

# Chapter 1

## Mathematical Foundation for Quantum System

**Abstract** This book introduces group representation theory in terms of quantum theory. For this purpose, this chapter introduces basic concepts of quantum theory, measurement, state, composite system, many-body system, and entanglement. It also prepares mathematical notations for quantum systems. Although these notations are specified to quantum systems, they are helpful for group representation. Hence, this book consistently deals with representation theory based on these notations.

### 1.1 System, State, and Measurement

In the framework of quantum theory for a microscopic system, the object of interest is called the **Quantum system** or the **System**, and is mathematically described as a complex vector space  $\mathcal{H}$  with a Hermitian inner product, which is finite-dimensional or infinite-dimensional. Such a complex vector space  $\mathcal{H}$  is called a **Hilbert space** even though it is finite-dimensional.<sup>1</sup> Since  $\mathcal{H}$  is a vector space with a Hermitian inner product, we can choose a **completely orthonormal system (CONS)**  $\{e_i\}$ . Each normalized base  $e_i$  represents a state in the quantum system that is distinguished from each other. An arbitrary state of the system is given as a normalized vector  $x \in \mathcal{H}$ . Once a CONS has been fixed as a standard basis, the vector  $x$  describing an arbitrary state is written as a linear combination  $\sum_i x_i e_i$ . In quantum theory, there are two methods to describe the element  $x \in \mathcal{H}$ . One is the description by a ket vector  $|x\rangle$ , and the other is that by a bra vector  $\langle x|$ . Although these descriptions are defined to satisfy the linearity with respect to real coefficients, the multiplication of a complex coefficient  $a \in \mathbb{C}$  is defined as

$$|ax\rangle = a|x\rangle, \quad \langle ax| = \bar{a}\langle x|. \quad (1.1)$$

In particular, for a base  $e_i$  of the standard basis,  $|e_i\rangle$  and  $\langle e_i|$  are simplified to  $|i\rangle$  and  $\langle i|$ , respectively. On the other hand, we define the Hermitian inner product  $\langle x|y\rangle$  for  $x, y \in \mathcal{H}$  to satisfy the condition  $\langle ax|by\rangle = \bar{a}b\langle x|y\rangle$  for  $a, b \in \mathbb{C}$ . Then, the inner

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<sup>1</sup>It is required to satisfy the **completeness** under the given inner product in the infinite-dimensional case. see Sect. 1.6.

product  $\langle x|y\rangle$  between  $x$  and  $y$  can be regarded as the multiplication  $\langle x| \cdot |y\rangle$  of the bra vector and the ket vector.

In addition to a state, a physical quantity is also an important concept. When the system obeys the classical mechanics, the value of the physical quantity is also determined according to the state of the system, hence, the physical quantity is given as a function whose input is the state of the system. However, the physical quantity does not necessarily take a fixed value, and is defined as a Hermitian linear map on the Hilbert space.<sup>2</sup> In the following, for the simplicity, we employ the terminologies in the finite-dimensional case.

The most important physical quantity is the **Hamiltonian**, which is written as  $H$ . This is because it is the physical quantity describing the time evolution. Since  $H$  is a Hermitian matrix,  $e^{itH}$  is a unitary, where the real number  $t$  describes the time. Then, the map  $|x\rangle \mapsto e^{itH}|x\rangle$  describes the evolution of the state of the system, i.e., the state change during time period  $t$ .

As mentioned above, a physical quantity  $A$  does not take a fixed value. What is its exact meaning? To answer this question, we need to consider the measurement of the physical quantity  $A$ . This is because the value of the physical quantity is determined via the measurement. In quantum theory, any physical quantity  $A$  is written as a Hermitian matrix or a self-adjoint operator on  $\mathcal{H}$ , and the Hermitian matrix or the self-adjoint operator is also written as  $A$  with this context. When a Hermitian matrix  $A$  has no multiplicity for eigenvalues, it is called **non-degenerate**. Otherwise, it is called **degenerate**. To consider the measurement, we focus on a non-degenerate Hermitian matrix  $A$ . Then, the eigenvalue decomposition of  $A$  is given as

$$A = \sum_i a_i |\phi_i\rangle \langle \phi_i|, \quad (1.2)$$

where  $a_i$  is an eigenvalue of  $A$  and  $\phi_i$  is an eigenvector corresponding to the eigenvalue  $a_i$ .

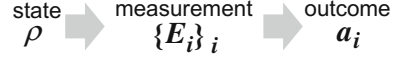
Once the physical quantity  $A$  is measured, the possible outcomes are limited to the eigenvalues  $a_i$  of the Hermitian matrix  $A$ . The realized outcome is determined according to the state of the system. The outcome is determined only probabilistically except for several special cases. When the state is a normalized vector  $x \in \mathcal{H}$ , the probability to obtain the outcome  $a_i$  is given to be

$$\langle x|\phi_i\rangle \langle \phi_i|x\rangle = |\langle x|\phi_i\rangle|^2. \quad (1.3)$$

The set of the above values gives the probability distribution because the relation  $\sum_i |\langle x|\phi_i\rangle|^2 = 1$  can be shown by the fact that  $\{\phi_i\}_i$  is a CONS. In particular, when the state is known to be a base of the CONS  $\{\phi_i\}_i$ , we can identify which base is the state  $|x\rangle$  via the above measurement. In general, once a CONS  $\{\phi_i\}_i$  is given, it is

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<sup>2</sup>It is defined as a self-adjoint operator in the infinite-dimensional case. The precise discussion is given in Sect. 1.6.

**Fig. 1.1** Measurement

possible to realize the measurement whose outcome corresponding to the base  $\phi_i$  is obtained with the probability (1.3) in the above way.

However, a Hermitian matrix might be a degenerate, i.e., might have multiplicity for eigenvalues, in general. The above fact can be generalized to the degenerate case by considering the spectral decomposition

$$A = \sum_i a_i E_i \quad (1.4)$$

instead of the eigenvalue decomposition (1.2). Then, the eigenvalues of  $A$  are  $\{a_i\}$ , and the eigenspace corresponding to  $a_i$  is the range of the projection  $E_i$ . When the physical quantity  $A$  is measured, the probability to obtain the outcome  $a_i$  is given to be  $\langle x|E_i|x\rangle = \text{Tr } E_i|x\rangle\langle x|$ . Hence, in general, given an orthogonal decomposition  $\oplus_i \mathcal{H}_i$  of the Hilbert space  $\mathcal{H}$ , a measurement can be defined by the set  $\{E_i\}_i$  of the projections  $E_i$  on the Hilbert space  $\mathcal{H}_i$ . Such a measurement is called a **projection-valued measurement (PVM)**. As Fig. 1.1, the outcome is given as  $a_i$ .

Here, we should remark that the above probability is determined by the one-dimensional projection  $|x\rangle\langle x|$  rather than the vector  $|x\rangle$ . Hence, even if the vector  $|x\rangle$  is changed to  $|e^{i\theta}x\rangle$  by multiplying the phase factor  $e^{i\theta}$ , the corresponding one-dimensional projection  $|x\rangle\langle x|$  does not change.

In general, it is difficult to prepare the state of the system to be a specific state  $|x\rangle$  exactly due to the difficulty of control of the quantum system. The mixture of two states  $|x\rangle$  and  $|y\rangle$  with a ratio  $(1 - p) : p$  is rather natural than the exact preparation of the state  $|x\rangle$ . In this case, when the above measurement is applied, the probability to obtain the outcome  $a_i$  is given to be

$$(1 - p) \text{Tr}(E_i|x\rangle\langle x|) + p \text{Tr}(E_i|y\rangle\langle y|) = \text{Tr } E_i((1 - p)|x\rangle\langle x| + p|y\rangle\langle y|). \quad (1.5)$$

How can we describe such a mixture of states? Since we cannot recognize the system by means other than measurements in the quantum system, it is better to identify a mixture of state with another mixture when they cannot be distinguished via any measurement. Thus, it is reasonable to define a mixed state by using the right hand side (RHS) of (1.5). That is, we describe the mixed state as a Hermitian matrix  $(1 - p)|x\rangle\langle x| + p|y\rangle\langle y|$ . In general, the state corresponding to the mixture of several states  $|\phi_i\rangle$  with the probability  $p_i$  is expressed as

$$\rho := \sum_i p_i |\phi_i\rangle\langle\phi_i|. \quad (1.6)$$

The above  $\rho$  is a Hermitian matrix, in which, the trace is 1 and the eigenvalues are not less than zero. Thanks to the above discussion, we can correctly describe the

probability to obtain each outcome of each physical quantity once we know the above matrix  $\rho$ . Conversely, when a Hermitian matrix  $\rho$  satisfies the two conditions, (1) the trace is 1 and (2) the eigenvalues are not less than zero, it can be described by the RHS of (1.6) via the eigenvalue decomposition of  $\rho$ . Here, the set of the states  $\{|\phi_i\rangle\}$  in the RHS of (1.6) does not necessarily form a CONS. In the following, a Hermitian matrix  $\rho$  is called a **density matrix** when it satisfies the above two conditions. In contrast, a state described by a normalized vector in  $\mathcal{H}$  is called a **wave function**. When a density matrix is written as a wave function, it is called a **pure state**. Otherwise, it is called a **mixed state**.

