# CHAPTER 1

# THREE PICTURES IN QUANTUM MECHANICS

In quantum mechanics, we may adopt three different pictures, that is, the Schrödinger picture, the Heisenberg picture, and the interaction picture to describe the dynamics of a quantum system. In fact, in the frame of classical mechanics, the dynamics of a classical material point can be described by different methods. For example, a material point can be described by the time development of a state vector with fixed coordinate vectors, or by the time development of the coordinate vectors with the fixed state vector. The mathematical representations of these two descriptions are different, but these two different descriptions give the same physical results. In quantum mechanics, the three different pictures adopted to describe a quantum system indicate that there exist three different ways of description. No matter which picture is applied to depict a quantum system, the laws of motion of the micro-system must be identical. This means that unitary transformation relations among the three pictures must exist. Which picture we actually choose to describe a quantum system depends on the characteristics of the system. Generally, we would rather choose the picture in which the physical properties of a system are more evident and the calculation are simple. In the following, we describe these three pictures.

## 1.1 The Schrödinger picture

In quantum mechanics when we describe a micro-system such as an atom, a system of an atom coupling to a single-mode field or two atoms interacting with a bimodal field, we usually assume that a state of the system is described by a state function $|\Psi(t)\rangle$. If the system is a single micro-particle, it can be represented by a state function $|\Psi(\mathbf{r},t)\rangle$, here $\mathbf{r}$ is the space coordinate of the system (micro-particle) and $t$ is the time coordinate. When the exact expression of the state function of the system is known at a given time, the time evolution of the system can be deduced. For example, we can learn the probability of the micro-particle at the position $\mathbf{r}$ at time $t$ which is defined by $\langle\Psi(\mathbf{r},t)|\Psi(\mathbf{r},t)\rangle$. And the probability of finding the particle in a volume $d^3\mathbf{r} = dxdydz$ about the point $\mathbf{r}$ at time $t$ is $\langle\Psi(\mathbf{r},t)|\Psi(\mathbf{r},t)\rangle d^3\mathbf{r}$. Since the probability of the particle over the space is equal to 1, the state function must obey the normalization condition, i.e.,

$$\int \langle\Psi(\mathbf{r},t)|\Psi(\mathbf{r},t)\rangle d^3\mathbf{r} = 1 \tag{1.1}$$

Another basic assumption in quantum mechanics is that the physical variables such as position, momentum or spin, are represented by operators. However, the property that any physical variable should be measurable requires that the eigenvalues of the corresponding operator must be restricted to a real number. Such operator is said to be Hermitian. An arbitrary Hermitian operator satisfies the following eigenvalue equation

$$A|u_n\rangle = \lambda_n|u_n\rangle \tag{1.2}$$

Here the symbol $|u_n\rangle$ is called the eigenfunction of the Hermitian operator $A$, and $\lambda_n$ is called the corresponding eigenvalue. An Hermitian operator has three important properties: (1). its eigenvalues $\lambda_n$ are real numbers, (2). its two eigenvectors $|u_n\rangle$ and $|u_m\rangle (n \neq m)$ belonging to different eigenvalues are orthogonal, (3). the eigenvectors of $A$ form a complete set $\{|u_m\rangle\}$, this completeness property allows the expansion of any state $|\Psi(t)\rangle$ of the system by means of the eigenkets of $A$, namely

$$|\Psi(t)\rangle = \sum_n |u_n\rangle\langle u_n|\Psi(t)\rangle = \sum_n C_n(t)|u_n\rangle \tag{1.3}$$

here

$$C_n(t) = \langle u_n|\Psi(t)\rangle$$

is the probability amplitude of the system characterized by $|\Psi(t)\rangle$ in the eigenvector set $\{|u_n\rangle\}$. So we can utilize the linear superposition of the set of eigenvectors $\{|u_n\rangle\}$ to represent the state vector of the quantum system.

Inasmuch as the description of a micro-system (for example, a single Hydrogen atom) needs a lot of physical variables such as position, momentum, angular momentum, energy, spin, etc., the question arises of the relationships among the operators of these physical variables. The actual relations among physical variables are determined by the physical characteristics of the system. In view of theoretical sense, there are two kinds of relations among arbitrary operators. If two operators $A$ and $B$ have a common eigenvector set, they satisfy the following commutation relation

$$[A, B] = AB - BA = 0$$

we say that the operators $A$ and $B$ commutate. If operators $A$ and $B$ do not have a common set of eigenvectors, $A$ and $B$ do not commutate. In this case,

$$[A, B] = iC \tag{1.4}$$

where $C$ may be a constant or another operator. The commutation relation eq.(1.4) reflects the physical correlation between the physical quantities $A$ and $B$ .

One of the main problems in quantum mechanics is how to determine the dynamic behavior of a quantum system. In quantum mechanics, the time development of the state vector $|\Psi(t)\rangle$ of the system is postulated to be determined by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle \tag{1.5}$$

here $H$ is an operator representing the energy of the system, which is usually interpreted as the Hamiltonian of the system. Generally an arbitrary system may be associated with a certain Hamiltonian. Thus the state vector $|\Psi(t)\rangle$ of the system can be determined by (1.5) and the initial condition. Consequently the time evolution of the system can be determined.

