1.5. Observables

According to the corresponding principle, any classical real function $A = A(\boldsymbol{x}, \boldsymbol{p})$ on the phase space becomes a quantum observable if $\boldsymbol{x}$ & $\boldsymbol{p}$ are replaced by their operator counterparts, provided all operator ordering issues are resolved. Since all measured values on the observable must be real, the operator

$$\hat{A} = A(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}) \tag{1.206}$$

must be hermitian. If the procedure leads to multiple possibilities, additional conditions, such as comparisons to experiments, must be imposed to remove any ambiguity [see Chap 8].

If $\hat{A}$ is hermitian, its eigenstates $| \, a \rangle$ defined by

$$\hat{A} \, | \, a \rangle = a \, | \, a \rangle \tag{1.207}$$

form a basis that spans the Hilbert space of the system. By properly dealing with any case of degeneracy, one can always select a set of orthonormal eigenstates that is also complete:

$$\langle \, a \, | \, a' \rangle = \delta_{a\,a'}$$
$$\sum_a | \, a \rangle \langle \, a \, | = 1 \tag{1.208}$$

By definition, any measurement on A gives the value a if the system is in state $| \, a \rangle$. Using (1.208), we can write

$$| \, \Psi(t) \rangle = \sum_a | \, a \rangle \langle \, a \, | \, \Psi(t) \rangle \tag{1.209}$$

The expectation value of A with respect to state Ψ is therefore

$$\left\langle \Psi(t) \, | \, \hat{A} \, | \, \Psi(t) \right\rangle = \sum_{a,\,a'} \langle \Psi(t) \, | \, a' \rangle \left\langle a' \, | \, \hat{A} \, | \, a \right\rangle \langle \, a \, | \, \Psi(t) \rangle \tag{1.209a}$$
$$= \sum_a a \, | \, \langle \, a \, | \, \Psi(t) \rangle \, |^2$$

which shows that the probability of getting the value a from a measurement of A when the system is in state Ψ is proportional to

$$| \, \langle \, a \, | \, \Psi(t) \rangle \, |^2 \tag{1.210}$$

For example, in the x-representation, the wave function

$$\Psi(\boldsymbol{x}, t) = \langle \, \boldsymbol{x} \, | \, \Psi(t) \rangle \tag{1.211}$$

is just the probability amplitude for finding the particle at $\boldsymbol{x}$. A slight generalization of (1.209a) gives

$$\left\langle \Phi(t) \, | \, \hat{A} \, | \, \Psi(t) \right\rangle = \int d^3 x' \int d^3 x \, \langle \, \Phi(t) \, | \, \boldsymbol{x}' \rangle \left\langle \boldsymbol{x}' \, | \, \hat{A} \, | \, \boldsymbol{x} \right\rangle \langle \, \boldsymbol{x} \, | \, \Psi(t) \rangle$$

If A takes the form (1.206), we have

$$\left\langle \boldsymbol{x}' \, | \, \hat{A} \, | \, \boldsymbol{x} \right\rangle = A\left(\boldsymbol{x}', \frac{\hbar}{i} \nabla'\right) \delta(\boldsymbol{x}' - \boldsymbol{x})$$
$$= A\left(\boldsymbol{x}, -\frac{\hbar}{i} \nabla\right) \delta(\boldsymbol{x}' - \boldsymbol{x})$$

so that, after an integration by part,

$$\left\langle \Phi(t) \, | \, \hat{A} \, | \, \Psi(t) \right\rangle = \int d^3 x' \int d^3 x \, \langle \, \Phi(t) \, | \, \boldsymbol{x}' \rangle \, \delta(\boldsymbol{x}' - \boldsymbol{x}) \, A\left(\boldsymbol{x}, \frac{\hbar}{i} \nabla\right) \langle \, \boldsymbol{x} \, | \, \Psi(t) \rangle$$
$$= \int d^3 x \, \langle \, \Phi(t) \, | \, \boldsymbol{x} \rangle \, A\left(\boldsymbol{x}, \frac{\hbar}{i} \nabla\right) \langle \, \boldsymbol{x} \, | \, \Psi(t) \rangle \tag{1.212}$$

$$= \int d^3x\, \Phi^*(\boldsymbol{x}, t)\, A\left(\boldsymbol{x}, \frac{\hbar}{i}\nabla\right) \Psi(\boldsymbol{x}, t)$$