Here, let us consider the measurement of the physical quantity  $A$ . Then, when the density matrix of  $\rho$ , the **expectation** of the outcome is given as

$$\sum_i a_i \text{Tr } E_i \rho = \text{Tr } A \rho. \quad (1.7)$$

Hence, the density matrix  $\rho$  can be regarded as a non-commutative extension of the probability distribution. On the other hand, the physical quantity  $A$  can be regarded as a non-commutative extension of a random variable. In probability theory, the expectation is the sum of the product of the possible values of the random variable and their probability. Since, in quantum theory, the expectation is the trace of the multiplication of a density matrix and a physical quantity, the above correspondence can be thought to be a natural non-commutative extension. Also, the **variance** is given as

$$\begin{aligned} \Delta_\rho^2 A &:= \sum_i a_i^2 \text{Tr } |\phi_i\rangle\langle\phi_i| \rho - (\text{Tr } A \rho)^2 \\ &= \text{Tr } A^2 \rho - (\text{Tr } A \rho)^2 = \text{Tr } (A - (\text{Tr } A \rho) I)^2 \rho. \end{aligned} \quad (1.8)$$

When two physical quantities  $A$  and  $B$  are commutative with each other, a simultaneous decomposition of  $A$  and  $B$ , i.e., the simultaneous measurement of  $A$  and  $B$ , is given as follows. Let  $a_i$ ,  $\mathcal{H}_i$ , and  $E_i$  be an eigenvalue of  $A$ , the eigenspace of  $A$  associated to  $a_i$ , and the projection to  $\mathcal{H}_i$ , respectively. Since  $B(A - a_i) = (A - a_i)B$ , any vector  $|x\rangle$  in  $\mathcal{H}_i$  satisfies  $(A - a_i)B|x\rangle = 0$ . So,  $B|x\rangle$  belongs to  $\mathcal{H}_i$ , i.e.,  $E_i B|x\rangle = B|x\rangle$ . For any element  $|y\rangle$ , we have  $E_i B E_i |y\rangle = B E_i |y\rangle$ , i.e.,  $E_i B E_i = B E_i$ . Since  $\sum_i E_i = I$ , we have

$$B = \sum_i E_i B E_i. \quad (1.9)$$

Thus, we can make the spectral decomposition  $\{E_{j,i}\}_j$  of  $E_i B E_i$  on  $\mathcal{H}_i$  as  $E_i B E_i = \sum_j b_{j,i} E_{j,i}$ . Since  $\sum_{j,i} E_{j,i} = I$ , the decomposition  $\{E_{j,i}\}_{j,i}$  forms a PVM. As (1.9) guarantees that  $\sum_{j,i} b_{j,i} E_{j,i} = B$ , the decomposition  $\{E_{j,i}\}_{j,i}$  gives the simultaneous measurement of  $A$  and  $B$ .

In this case, the covariance of two outcomes is given as

$$\begin{aligned} & \Delta_\rho A \circ B \\ &:= \frac{1}{2} \text{Tr}[(B - (\text{Tr } B\rho))(A - (\text{Tr } A\rho)) + (A - (\text{Tr } A\rho))(B - (\text{Tr } B\rho))]\rho. \end{aligned} \quad (1.10)$$

Now, we consider the case when  $A$  and  $B$  are non-commutative. Although  $\Delta_\rho A \circ B$  can be defined and can be regarded as a kind of correlation between the two physical quantities  $A$  and  $B$ , it cannot be thought to be a covariance because the simultaneous measurement of  $A$  and  $B$  cannot be defined.

In the above formulation, a measurement is given from a CONS. This formulation can be generalized as follows. Given a set  $\{|\phi_i\rangle\}_i$  of non-normalized vectors in  $\mathcal{H}$ , we assume that

$$\sum_i |\phi_i\rangle\langle\phi_i| = I, \quad (1.11)$$

where  $I$  is the unit matrix. Then, the set  $\{|\phi_i\rangle\langle\phi_i|\}_i$  gives a decomposition of the unit matrix  $I$ , which gives a measurement as well [58]. Such a decomposition is called a positive operator-valued measure (POVM). When the above measurement is applied to the system whose state is given as the density matrix  $\rho$ , the measurement outcome  $i$  is obtained with the probability  $\langle\phi_i|\rho|\phi_i\rangle$ . Such a measurement is possible within the framework of PVMs by extending the system [46, 54, 58]. Such a type of measurement can be generalized to the continuous case. That is, when normalized vectors  $\{|\phi_\theta\rangle\}_{\theta \in \Theta}$  are parameterized by the set  $\Theta$  and the measure on the parameter space  $\Theta$  satisfies the condition

$$\int_{\Theta} |\phi_\theta\rangle\langle\phi_\theta| \mu(d\theta) = I, \quad (1.12)$$

the decomposition of the unit matrix is called a POVM and gives a measurement in the above-mentioned sense.

In summary, the key points of quantum theory are summarized as the following basic concepts, a physical quantity (especially the Hamiltonian), its spectral decomposition, a wave function as an element of  $\mathcal{H}$ , and a density matrix.

**Exercise 1.1** Define the POVM  $M = \{M_i\}_{i=1}^3$  and the density matrix  $\rho$  as  $M_1 = \begin{pmatrix} \frac{1}{2} & \frac{i}{4} \\ \frac{i}{4} & \frac{1}{8} \end{pmatrix}$ ,  $M_2 = \begin{pmatrix} \frac{1}{2} & -\frac{i}{4} \\ -\frac{i}{4} & \frac{1}{8} \end{pmatrix}$ ,  $M_3 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{3}{4} \end{pmatrix}$ , and  $\rho = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ . Calculate the distribution  $P_M^\rho$ .

**Exercise 1.2** Give the spectral decomposition of  $A = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$  and  $B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ .

**Exercise 1.3** Calculate the expectation when the measurement is the spectral decomposition of  $A$  given in Exercise 1.2 and the state is  $\rho = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ .

**Exercise 1.4** Calculate the variance  $\Delta_\rho A$  in Exercise 1.3.

**Exercise 1.5** Calculate the value  $\Delta_\rho A \circ B$  when  $A$ ,  $B$  and  $\rho$  are given in Exercises 1.2 and 1.3, respectively.

## 1.2 Composite System

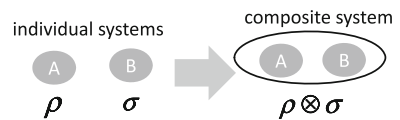
### 1.2.1 Tensor Product System

When we have two quantum systems  $\mathcal{H}_A$  and  $\mathcal{H}_B$  and we treat them as one quantum system, we need a description for the whole system as Fig. 1.2. For example, when the system  $\mathcal{H}_A$  describes the internal freedom of a particle and the system  $\mathcal{H}_B$  does its position, we need the quantum system that describing the whole freedom of the particle, whose typical example is given in Sect. 5.4. Such a quantum system is called the composite system of  $\mathcal{H}_A$  and  $\mathcal{H}_B$ . The composite system is given by the **tensor product space**  $\mathcal{H}_A \otimes \mathcal{H}_B$ . When  $\mathcal{H}_A$  and  $\mathcal{H}_B$  have their CONSs  $\{|v_i\rangle\}_{i=1}^k$  and  $\{|u_j\rangle\}_{j=1}^l$ , respectively, the tensor product space  $\mathcal{H}_A \otimes \mathcal{H}_B$  is given as the linear space whose CONS is  $\{|v_i, u_j\rangle\}_{1 \leq i \leq k, 1 \leq j \leq l}$ . One might consider that the composite system is given as the product space  $\mathcal{H}_A \oplus \mathcal{H}_B$ . However, the composite system is as the tensor product space  $\mathcal{H}_A \otimes \mathcal{H}_B$ . To understand the reason, we consider the typical classical case. Remember that the product space  $\mathcal{H}_A \oplus \mathcal{H}_B$  has the CONS  $\{|v_i\rangle\}_{i=1}^k \cup \{|u_j\rangle\}_{j=1}^l$ .