It is very important to choose an appropriate picture in studying the dynamic behavior of a quantum system. In quantum mechanics, one important picture is the Schrödinger picture. The key point of this picture is that the state vector $|\Psi(t)\rangle$ describing the dynamic behavior of the system changes continuously according to the Schrödinger equation from an initial state $|\Psi(t_0)\rangle$ to a final state $|\Psi(t)\rangle$ at time $t$, but the operators of physical variables (such as $H$, $\mathbf{P}, \mathbf{r}$) are time-independent. In order to distinguish this picture from others, the subscript (or superscript) $S$ is used to indicate that the operators and the state vectors are in the Schrödinger picture. Thus we write $H_S$ , $q_S$ , $p_S$ , $|\Psi_S(t)\rangle$ and the like. In general, if the subscript or superscript of picture is not explicitly written, we mean that the quantities are in the Schrödinger picture. Inasmuch as physical quantity $A_S$ is time-independent in the Schrödinger picture, the eigenvectors of $A_S$ are stationary (time-independent). Therefore, in the Schrödinger picture the eigenvectors of an arbitrary Hermitian operator can form a fixed basis vectors to describe the state vector of the system. That is to say, the basis vectors are stationary and the dynamical state vector changes in time in the Schrödinger picture. From the Schrödinger equation (1.5) and the state vector $|\Psi_S(t_0)\rangle$ of the system at time $t_0$ , the state vector $|\Psi_S(t)\rangle$ at time $t$ can be obtained as

$$|\Psi_S(t)\rangle = U(t,t_0)|\Psi_S(t_0)\rangle \tag{1.6}$$

where $U(t,t_0)$ is a time evolution operator which depends on the Hamiltonian of the system. Substituting (1.6) into (1.5), then

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)|\Psi_S(t_0)\rangle = H_S U(t,t_0)|\Psi_S(t_0)\rangle \tag{1.7}$$

Since $|\Psi_S(t_0)\rangle$ is arbitrary, the time evolution operator obeys

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H_S U(t,t_0) \tag{1.8}$$

Integrating the above equation, gives

$$U(t,t_0) = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} H_S(t')dt'\right] \tag{1.9}$$

Here $H_S$ is a Hermitian operator, so $U(t,t_0)$ is a unitary operator. If the system is conservative and $H_S$ is explicitly independent of time, then equation (1.9) reduces to

$$U(t,t_0) = \exp\left[-\frac{i}{\hbar}H_S(t-t_0)\right] \tag{1.10}$$

Inserting (1.9) or (1.10) into (1.6), the state vector of the system at time $t$ can be obtained. Thus, at time $t$ the probability of the system in the eigenket $|u_n\rangle$ of the operator $A$ gives

$$|\langle u_n|\Psi_S(t)\rangle|^2 = |\langle u_n|U(t,t_0)|\Psi_S(t_0)\rangle|^2 \tag{1.11}$$

and the expectation value of $A_S$ at time $t$ is

$$\langle A\rangle_S = \langle\Psi_S(t)|A_S|\Psi_S(t)\rangle \tag{1.12}$$

It must be mentioned that when the two Hermitian operators $A$ and $B$ do not commutate (shown in equation (1.4b)), which means that they do not have the same eigenket set, then the physical quantities represented by $A$ and $B$ can not be measured simultaneously. In this case, the mean-square deviations or fluctuations $(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2$ and $(\Delta B)^2 = \langle B^2\rangle - \langle B\rangle^2$ satisfy the inequality

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}|\langle C\rangle|^2 \tag{1.13}$$

where

$$\langle C\rangle = \langle\Psi(t)|C|\Psi(t)\rangle \tag{1.14}$$

$$(\Delta A)^2 = \langle\Psi(t)|A^2|\Psi(t)\rangle - \langle\Psi(t)|A|\Psi(t)\rangle^2 \tag{1.15}$$

The inequality (1.13) is called the Heisenberg uncertainty relation. It expresses a fundamental relation between quantities corresponding to noncommutative operators. If $\langle C\rangle = 0$, namely $C$=0, then $A$ and $B$ commute. In this case, the physical observables $A$ and $B$ can be measured simultaneously and both have precise values. If operator $A$ is the coordinate operator $q$ and $B$ is the momentum operator $p$, then the commutation relation between $q$ and $p$ is

$$[q, p] = i\hbar \tag{1.16}$$

correspondingly, (1.13) may be written as

$$(\Delta p)^2(\Delta q)^2 \geq \frac{1}{4}\hbar^2 \tag{1.17}$$

This is the well-known Heisenberg momentum-position uncertainty relation.

When $A$ is the $x$-component $L_x$ of angular momentum and $B$ is the $y$-component $L_y$ , the commutation relation between $L_x$ and $L_y$ gives

$$[L_x, L_y] = i\hbar L_z \tag{1.18}$$

Evidently

$$(\Delta L_x)^2(\Delta L_y)^2 \geq \frac{1}{4}\hbar^2|\langle L_z\rangle|^2 \tag{1.19}$$

Equation (1.19) is the uncertainty relation of $x - y$ components of the angular momentum, so that the product $(\Delta L_x)^2(\Delta L_y)^2$ is determined by the expectation value $\langle L_z\rangle$.