the usual trace for the subsystem  $B$ :  $\text{Tr}[|b_1\rangle\langle b_2|] = \langle b_2|b_1\rangle$ . In addition to Eq. (2.11), we also require that the partial trace is linear, i.e.,  $\text{Tr}_B[M^{AB} + N^{AB}] = \text{Tr}_B[M^{AB}] + \text{Tr}_B[N^{AB}]$  for any two operators  $M^{AB}$  and  $N^{AB}$ . In this way, the partial trace is defined for all density operators. The physical meaning of the partial trace lies in the fact that it is the unique operation for obtaining correct measurement statistics for the subsystem  $A$  [1, p. 105ff.].

## 2.4 Entropy and Mutual Information

The *von Neumann entropy* of a quantum state with density operator  $\rho$  is defined as

$$S(\rho) = -\text{Tr}[\rho \log_2 \rho], \quad (2.12)$$

where the logarithm of the density operator  $\rho$  is defined via its eigenvalues  $\lambda_i$  and eigenstates  $|i\rangle$  in the following way:  $\log_2 \rho = \sum_i \log_2(\lambda_i) |i\rangle \langle i|$ . With this definition, the entropy can be written as

$$S(\rho) = -\sum_i \lambda_i \log_2 \lambda_i, \quad (2.13)$$

where it is defined that  $0 \log_2 0 = 0$ .

The von Neumann entropy is the quantum version of the classical *Shannon entropy*. For a discrete random variable  $X$  which can take a value  $x$  with probability  $p_x$ , the Shannon entropy is defined as

$$H(X) = -\sum_x p_x \log_2 p_x. \quad (2.14)$$

Similar to the Shannon entropy, which measures the uncertainty of a classical random variable, the von Neumann entropy measures the uncertainty of a quantum state. Pure states represent full knowledge about a quantum system: their von Neumann entropy is zero. On the other hand, for a  $d$ -dimensional Hilbert space, maximal uncertainty is represented by the completely mixed density operator  $\mathbb{1}/d$  with the von Neumann entropy  $\log_2 d$ .

For two parties, the von Neumann entropy can be used to define the *mutual information* between the parties. If the total state is given by the density operator  $\rho^{AB}$  with reduced density operators  $\rho^A$  and  $\rho^B$ , the mutual information is defined as

$$I(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}). \quad (2.15)$$

The mutual information is zero if the state is completely uncorrelated, i.e., if the density operator has the form  $\rho^{AB} = \rho^A \otimes \rho^B$ . Otherwise, the mutual information is greater than zero: it measures the amount of correlations between  $A$  and  $B$ .

Closely related to the von Neumann entropy is the *quantum relative entropy*. For two density operators  $\rho$  and  $\sigma$  it is defined as

$$S(\rho||\sigma) = \text{Tr}[\rho \log_2 \rho] - \text{Tr}[\rho \log_2 \sigma] \quad (2.16)$$

if the support of  $\rho$  is contained in the support of  $\sigma$ , and  $S(\rho||\sigma) = +\infty$  otherwise. The quantum relative entropy is nonnegative, and zero if and only if  $\rho = \sigma$ . The mutual information defined in Eq. (2.15) can be written as the relative entropy between

the density operator  $\rho^{AB}$  and the tensor product of the reduced density operators  $\rho^A \otimes \rho^B$  [2]:

$$I(\rho^{AB}) = S(\rho^{AB} || \rho^A \otimes \rho^B). \quad (2.17)$$

## 2.5 Distance Between Density Operators

Given two quantum states, how “close” are they to each other? This question, posed in [1, p. 403], can be answered by defining an appropriate distance onto the set of density operators. One important and frequently used distance is the *trace distance*

$$D_t(\rho, \sigma) = \frac{1}{2} \text{Tr} |\rho - \sigma|, \quad (2.18)$$

where  $\rho$  and  $\sigma$  are any two density operators,  $\text{Tr}|M| = \text{Tr}\sqrt{M^\dagger M}$  is the trace norm of an operator  $M$ , and the square root of a Hermitian operator  $M^\dagger M$  with nonnegative eigenvalues  $\lambda_i$  and eigenstates  $|i\rangle$  is defined as  $\sqrt{M^\dagger M} = \sum_i \sqrt{\lambda_i} |i\rangle \langle i|$ . The trace distance satisfies all properties of a general distance  $D$ :

- $D(\rho, \sigma) \geq 0$ , and  $D(\rho, \sigma) = 0$  holds if and only if  $\rho = \sigma$ ,
- $D$  is symmetric:  $D(\rho, \sigma) = D(\sigma, \rho)$ ,
- $D$  satisfies the triangle inequality:  $D(\rho, \tau) \leq D(\rho, \sigma) + D(\sigma, \tau)$  for any three density operators  $\rho$ ,  $\sigma$ , and  $\tau$ .

In quantum information theory, the trace distance has an important interpretation:  $\frac{1}{2} + \frac{1}{2}D_t(\rho, \sigma)$  is the optimal probability of success for distinguishing two quantum states with density operators  $\rho$  and  $\sigma$  [3].

Another frequently used quantity is the *fidelity*. For two density operators  $\rho$  and  $\sigma$  it is defined as

$$F(\rho, \sigma) = \left( \text{Tr} \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}} \right)^2. \quad (2.19)$$

The fidelity itself is not a distance, since it is one if and only if  $\rho = \sigma$ , and smaller than one otherwise. However, the fidelity can be used to define the *Bures distance*:  $D_B(\rho, \sigma) = 2(1 - \sqrt{F(\rho, \sigma)})$ , which satisfies all properties of a mathematical distance.

Both, the trace distance and the Bures distance have also another important property, namely they are *nonincreasing under quantum operations*:

$$D(\Lambda(\rho), \Lambda(\sigma)) \leq D(\rho, \sigma), \quad (2.20)$$

where  $\rho$  and  $\sigma$  are any two density operators, and  $\Lambda$  is any quantum operation. This property is frequently used in quantum information theory, especially in studying entanglement and other quantum correlations.

Note that the inequality (2.20) does not follow from the general properties of a mathematical distance, and thus there exist distances which violate it. One such distance is the *Hilbert-Schmidt distance*

$$D_{HS}(\rho, \sigma) = \|\rho - \sigma\|, \quad (2.21)$$

where  $\|M\| = \sqrt{\text{Tr}[M^\dagger M]}$  is the Hilbert-Schmidt norm of an operator  $M$ . For the Hilbert-Schmidt distance violation of Eq. (2.20) was shown in [4, 5].

Finally, the relative entropy introduced in Eq. (2.16) is not a distance in the mathematical sense since it is not symmetric, and also does not satisfy the triangle inequality. However, the relative entropy is nonincreasing under quantum operations, i.e., it satisfies the inequality (2.20) [6].

## References

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