In the classical case, the state is given as a probability distribution over the set of events. That is, to identify the system, we need to identify the set of events. The basis of the quantum system corresponds to the set of events. In the classical case, an event of the composite system is given as a pair of events of the respective systems. That is, the set of events of the composite system is the product set of the sets of events of the respective systems. Considering the relation between the basis of the quantum system and the events of the classical system, we find that the basis of the composite system is  $\{|v_i, u_j\rangle\}_{1 \leq i \leq k, 1 \leq j \leq l}$  and is not  $\{|v_i\rangle\}_{i=1}^k \cup \{|u_j\rangle\}_{j=1}^l$ . Thus, the composite system is the tensor product system  $\mathcal{H}_A \otimes \mathcal{H}_B$ . When we need to identify the basis of the composite system with a single number, we number it as  $|e_{i+k(j-1)}\rangle = |v_i, u_j\rangle$ .

Next, let us consider the case when the respective states of the systems  $\mathcal{H}_A$  and  $\mathcal{H}_B$  are independently prepared to be the density matrices  $\rho$  and  $\sigma$ . When  $\rho = \sum_{i,i'=1}^k a_{i,i'} |v_i\rangle\langle v_{i'}|$  and  $\sigma = \sum_{j,j'=1}^l b_{j,j'} |u_j\rangle\langle u_{j'}|$ , the state of the composite system is given as the **tensor product state**  $\rho \otimes \sigma := \sum_{i,i'=1}^k \sum_{j,j'=1}^l a_{i,i'} b_{j,j'} |v_i, u_j\rangle\langle v_{i'}, u_{j'}|$ .

**Fig. 1.2** Composite system of two quantum systems



$\langle v_{i'}, u_{j'} |$ . In the following, for simplicity, we consider the case when these density matrices are diagonal, i.e.,  $\rho = \sum_{i=1}^k a_i |v_i\rangle\langle v_i|$  and  $\sigma = \sum_{j=1}^l b_j |u_j\rangle\langle u_j|$ . Since  $\rho \otimes \sigma = \sum_{i=1}^k \sum_{j=1}^l a_i b_j |v_i, u_j\rangle\langle v_i, u_j|$ , the event  $(v_i, u_j)$  occurs with the probability  $a_i b_j$ . Hence, the above independent situation does not contradict the independence in the classical case. Therefore, when the respective states are independently prepared in the quantum system, the state of the composite system is given as the tensor product state.

Here, we should remark that the tensor product  $|v\rangle \otimes |u\rangle = \sum_{i=1}^k \sum_{j=1}^l c_i f_j |v_i, u_j\rangle$  of two wave functions  $|v\rangle = \sum_{i=1}^k c_i |v_i\rangle$  and  $|u\rangle = \sum_{j=1}^l f_j |u_j\rangle$  is independent of the choice of the bases of the respective systems. To check this fact, it is sufficient to show that the tensor product based on other CONSs  $\{|\tilde{v}_i\rangle\}_{i=1}^k$  and  $\{|\tilde{u}_j\rangle\}_{j=1}^l$  of the respective systems  $\mathcal{H}_A$  and  $\mathcal{H}_B$  equals the tensor product  $|v\rangle \otimes |u\rangle = \sum_{i=1}^k \sum_{j=1}^l c_i f_j |v_i, u_j\rangle$  based on the original bases. When the wave functions  $|v\rangle$  and  $|u\rangle$  are given as  $|v\rangle = \sum_{s=1}^k \tilde{c}_s |\tilde{v}_s\rangle$  and  $|u\rangle = \sum_{t=1}^l \tilde{f}_t |\tilde{u}_t\rangle$ , the tensor product based on the basis  $\{|\tilde{v}_s\rangle\}_{s=1}^k$  and  $\{|\tilde{u}_t\rangle\}_{t=1}^l$  is  $\sum_{s,t} \tilde{c}_s \tilde{f}_t |\tilde{v}_s, \tilde{u}_t\rangle$ . Now, we employ the unitary matrices  $U$  and  $V$  defined as  $|\tilde{v}_s\rangle = \sum_i V_{s,i} |v_i\rangle$  and  $|\tilde{u}_t\rangle = \sum_j U_{t,j} |u_j\rangle$ . Then, we have  $c_s = \sum_i \tilde{c}_s V_{s,i}$  and  $f_t = \sum_j \tilde{f}_t U_{t,j}$ , which implies that

$$\sum_{s,t} \tilde{c}_s \tilde{f}_t |\tilde{v}_s, \tilde{u}_t\rangle = \sum_{s,t,i,j} \tilde{c}_s \tilde{f}_t V_{s,i} U_{t,j} |v_i, u_j\rangle = \sum_{i,j} c_i f_j |v_i, u_j\rangle.$$

Thus, given a matrix  $X$  on  $\mathcal{H}_A$  and a matrix  $Y$  on  $\mathcal{H}_B$ , their tensor product is defined as a linear map on the composite system  $\mathcal{H}_A \otimes \mathcal{H}_B$  as follows.

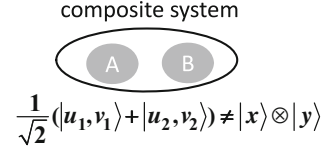
$$X \otimes Y(|v\rangle \otimes |u\rangle) := (X|v\rangle) \otimes (Y|u\rangle). \quad (1.13)$$

Since the tensor product of  $|v\rangle$  and  $|u\rangle$  is defined independently of the choice of the bases, the definition of the linear map  $X \otimes Y$  does not depend on the choice of the bases. Hence, the tensor product state  $\rho \otimes \sigma$  of  $\rho = \sum_{i,i'=1}^k a_{i,i'} |v_i\rangle\langle v_{i'}|$  and  $\sigma = \sum_{j,j'=1}^l b_{j,j'} |u_j\rangle\langle u_{j'}|$  is defined as  $\sum_{i,i'=1}^k \sum_{j,j'=1}^l a_{i,i'} b_{j,j'} |v_i, u_j\rangle\langle v_{i'}, u_{j'}|$ , which does not depend on the choice of the bases. States of the composite system  $\mathcal{H}_A \otimes \mathcal{H}_B$  cannot be restricted to tensor product states  $\rho \otimes \sigma$  or their convex combinations  $\sum_j p_j \rho_j \otimes \sigma_j$ , which are called **separable states**, where  $p_j$  is a probability and  $\rho_j$  and  $\sigma_j$  are density matrices on  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively.

### 1.2.2 Entangled State

We need to notice that all states on the composite system are not necessarily separable, i.e., do not necessarily have the form  $\sum_j p_j \rho_j \otimes \sigma_j$ . For example, the pure state corresponding to the vector  $\sum_j \sqrt{p_j} |v_j, u_j\rangle$  cannot be described as a convex combination of tensor product states unless  $p_j$  is a deterministic distribution. For

**Fig. 1.3** Entangled state between two quantum systems



example, the state  $\frac{1}{\sqrt{2}}(|u_1, v_1\rangle + |u_2, v_2\rangle)$  cannot be written with any convex combination (Fig. 1.3). It is not a separable state. Such a state is called an **entangled state**, which has been studied as a resource of quantum information processing. In particular, such a property is called **entanglement**.

