4 The Postulates—a General Discussion

4.1 Postulates

1. The state of a particle is represented by a ket $|\psi(t)\rangle$ in the Hilbert space.

2. x and p of classical mechanics are represented by Hermitian operators X and P defined by

$$\langle x|\hat{X}|x'\rangle = x\delta(x - x') \tag{18}$$

$$\langle x|\hat{P}|x'\rangle = -i\hbar\delta'(x - x'). \tag{19}$$

   The operator corresponding to the dynamical variable $\Omega(x, p)$ is given by the function of corresponding operators while preserving its form:

$$\hat{\Omega}(\hat{X}, \hat{P}) = \Omega(\hat{X}, \hat{P}). \tag{20}$$

3. Measurement of the variable Ω yield one of the eigenvalues ω with probability $P(\omega) \propto |\langle\omega|\psi\rangle|^2$, where the $|\psi\rangle$ is the state of the particle. After the measurement, the state will change to the corresponding eigenstate $|\omega\rangle$.

4. The time evolution of the state $|\psi(t)\rangle$ is given by the Schrdinger equation:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle, \tag{21}$$

   where $\hat{H}$ is the Hamiltonian operator.

4.2 Statistical Quantities

4.2.1 Expectation Value

Using the definition of an expectation value, the third postulate and the notion of the eigenequation, we can rewrite $\langle\Omega\rangle$ as

$$\langle\Omega\rangle = \int P(\omega)\omega\mathrm{d}\omega = \int |\langle\omega|\psi\rangle|^2\,\omega\mathrm{d}\omega = \int \langle\psi|\omega\rangle\langle\omega|\psi\rangle\omega\mathrm{d}\omega = \int \langle\psi|\hat{\Omega}|\omega\rangle\langle\omega|\psi\rangle\mathrm{d}\omega.$$

Thus,

$$\langle\Omega\rangle = \langle\psi|\hat{\Omega}|\psi\rangle \tag{22}$$

holds.

4.2.2 Uncertainty

Since the variance is the expectation value of $(\Omega - \langle\Omega\rangle)^2$, the root-mean-square deviation or the uncertainty in Ω is given by:

$$\Delta\Omega = \sqrt{\langle\psi|(\hat{\Omega} - \langle\Omega\rangle)^2|\psi\rangle}. \tag{23}$$

4.3 Commuting Operators

4.3.1 Compatibility

If the commutator of two operators $\hat{\Omega}$ and $\hat{\Lambda}$, $[\hat{\Omega}, \hat{\Lambda}] = \hat{\Omega}\hat{\Lambda} - \hat{\Lambda}\hat{\Omega}$, vanishes, there can exist an eigenbasis that is of both two simultaneously. Such operators are said to be compatible.

In the degenerate case, the second measurement may disturb the state. However, whether the eigenvalue is degenerated or not, the probability of obtaining $\Omega = \omega$ and $\Lambda = \lambda$ is independent of the order of measurements.

4.3.2 Canonical Commutativity

Two operators corresponding to canonical conjugate variables obey the canonical commutation relation rule:

$$[\hat{X}, \hat{P}] = i\hbar. \tag{24}$$

In this case, there cannot exist a simultaneous eigenket. This is known as Heisenberg's uncertainty principle.

4.4 Density Operator

Let us consider an ensemble consisting with k kets $|1\rangle, \cdots, |k\rangle$. The density operator of the ensemble is defined by

$$\rho = \sum_i p_i |i\rangle\langle i|, \tag{25}$$

where p_i is the proportion of particles with the state $|i\rangle$ in the whole ensemble.

The average of Ω over both different states and different eigenvalues obtained as the trace of $\Omega\rho$:

$$\langle\bar{\Omega}\rangle = \sum_i p_i \langle i|\Omega|i\rangle = \sum_{i,j} p_i \langle i|j\rangle\langle j|\Omega|i\rangle = \sum_j \langle j|\Omega\rho|j\rangle = \text{tr } \Omega\rho. \tag{26}$$

Since the probability of obtaining a particular eigenvalue ω is given by the projection operator as

$$P(\omega) = |\langle\omega|\psi\rangle|^2 = \langle\psi|\omega\rangle\langle\omega|\psi\rangle = \langle\psi|\mathbb{P}_\omega|\psi\rangle = \langle\mathbb{P}_\omega\rangle,$$

its ensemble average is given by

$$\overline{P(\omega)} = \text{tr } \mathbb{P}_\omega\rho.$$

4.5 Schrdinger Equation

4.5.1 Time–Independent Schrdinger Equation

If the Hamiltonian does not depend on t explicitly, the general solution of the Schrdinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle$$

takes the form

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle\,,$$

where the time-evolution operator

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}. \tag{27}$$

We can expand $|\psi\rangle$ as

$$|\psi(t)\rangle = \int |E\rangle\langle E|\psi(t)\rangle\,\mathrm{d}E = \int c_E(t)\,|E\rangle\,\mathrm{d}E.$$

by acting $(i\hbar\partial/\partial t - H)$ both sides, we obtain

$$i\hbar\dot{c}_E(t) = Ec_E,$$

thus we get

$$U(t) = \int |E\rangle\langle E|e^{-iEt/\hbar}\mathrm{d}E. \tag{28}$$

For this reason, the eigenequation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle \tag{29}$$

is called the time-independent Schrdinger equation.

The normal modes

$$|E(t)\rangle = |E\rangle\,e^{-iEt/\hbar} \tag{30}$$

are also called stationary states, since

$$P(\omega,t) = |\langle\omega|E(t)\rangle|^2 = |\langle\omega|E\rangle|^2 = P(\omega,0) \tag{31}$$

in this state.

4.5.2 Time–Dependent Hamiltonian

If the Hamiltonian depends on time, we can introduce the first-order approximation

$$|\psi(\delta t)\rangle = |\psi(0)\rangle + \left.\frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t}\right|_0 \delta t = \left[1 - \frac{i\delta t}{\hbar}\hat{H}(0)\right]|\psi(0)\rangle = e^{i\hat{H}(0)\delta t/\hbar}|\psi(0)\rangle + \mathcal{O}(\delta t^2).$$

Therefore, the time-evolution operator is now expressed as the time-ordered exponential:

$$U(t) = \mathcal{T}\left\{\exp\left[-\frac{i}{\hbar}\int_0^t \hat{H}(t')\mathrm{d}t'\right]\right\} = \lim_{\delta t\to 0} e^{i\hat{H}(t-\delta t)\delta t/\hbar}\cdots e^{i\hat{H}(0)\delta t/\hbar}.$$

Of course, whether the Hamiltonian depends on time or not,

$$U(t_3,t_2)U(t_2,t_1) = U(t_3,t_1), \quad U^\dagger(t_2,t_1) = U(t_1,t_2), \quad U(t,t) = \mathbb{I}.$$