When the state of the composite system  $\mathcal{H}_A \otimes \mathcal{H}_B$  is given as the density matrix

$$\rho = \sum_{i,i'=1}^k \sum_{j,j'=1}^l c_{i,j,i',j'} |v_i, u_j\rangle \langle v_{i'}, u_{j'}|,$$

there exists a density matrix  $\text{Tr}_{\mathcal{H}_B} \rho$  such that

$$\text{Tr}(\text{Tr}_{\mathcal{H}_B} \rho) X = \text{Tr} \rho (X \otimes I_{\mathcal{H}_B})$$

for any matrix  $X$  on the system  $\mathcal{H}_A$ . Thus, it is natural to consider that the state of the smaller system  $\mathcal{H}_A$  is given as the density matrix  $\text{Tr}_{\mathcal{H}_B} \rho$ . The state  $\text{Tr}_{\mathcal{H}_B} \rho$  is called the **partial trace** of  $\rho$ , and is calculated as

$$\text{Tr}_{\mathcal{H}_B} \rho = \sum_{i,i'=1}^k \sum_{j=1}^l c_{i,j,i',j} |v_i\rangle \langle v_{i'}|.$$

When the density matrix  $\rho$  is diagonal under the basis  $\{|v_i, u_j\rangle\}_{i,j}$ , the partial trace coincides with the marginal distribution of the distribution composed of the diagonal elements. The partial trace can be defined when  $\rho$  is not necessarily a density matrix. When it is a density matrix, the partial trace is also called the **reduced density matrix** of  $\rho$ . In the following, when there is no possibility for confusion,  $\text{Tr}_{\mathcal{H}_B}$  is simplified to  $\text{Tr}_B$ .

Now, we consider the linear space of Hermitian matrices on  $\mathcal{H}_A$  as the normed linear space  $\mathcal{B}(\mathcal{H}_A)$  with respect to the matrix norm. The partial trace  $\text{Tr}_{\mathcal{H}_B}$  can be regarded as a linear map from  $\mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$  to  $\mathcal{B}(\mathcal{H}_A)$ . The norm of the linear map is  $\min\{\dim \mathcal{H}_B, \dim \mathcal{H}_A\}$  because the relation

$$\frac{\|\text{Tr}_{\mathcal{H}_B} X\|}{\|X\|} \leq \min\{\dim \mathcal{H}_B, \dim \mathcal{H}_A\} \quad (1.14)$$

holds for a Hermitian matrix  $X$  on  $\mathcal{H}_A \otimes \mathcal{H}_B$ .



In this book, if there is no possibility for confusion, for a matrix  $X$  on  $\mathcal{H}_A$  and a matrix  $Y$  on  $\mathcal{H}_B$ , the matrices  $X \otimes I_{\mathcal{H}_B}$  and  $I_{\mathcal{H}_A} \otimes Y$  on  $\mathcal{H}_A \otimes \mathcal{H}_B$  are simplified to  $X$  and  $Y$ . Hence,  $X \otimes Y$  is written as  $XY$ . Once standard bases of the systems  $\mathcal{H}_A$  and  $\mathcal{H}_B$  are fixed, we use the following simplified notations. Since two quantum systems are addressed, the ket vectors of their standard bases are distinguished as  $|j\rangle_A, |j\rangle_B$ . Hence, the basis of the composite system  $\mathcal{H}_A \otimes \mathcal{H}_B$  is  $|k\rangle_A \otimes |j\rangle_B$ , which is simplified to  $|k, j\rangle_{A,B}$ .

In the following, given a matrix  $X = (x_{k,j})$ , we denote the **complex conjugate matrix** (The entries are given as the complex conjugate of the original entries.) under the standard basis by  $\overline{X}$ , and the **transposed matrix** under the standard basis by  $X^T$ . Then, we denote the **complex conjugate transposed matrix** by  $X^\dagger$ . Although the matrices  $\overline{X}$  and  $X^T$  depend on the choice of the standard basis, the matrix  $X^\dagger$  depends only on the Hermitian matrix and does not depend on the choice of the standard basis. Using the matrix  $X = (x_{k,j})$ , we denote the vector  $\sum_{k,j} x_{k,j} |k, j\rangle_{A,B}$  on the composite system  $\mathcal{H}_A \otimes \mathcal{H}_B$  by  $|X\rangle_{A,B}$ . Then, we have

$$Y \otimes Z |X\rangle_{A,B} = |YXZ^T\rangle_{A,B}. \quad (1.15)$$

The inner product of two vectors  $|X\rangle_{A,B}$  and  $|Y\rangle_{A,B}$  is given as

$$A, B \langle X | Y \rangle_{A,B} = \text{Tr } X^\dagger Y. \quad (1.16)$$

Hence, the vector  $|X\rangle_{A,B}$  is a wave function, i.e., its norm is 1 if and only if

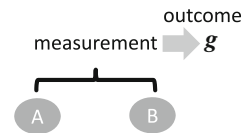
$$\text{Tr } X^\dagger X = 1. \quad (1.17)$$

We also have the following formula for the partial trace;

$$\text{Tr}_B |X\rangle_{A,B} {}_{A,B} \langle X| = X X^\dagger, \quad \text{Tr}_A |X\rangle_{A,B} {}_{A,B} \langle X| = X^T \overline{X}. \quad (1.18)$$

Further, the states  $\left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\rangle_{A,B}$ ,  $\left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\rangle_{A,B}$ ,  $\left| \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\rangle_{A,B}$ , and  $\left| \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\rangle_{A,B}$  are called Bell states. Since they form a CONS on  $\mathbb{C}^2 \otimes \mathbb{C}^2$  (see Exercise 1.7), they give a PVM, i.e., a measurement on the composite system  $\mathbb{C}^2 \otimes \mathbb{C}^2$ . The measurement is called Bell measurement. To realize this measurement, the measurement device needs to handle the quantum correlation between two systems (Fig. 1.4).

**Fig. 1.4** Bell measurement



**Exercise 1.6** Assume that  $X$  is a  $2 \times 2$  matrix. Show that the state  $|X\rangle\rangle_{A,B} \langle\langle X|$  is entangled if and only if  $\det X \neq 0$ .

**Exercise 1.7** Show that  $\left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\rangle\rangle_{A,B}, \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\rangle\rangle_{A,B}, \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\rangle\rangle_{A,B}$ , and  $\left| \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\rangle\rangle_{A,B}$  forms a CONS on  $\mathbb{C}^2 \otimes \mathbb{C}^2$ .

### 1.3 Many-Body System

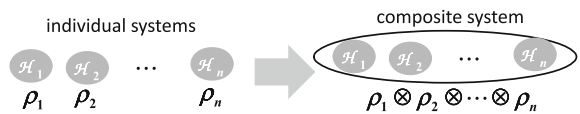
Consider the case when there are  $n$  particles and their quantum systems are given as  $\mathcal{H}_i$  ( $i = 1, \dots, n$ ) (Fig. 1.5). When they can be distinguished from each other, the composite system of these  $n$  particles is given as  $((\mathcal{H}_1 \otimes \mathcal{H}_2) \cdots) \otimes \mathcal{H}_n$ . Since the tensor product space does not depend on the order of the tensor products, the above tensor product space is the same as  $(\mathcal{H}_1(\cdots(\mathcal{H}_{n-1} \otimes \mathcal{H}_n)))$ . Hence, we denote it by  $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$ . In particular, when each system  $\mathcal{H}_i$  is isometric to  $\mathcal{H}$ , the tensor product space is simplified to  $\mathcal{H}^{\otimes n}$ .

However, when these particles are the same particles and cannot be distinguished from each other, we cannot use the above notation. Such a difficult case will be addressed as bosonic system or fermionic system in the latter chapter (Sects. 4.4.2 and 7.4). Even if these  $n$  particles are the same particles, they might be distinguished from each other. For example, when the system  $\mathcal{H}_i$  describes the internal freedom of the particle and the position of each particle can be distinguished with probability 1, the composite system is given as  $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$ .

When the state of each system  $\mathcal{H}_i$  is independently prepared to be the density matrix  $\rho_i$ , the state of the composite system is given as  $((\rho_1 \otimes \rho_2) \cdots) \otimes \rho_n$ . Since the tensor product of the matrices does not depend on the order of the tensor product, the density matrix given by the tensor product is written as  $\rho_1 \otimes \rho_2 \cdots \otimes \rho_n$ . In particular, when  $\rho_i = \rho$ , i.e., the state  $\rho$  is independently prepared in  $n$  quantum systems, the density matrix of the composite system is simplified to  $\rho^{\otimes n}$ , and is called an  $n$ -fold **tensor product state** of  $\rho$ . This notation can be applied to the case when  $\rho$  and  $\rho_i$  are not restricted to density matrices.

Given a matrix  $A$  on the tensor product system  $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$ , we denote the partial trace of  $A$  with respect to the system  $\mathcal{H}_i$  by  $\text{Tr}_{\mathcal{H}_i} A$ . Conversely, we denote the partial trace with respect to the all systems except for the system  $\mathcal{H}_i$  by  $\text{Tr}_{\check{\mathcal{H}}_i} A$ . In particular, when  $A$  is a density matrix  $\rho$ ,  $\text{Tr}_{\check{\mathcal{H}}_i} \rho$  is simplified to  $\rho_{\mathcal{H}_i}$  or  $\rho_i$ . On the other hand, given a matrix  $A$  on the system  $\mathcal{H}_i$ , the matrix  $I^{\otimes i-1} \otimes A \otimes I^{\otimes n-i}$  on

**Fig. 1.5** Composite system of  $n$  quantum systems



the composite system  $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n$  is simplified to  $A_i$ . We also abbreviate the matrix  $\sum_{i=1}^n A_i$  to  $A^{(n)}$ .

As mentioned above, to consider the quantum system, we need to discuss a physical quantity (especially Hamiltonian), its spectral decomposition, a wave function, and a density matrix. However, even when the respective systems  $\mathcal{H}_i$  are 2-dimensional, the composite system has the dimension  $2^n$  and requires very complicated treatment. So, we have serious troubles to handle physical quantities and density matrices. However, when they have invariance with respect to physical transformation, the number of parameters to describe them can be reduced so that their mathematical treatment is simplified. The purpose of this book is to provide the systematic method to treat physical quantities and density matrices by reducing the freedom under the suitable physical invariance.

**Exercise 1.8** Give the spectral decomposition of  $\rho^{\otimes n}$  when  $\rho = \frac{1}{3}E_0 + \frac{2}{3}E_1$  on  $\mathbb{C}^2$ .

## 1.4 Hamiltonian

### 1.4.1 Dynamics and Hamiltonian

In the isolated quantum system, time evolution of the state of the system is given by the time span  $t$  and the **Hamiltonian**  $H$  as

$$\rho \mapsto U\rho U^\dagger, \quad (1.19)$$

where the unitary matrix  $U$  is defined as  $U := e^{itH}$  (Fig. 1.6). However, when we cannot estimate the time  $t$ , we need to take the average with respect to  $T$  as

$$\frac{1}{T} \int_0^T e^{itH} \rho e^{-itH} dt. \quad (1.20)$$

In particular, taking the limit  $T \rightarrow \infty$ , we have the state  $\sum_j E_j \rho E_j$  when the Hamiltonian  $H$  has the spectral decomposition  $\sum_j h_j E_j$  (see Exercise 1.9). Then, only eigenvectors are stable. Hence, it is an important topic to calculate eigenvectors of the Hamiltonian  $H$ . That is, we need to the following equation;

$$H|x\rangle = E|x\rangle \quad (1.21)$$

with eigenvalue  $E$ , which is called **Schrödinger equation**.

**Fig. 1.6** Time evaluation



Hamiltonian has another role in quantum theory. When the system is correlated to a huge system called an environment system or a heat bath during a long time, the state of the system approaches to the state  $e^{-\beta H} / \text{Tr } e^{-\beta H}$  called the thermal equilibrium state or thermal state, where the parameter  $\beta$  is called the inverse temperature. On the other hand, under the limit that the inverse temperature  $\beta$  goes to infinity, the state converges to an eigenvector of  $H$  associated with the minimum eigenvalue. Especially, when the eigenspace is the one-dimensional, the state is called the ground state. Such a state can be realized by keeping the system at a lower temperature. Therefore, it is a central issue to derive the ground state for a given Hamiltonian. In general, the number of particles in the given system is not necessarily one. When the particle is the type of fermion, more than one particles cannot share the same state. That is, when one particle takes the ground state, another particle takes a state orthogonal to the ground state. Hence, to clarify all of states of these particles, we need to calculate several eigenvectors of the Hamiltonian  $H$  associated to lower eigenvalues.

However, in general, it is often difficult to describe the exact form of the Hamiltonian. In some cases, the main term  $H_0$  of the Hamiltonian is given and the fluctuation  $\Delta H$  is given as a small constant  $\epsilon$  times of another Hermitian matrix  $H_1$ . In particular, when  $H_0$  and  $H_1$  are commutative with each other, we have common eigenvectors as a basis. Then, we can take a eigenvector system of  $H$  independently of the coefficient  $\epsilon$ .

**Exercise 1.9** Show that  $\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T e^{itH} \rho e^{-itH} dt = \sum_j E_j \rho E_j$  when  $H = \sum_j h_j E_j$ .

### 1.4.2 Simultaneous Diagonalization

Now, we consider the diagonalization of a given Hamiltonian  $H$  on a given composite system  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . Usually, this task needs our complicated operation for the composite system  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . However, when a non-degenerate Hermitian matrix  $A$  on  $\mathcal{H}_2$  is commutative with  $H$  as a Hermitian matrix on  $\mathcal{H}_1 \otimes \mathcal{H}_2$ , this task can be decomposed to several operations on the subsystems  $\mathcal{H}_1$  and  $\mathcal{H}_2$  as follows. First, we diagonalize  $A$  as  $\sum_i a_i |x_i\rangle\langle x_i|$ . When  $|x_i\rangle\langle x_i|$  is identified with  $|x_i\rangle\langle x_i| \otimes I_{\mathcal{H}_2}$ , this diagonalization can be regarded as the diagonalization of a matrix on the composite system  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . Then, we have a Hermitian matrix  $H_i := \text{Tr}_{\mathcal{H}_2} |x_i\rangle\langle x_i| H |x_i\rangle\langle x_i|$  on  $\mathcal{H}_1$ . Now, we diagonalize  $H_i$  as  $H_i = \sum_j h_{j,i} E_{j,i}$ . Since

$$|x_i\rangle\langle x_i| H |x_i\rangle\langle x_i| = \sum_j h_{j,i} (E_{j,i} \otimes |x_i\rangle\langle x_i|), \quad (1.22)$$

we obtain the spectral decomposition of  $H$  as  $H = \sum_{j,i} h_{j,i} E_{j,i} \otimes |x_i\rangle\langle x_i|$ . from the discussion before (1.10). This method is employed in Sect. 5.1.

Notice that this method does not work when the Hermitian matrix  $A$  is degenerate because (1.22) does not hold in general. To resolve this problem, we consider a set of Hermitian matrices  $\{A_k\}_k$  on  $\mathcal{H}_2$  such that the simultaneous measurement of the Hermitian matrices  $\{A_k\}_k$  is composed of rank-one projections, i.e., has the form  $\{|x_i\rangle\langle x_i|\}_i$ . In this case, we can show that  $|x_i\rangle\langle x_i|H|x_i\rangle\langle x_i| = H|x_i\rangle\langle x_i|$ , which implies that

$$H = \sum_i |x_i\rangle\langle x_i|H|x_i\rangle\langle x_i|. \quad (1.23)$$

Then, we can define the Hermitian matrix  $H_i$  on  $\mathcal{H}_1$  in the same way. Using the spectral decomposition of  $H_i$ , we obtain that of  $H$  in the above way.

**Exercise 1.10** Give the simultaneous diagonalization of  $A \otimes I$  and  $I \otimes B$ , where  $A$  and  $B$  are given in Exercise 1.2.

### 1.4.3 Relation to Representation

Due to the above discussion, it is important to derive the spectral decompositions of the Hamiltonian  $H$  and the related Hermitian matrices. When the system  $\mathcal{H}$  is too large and/or is too complicated, it is very difficult to find their spectral decompositions. That is, it is almost impossible to derive them without reducing the problem to an easier problem.

When a set of Hermitian matrices  $\{A_j\}_j$  satisfies the following condition, the condition almost determines the structure of these Hermitian matrices. There exists a set of real numbers  $c_{k,j,l}$  such that

$$i[A_j, A_k] = \sum_l c_{k,j,l} A_l, \quad (1.24)$$

where  $[X, Y] := XY - YX$ . Indeed, the condition vanishes a larger part of the freedom of these Hermitian matrices. Then, the difficulty of the spectral decomposition is transformed to an algebraic problem. When we use terminologies roughly, this commutation condition (1.24) is called a representation of Lie algebra, and brings very powerful methods. This method is related to the fact that the set of skew-Hermitian matrices is closed with respect to the commutation relation.

Next, we focus on the set of unitary matrices. The set of unitary matrices is closed with respect to the matrix product. Now, we assume that a subset  $\mathcal{S}$  of the set of unitary matrices are closed with respect to the matrix product. When the Hamiltonian  $H$  is invariant for  $\mathcal{S}$ , i.e.,  $UHU^\dagger = H$  for any element  $U \in \mathcal{S}$ , the algebraic structure of  $\mathcal{S}$  for the matrix product determines a larger part of the structure of  $H$ . At least, the structure vanishes a larger part of freedom of the Hilbert space  $\mathcal{H}$ . Hence, the problem of the analysis of the Hamiltonian can be reduced to much more simple

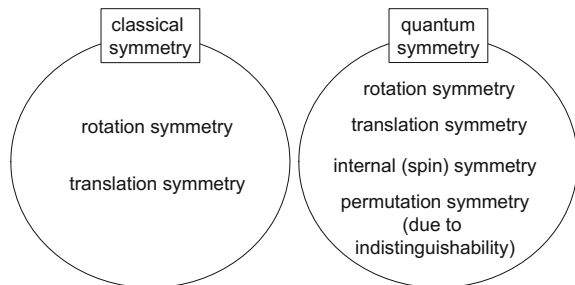
problem. When we use terminologies roughly, the condition for the subset  $\mathcal{S}$  is called a representation of a group. A representation of a group is a powerful tool as well as a representation of Lie algebra. To discuss a representation of a group, we need more rigorous formulation. So, in the next chapter, we start our study of a representation of a group with the formal definition of a group. Since a representation of Lie algebra requires much more preparation, we can start its discussion in the middle in Chap. 3.

## 1.5 Relation to Symmetry

As above-mentioned, symmetry plays an important role in the derivation of Schrödinger equation. In fact, the three dimensional space has natural symmetry with respect to the three-dimensional rotation and displacement. The symmetry of three-dimensional rotation is crucial to discuss quantum system. These symmetries are related to the freedom of the physical space and appear even in classical mechanics.

However, quantum mechanics has a different type of symmetry as Fig. 1.7. Since quantum mechanical object is composed of microscopic particles, we cannot distinguish them when they are the same kind of particles, like, electrons. This problem appears when we have more than one particles while this problem does not occur for the single particle case. Indeed, in quantum theory, it is the most important thing to identify the Hilbert space  $\mathcal{H}$  to describe the quantum system because we cannot discuss anything without identifying the Hilbert space  $\mathcal{H}$ . Hence, we need a proper Hilbert space  $\mathcal{H}$  to describe the possible physical freedom reflecting the indistinguishability. Since the indistinguishability is related to a special kind of symmetry, this description is closely related to the symmetry, which never appear in the classical mechanics. The symmetry is rooted in group representation theory and requires many preparations. Indeed, at least, we have two kinds of indistinguishable particles, boson and fermion. We need different type of symmetry dependently of the type of indistinguishable particles. Hence, we discuss both types of indistinguishable particles in Sect. 4.4.2 after many discussions for group representation theory. Then, we apply this description of the Hilbert space  $\mathcal{H}$  to several important real physical systems in Chaps. 5 and 7.

**Fig. 1.7** Classical and quantum symmetries



As another relation between quantum system and symmetry, we have discrete symmetry of available unitaries. When we artificially control the quantum system, we need to consider the set of possible unitaries, which usually forms a finite set because it is quite hard to prepare the devices corresponding to infinitely many unitaries. In this case, it is important to discuss what subset of unitaries generates the given subset of unitaries. To discuss this issue, we need algebraic structure of the set based on the matrix product. In this context, representation theory plays a crucial role for the design of quantum operation. To protect quantum state from the noises, we often use the quantum noise based on this algebraic structure. Hence, this algebraic structure brings us an essential utility for quantum technologies. Since this kind of symmetry has analogy with boson, we discuss it in Chap. 8 after Chap. 7 that discusses the detail of boson.

## 1.6 Remark for Unbounded Case\*

Finally, we remark several mathematical issues for precise description. If a reader is not interested in such mathematical issues, he/she can skip this part. When the system  $\mathcal{H}$  is infinite-dimensional, we need more careful discussions. Firstly, the system  $\mathcal{H}$  needs to satisfy the **completeness** under the given inner product, i.e., the system  $\mathcal{H}$  needs to contain the limit of Cauchy sequences in  $\mathcal{H}$ . When it does not satisfy the condition, we need to attach the **completion** for a given vector space  $\tilde{\mathcal{H}}$  with Hermitian inner product, which is explained below. First, consider the set of Cauchy sequences  $\{x_n\}$  in  $\tilde{\mathcal{H}}$ . Second, we introduce the equivalence of the set as follows. Given two Cauchy sequences  $\{x_n\}$  and  $\{y_n\}$ , we define equivalence  $\{x_n\} \sim \{y_n\}$  when the sequence  $\{\|x_n - y_n\|\}$  goes to zero. Finally, we take the quotient space composed of sequences with respect to this equivalence. So, the resultant vector space satisfies the completeness.

Even though the system  $\mathcal{H}$  satisfies the completeness, we need to care about the operator norm  $\|H\| := \sup_{x \in \mathcal{H}} \frac{\|Hx\|}{\|x\|}$  for an operator  $H$  on  $\mathcal{H}$ . When the operator norm  $\|H\|$  takes finite value, the operator is called **bounded**. Otherwise, it is called **unbounded** and we need another mathematical delicate problem. In the infinite-dimensional case, there is a possibility that an operator  $H$  on  $\mathcal{H}$  is unbounded. In such a case, the operator  $H$  is called unbounded and requires a more delicate treatment. When we omit this careful treatment, the discussion contains several inconsistencies.<sup>3</sup>

When the operator norm of an operator  $H$  is infinite, we need to restrict the domain of  $H$  to a subspace  $\mathcal{D}(H)$  of  $\mathcal{H}$  so that  $\|Hx\| < \infty$  for  $x \in \mathcal{D}(H)$ . Then, we define the graph norm  $\|x\|_H := \sqrt{\|x\|^2 + \|Hx\|^2}$ . When the domain  $\mathcal{D}(H)$  is closed in the sense of the graph norm,  $H$  is called a **closed operator**. Now, we define the **adjoint operator**  $H^\dagger$  of  $H$  on the domain

$$\mathcal{D}(H^\dagger) := \{x \in \mathcal{H} | \exists y \in \mathcal{H} \text{ such that } \langle y | z \rangle = \langle x | Hz \rangle \text{ for } \forall z \in \mathcal{D}(H)\}$$

---

<sup>3</sup>Even if a reader ignores such inconsistencies, so serious problem will not be caused when the Hilbert space  $L^2(\mathbb{R}^d)$  is discussed. So, it is possible to skip this section.

as

$$\langle H^\dagger x | z \rangle = \langle x | H z \rangle \quad (1.25)$$

for  $z \in D(H)$ . When  $D(H) \subset D(H^\dagger)$  and  $Hx = H^\dagger x$  for  $x \in D(H)$ ,  $H$  is called **symmetric**. When  $D(H) = D(H^\dagger)$  and  $Hx = H^\dagger x$  for  $x \in D(H)$ ,  $H$  is called **self-adjoint**.

In general, it is quite difficult to directly define a self-adjoint operator  $H$  on the proper domain  $D(H)$  because the domain cannot be described explicitly in many cases. Hence, we often define a self-adjoint operator indirectly as follows. Firstly, we usually define an operator  $\tilde{H}$  on a dense subspace  $D(\tilde{H})$  of  $\mathcal{H}$  so that  $\tilde{H}$  is symmetric. Then, we take the completion of the subspace  $D(\tilde{H})$  in the sense of the graph norm of  $\tilde{H}$ . The completion (the resultant Hilbert space of the completion) is different from  $\mathcal{H}$  because we consider the graph norm of  $\tilde{H}$  not the norm of the original Hilbert space  $\mathcal{H}$ . Then, we denote the completion by  $D(H)$  and the operator  $\tilde{H}$  on  $D(H)$  by  $H$ . Since the operator  $H$  is automatically a closed operator, it is called the **closed extension** of  $\tilde{H}$ . When  $\tilde{H}$  is symmetric, the closed extension  $H$  is also symmetric. However, in general, the closed extension  $H$  is not necessarily self-adjoint even though  $\tilde{H}$  is symmetric. Indeed, when an operator  $\tilde{H}$  has a closed extension  $H$  that is self-adjoint, it is called **essentially self-adjoint**.

For a self-adjoint operator  $H$ , we have the following lemma.

**Lemma 1.1** *For a self-adjoint operator  $H$ , there exists a PVM  $E$  on  $\mathbb{R}$  such that*

$$\langle y | H x \rangle = \int_{\mathbb{R}} s \langle y | E(ds) x \rangle. \quad (1.26)$$

Conversely, we have the following lemma.

**Lemma 1.2** *Given a PVM  $E$  taking the outcome in  $\mathbb{R}$ , we define the operator  $X_E$  as*

$$X_E x := \int_{\mathbb{R}} s E(ds) x \quad (1.27)$$

on

$$D(X_E) := \left\{ x \in \mathcal{H} \mid \int_{\mathbb{R}} s^2 \langle x | E(ds) x \rangle < \infty \right\}. \quad (1.28)$$

Then,  $X_E$  is a self-adjoint operator.

Due to this lemma, for any self-adjoint operator  $X$  and any real-valued function  $f$ , we can define the self-adjoint operator  $f(X)$  as  $\int_{\mathbb{R}} f(s) E_X(ds)$ , where  $E_X$  is the PVM defined for the self-adjoint operator  $X$  in Lemma 1.1.



*Proof* Assume that, for an element  $x \in \mathcal{H}$ , there exists an element  $y \in \mathcal{H}$  such that

$$\langle x | X_E z \rangle = \langle y | z \rangle \quad (1.29)$$

for any element  $z \in D(X_E)$ . Hence, it is sufficient to show that  $\int_{\mathbb{R}} s^2 \langle x | E(ds)x \rangle < \infty$ . Firstly, we define the bounded subset  $S_R := \{s \in \mathbb{R} | |s| < R\}$ . Then, we have

$$\langle y | z \rangle = \langle x | X_E z \rangle = \lim_{R \rightarrow \infty} \left\langle x \left| \int_{S_R} s E(ds) z \right. \right\rangle = \lim_{R \rightarrow \infty} \left\langle \int_{S_R} s E(ds) x \left| z \right. \right\rangle \quad (1.30)$$

for any element  $z \in D(X_E)$ . Since  $D(X_E)$  is a dense subset of  $\mathcal{H}$ ,  $\int_{S_R} s E(ds)x$  converges to  $y$  as  $R \rightarrow \infty$ . Thus,  $\int_{\mathbb{R}} s^2 \langle x | E(ds)x \rangle = \langle \int_{S_R} s E(ds)x | \int_{S_R} s E(ds)x \rangle < \infty$ , which is the desired statement.  $\blacksquare$

When a Hamiltonian is given as a self-adjoint operator  $H$ , the unitary matrix  $U$  describing the time evolution is given as  $U := \int_{\mathbb{R}} e^{its} E(ds)$ .

Next, we consider the case when the Hilbert space  $\mathcal{H}$  is given as the set of square summable sequences with an index  $n = 0, 1, 2, \dots, \infty$ . An infinite-dimensional matrix  $\{h_{i,j}\}_{i,j \geq 0}$  is called a band-diagonal matrix with width  $l$  when  $h_{i,j} = 0$  for  $|i - j| > l$ .

**Lemma 1.3** *For two band-diagonal matrices  $\{h_{i,j}\}_{i,j \geq 0}$  and  $\{g_{i,j}\}_{i,j \geq 0}$  with width  $l$ , the sum  $\{h_{i,j} + g_{i,j}\}_{i,j \geq 0}$  is a band-diagonal matrix with width  $l$ , and the product  $\{f_{i,j}\}_{i,j \geq 0}$  is a band-diagonal matrix with width  $2l$ , where  $f_{i,j} := \sum_{j'=i-l}^{i+l} h_{i,j} g_{j',j}$ .*

The above lemma shows that the set of band-diagonal matrices are closed with respect to the sum and the matrix multiplication. A band-diagonal matrix  $\{h_{i,j}\}_{i,j \geq 0}$  is called **Hermitian** when  $h_{i,j} = \overline{h_{j,i}}$ .

**Lemma 1.4** ([68, Theorem 2.3]). *For a band-diagonal matrix  $\{h_{i,j}\}_{i,j \geq 0}$ , we define an operator  $H$  on*

$$D(H) := \left\{ \{a_k\}_{k=0}^{\infty} \in \mathcal{H} \left| \sum_{n=0}^{\infty} \left| \sum_{k=-l}^l h_{nn+k} a_{n+k} \right|^2 < \infty \right. \right\} \quad (1.31)$$

as

$$(Ha)_n := \sum_{k=-l}^l h_{nn+k} a_{n+k} \quad (1.32)$$

for  $a \in D(H)$ . When  $\{h_{i,j}\}_{i,j \geq 0}$  is Hermitian, the operator  $H$  is self-adjoint.

This lemma shows that any band-diagonal matrix can be regarded as a self-adjoint operator.

*Proof* Since  $a \in D(H)$  satisfies  $H^\dagger a = Ha$ , it is sufficient to show that for an element  $x \in \mathcal{H} \setminus D(H)$ , no element  $y \in \mathcal{H}$  satisfies that

$$\langle x | H z \rangle = \langle y | z \rangle \quad (1.33)$$

for  $z \in D(H)$ . When  $y \in \mathcal{H}$  satisfies the above condition, the conditions with  $z = \{\delta_{m,n}\}_{n=0}^\infty$  implies that  $y_m = \sum_{k=-l}^l h_{m,m+k} x_{m+k}$ . Since  $\sum_{n=0}^\infty |y_n|^2 < \infty$ ,  $x \in D(H)$ . This, we obtain the desired statement. ■

**Lemma 1.5** *Let  $\{h_{i,j}\}_{i,j \geq 0}$  be a Hermitian band-diagonal matrix. When a dense subspace  $D(\tilde{H})$  of  $\mathcal{H}$  contains the sequence  $\{\delta_{m,n}\}_{n=0}^\infty$  for any non-negative integer  $m$  and is included in  $D(H)$ , the operator  $\tilde{H}$  defined by the Hermitian band-diagonal matrix  $\{h_{i,j}\}_{i,j \geq 0}$  on  $D(\tilde{H})$  is symmetric. Also, the closed extension of  $\tilde{H}$  is  $H$ .*

*Proof* The first part is trivial because it is included in  $D(H)$ . Since the domain of the closed extension of  $\tilde{H}$  is included in  $D(H)$ , it is enough to show that any element of  $D(H)$  is contained in the domain of the closed extension of  $\tilde{H}$ . Any finite sequence  $\{a_n\}_{n=0}^m$  is contained in the domain of the closed extension of  $\tilde{H}$ . When a sequence  $\{a_n\}_{n=0}^\infty$  satisfies  $\sum_{n=0}^\infty |\sum_{k=-l}^l h_{n,n+k} a_{n+k}|^2 < \infty$  and  $\sum_{n=0}^\infty |a_n|^2 < \infty$ , the sequence  $\{a_n\}_{n=0}^\infty$  belongs to the domain of the closed extension of  $\tilde{H}$ , which implies the desired statement. ■

We often consider the case when the Hilbert space  $\mathcal{H}$  is given as  $L^2(\mathbb{R})$ , which is defined as follows. Firstly, we consider the set  $\mathcal{S}(\mathbb{R})$  of rapidly decreasing functions as

$$\mathcal{S}(\mathbb{R}) := \left\{ \phi \in C^\infty(\mathbb{R}) \mid \sup_{x \in \mathbb{R}} |x^\alpha \frac{d^\beta}{dx^\beta} f(x)|^2 < \infty, \forall \alpha, \beta \in \mathbb{Z}_+ \right\}, \quad (1.34)$$

where  $C^\infty(\mathbb{R})$  is the set of smooth functions. Then, we define the space  $L^2(\mathbb{R})$  as the completion of the  $L^2$  norm defined as  $\|\phi\|^2 := \int_{\mathbb{R}} |\phi(x)|^2 dx$ . The multiplication operator  $\phi(x) \mapsto x\phi(x)$  and the differential operator  $\phi(x) \mapsto \frac{d}{dx}\phi(x)$  are defined in the following way. So, we can define the symmetric operators  $\tilde{Q}$  and  $\tilde{P}$  on  $\mathcal{S}(\mathbb{R})$  by

$$(\tilde{Q}\phi)(x) := x\phi(x), \quad (\tilde{P}\phi)(x) := -i \frac{d}{dx}\phi(x). \quad (1.35)$$

The set  $\mathcal{S}(\mathbb{R})$  contains the  $n$ -th Hermitian function  $\psi_n(x) := \frac{1}{\sqrt{n!2^n\sqrt{\pi}}} e^{\frac{x^2}{2}} \frac{d^n}{dx^n} e^{-x^2}$ , which is identified with  $|n\rangle$ . We define the operators  $\tilde{a}$  and  $\tilde{a}^\dagger$  as  $\tilde{a} := \frac{1}{\sqrt{2}}(\tilde{Q} + i\tilde{P})$  and  $\tilde{a}^\dagger := \frac{1}{\sqrt{2}}(\tilde{Q} - i\tilde{P})$ , respectively. Since  $\tilde{a}|n\rangle = \sqrt{n}|n-1\rangle$  and  $\tilde{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ , the operators  $\tilde{a}$  and  $\tilde{a}^\dagger$  have band-diagonal forms. So, the operators  $\tilde{Q}$  and  $\tilde{P}$  have Hermitian band-diagonal forms. Due to Lemmas 1.4 and 1.5, the closed extensions  $Q$  and  $P$  of  $\tilde{Q}$  and  $\tilde{P}$  are self-adjoint. Now, we consider a two-variable ordered polynomial  $f$ . That is, when the degree is 2,  $f(a, b)$  is written as linear sum of  $a, b, a^2, ab, ba$ , and  $b^2$ . Then, an operator  $f(\tilde{Q}, \tilde{P})$  is defined on  $\mathcal{S}(\mathbb{R})$  as a linear sum of multiplications of  $\tilde{P}$  and  $\tilde{Q}$ , and it has a band-diagonal form. In this case, the ordered polynomial  $f$  equals the opposite ordered polynomial

of  $f$  if and only if  $f(a, b)$  is written as linear sum of  $a, b, a^2, ab + ba$ , and  $b^2$ . When this condition is additionally assumed, the operator  $f(\tilde{Q}, \tilde{P})$  is symmetric and has a Hermitian band-diagonal form. Due to Lemma 1.5, the closed extension  $f(Q, P)$  of  $f(\tilde{Q}, \tilde{P})$  is self-adjoint. So, the operators  $\mathbf{a}$  and  $\mathbf{a}^\dagger$  are defined as the closed operators in this way.

Further, we can define the set  $\mathcal{S}(\mathbb{R}^d)$  of  $d$ -dimensional space rapidly decreasing functions in the same way. Taking the completion, we can define the  $d$ -dimensional  $L^2$  space  $L^2(\mathbb{R}^d)$ . Then, we can define self-adjoint operators  $\mathbf{Q}_j, \mathbf{P}_j$  and  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d, \mathbf{P}_1, \dots, \mathbf{P}_d)$  in the above way when  $f$  is  $2d$ -variable ordered polynomial and it equals the opposite ordered polynomial of  $f$ .

Now, we consider the case with the Coulomb potential. Firstly, we define the self-adjoint operator  $\sum_{j=1}^3 \mathbf{Q}_j^2$  on a dense subspace of  $L^2(\mathbb{R}^3)$ . Then, according to the method explained after Lemma 1.2, we define the self-adjoint operator— $(\sum_{j=1}^3 \mathbf{Q}_j^2)^{-\frac{1}{2}}$ , which is called the Coulomb potential. This operator is also constructed by a closed extension of an operator defined in the domain  $\mathcal{S}(\mathbb{R}^3)$ .

**Lemma 1.6** *Let  $f$  be a smooth function densely defined on  $\mathbb{R}^d$ . Then, we can define the self-adjoint operator  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)$  according to the method explained after Lemma 1.2. We also define the operator  $f(\tilde{\mathbf{Q}}_1, \dots, \tilde{\mathbf{Q}}_d)$  on  $\mathcal{S}(\mathbb{R}^d)$ . Then, the closed extension of  $f(\tilde{\mathbf{Q}}_1, \dots, \tilde{\mathbf{Q}}_d)$  is  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)$ .*

*Proof* Since the domain of  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)$  includes  $\mathcal{S}(\mathbb{R}^d)$ , the domain of  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)$  includes the domain of the closed extension of  $f(\tilde{\mathbf{Q}}_1, \dots, \tilde{\mathbf{Q}}_d)$ . So, it is sufficient to show that any element  $g$  of the domain of  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)$  is expressed as the limit of sequence in  $\mathcal{S}(\mathbb{R}^d)$  in the sense of the graph norm.

Given  $R > 0$ , we choose a function  $\tilde{g}_R \in \mathcal{S}(\mathbb{R}^d)$  such that  $\tilde{g}_R(x) = 1$  for  $|f(x)| < R$  and  $\tilde{g}_R(x) = 0$  for  $|f(x)| > 2R$ . We also choose a sequence of functions  $g_n \in \mathcal{S}(\mathbb{R}^d)$  such that  $\|g - g_n\| \rightarrow 0$  as  $n \rightarrow \infty$ . Now, we choose an integer  $n_R$  such that  $\|\tilde{g}_R(g - g_{n_R})\| < \frac{1}{R^2}$ .

Then, we have  $\tilde{g}_m g_{n_m} \in \mathcal{S}(\mathbb{R}^d)$ . Now, we show that  $\tilde{g}_m g_{n_m}$  converges to  $g$  in the sense of graph norm as follows. We have

$$\|\tilde{g}_m g_{n_m} - g\| \leq \|\tilde{g}_m g_{n_m} - \tilde{g}_m g\| + \|\tilde{g}_m g - g\| \rightarrow 0. \quad (1.36)$$

and

$$\begin{aligned} & \|f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)(\tilde{g}_m g_{n_m} - g)\| \\ & \leq \|f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)(\tilde{g}_m g_{n_m} - \tilde{g}_m g)\| + \|f(\mathbf{Q}_1, \dots, \mathbf{Q}_d)(\tilde{g}_m g - g)\| \\ & \leq 2m \|(\tilde{g}_m g_{n_m} - \tilde{g}_m g)\| + \sqrt{\int_{|s| > n_m} |g(s)|^2 ds} \\ & \leq 2m \frac{1}{m^2} + \sqrt{\int_{|s| > m} |g(s)|^2 ds} \rightarrow 0. \end{aligned} \quad (1.37)$$

■

Although the self-adjoint operator  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d, \mathbf{P}_1, \dots, \mathbf{P}_d)$  is defined only on a dense subspace of the Hilbert space  $\mathcal{H}$ , to avoid the complexity of description, we simply say that the self-adjoint operator  $f(\mathbf{Q}_1, \dots, \mathbf{Q}_d, \mathbf{P}_1, \dots, \mathbf{P}_d)$  is defined on the Hilbert space  $\mathcal{H}$  in this book when the self-adjoint operator is defined in the above way.

**Exercise 1.11** Show that the functions  $xf(x)$  and  $\frac{d}{dx}(x)$  for a function  $f$  in  $\mathcal{S}(\mathbb{R}^d)$  also belong to  $\mathcal{S}(\mathbb{R}^d)$ .

**Exercise 1.12** Consider two functions  $f$  and  $g$  in  $\mathcal{S}(\mathbb{R}^d)$ . Show that the product  $f(x)g(x)$  also belongs to  $\mathcal{S}(\mathbb{R}^d)$ .

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