1.5.1. Uncertainty Relation

The following shows that the uncertainty principle

$$\Delta x_i \Delta p_j \geq \hbar\, \delta_{ij} \tag{1.213}$$

is a consequence of the canonical commutation relations

$$\left[\hat{x}_i, \hat{p}_j\right] = i\hbar\, \delta_{ij} \tag{1.214}$$

In general, the only measurable values of an observable A are the eigenvalues a of the operator $\hat{A}$ defined by

$$\hat{A} \mid a \rangle = a \mid a \rangle \tag{1.215}$$

If the system is in one of the eigenstates, $\mid a \rangle$, then the measured value is a and the system stays in state $\mid a \rangle$ afterwards. If the system is in a normalized state

$$\mid \Psi(t) \rangle = \sum_a \mid a \rangle \langle a \mid \Psi(t) \rangle \tag{1.216}$$

the probability of measuring a value a' is $\mid \langle a' \mid \Psi(t) \rangle \mid^2$. Immediately after getting a value a', the system collapses to state $\mid a' \rangle$.

If the measurement of another observable B does not affect the measurement of A, the eigenstates $\mid a \rangle$ must also be eigenstates of B, i.e.,

$$\hat{B} \mid a \rangle = b_a \mid a \rangle \tag{1.217}$$

then

$$\hat{A}\hat{B} \mid a \rangle = b_a \hat{A} \mid a \rangle = b_a\, a \mid a \rangle$$

$$\hat{B}\hat{A} \mid a \rangle = a \hat{B} \mid a \rangle = a\, b_a \mid a \rangle$$

$$\rightarrow \quad \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) \left| a \right\rangle = 0 \qquad \forall \mid a \rangle \tag{1.218}$$

$$\therefore \quad \left[\hat{A}, \hat{B}\right] = 0 \tag{1.219}$$

Thus, (1.219) implies A an B are not subject to the uncertainty principle, i.e.,

$$\Delta A\, \Delta B = 0$$

Conversely, (1.213) must be due to (1.214).

1.5.2. Density Matrix and Wigner Function

The density operator for a pure state Ψ is defined as

$$\hat{\rho}(t) = \mid \Psi(t) \rangle \langle \Psi(t) \mid \tag{1.220}$$

In the x-representation, the density matrix has elements

$$\rho(\boldsymbol{x}_1, \boldsymbol{x}_2; t) = \left\langle \boldsymbol{x}_1 \middle| \hat{\rho}(t) \middle| \boldsymbol{x}_2 \right\rangle = \langle \boldsymbol{x}_1 \mid \Psi(t) \rangle \langle \Psi(t) \mid \boldsymbol{x}_2 \rangle \tag{1.221}$$

The expectation value of any operator $f(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}})$ with respect to Ψ can be written as

$$\langle \Psi(t) \mid f(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}) \mid \Psi(t) \rangle = \int d^3x\, \langle \Psi(t) \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid f(\boldsymbol{x}, \hat{\boldsymbol{p}}) \mid \Psi(t) \rangle$$

$$= \int d^3x\, \langle \boldsymbol{x} \mid f(\boldsymbol{x}, \hat{\boldsymbol{p}}) \mid \Psi(t) \rangle \langle \Psi(t) \mid \boldsymbol{x} \rangle$$

$$= \int d^3x\, \langle \boldsymbol{x} \mid f(\boldsymbol{x}, \hat{\boldsymbol{p}})\, \hat{\rho}(t) \mid \boldsymbol{x} \rangle$$

$$= \mathrm{tr}\left[f(\boldsymbol{x}, \hat{\boldsymbol{p}})\, \hat{\rho}(t) \right] \tag{1.222}$$

Thus, $\hat{\rho}$ acts like the statistical operator in statistical mechanics.

Expanding $|\Psi(t)\rangle$ in terms of the energy eigenstates $|E_n\rangle$, we have

$$|\Psi(t)\rangle = \sum_n |E_n\rangle\langle E_n|\Psi(t)\rangle$$

$$\langle\Psi(t)| = \sum_m \langle\Psi(t)|E_m\rangle\langle E_m|$$

and (1.220) becomes

$$\hat{\rho}(t) = \sum_{n,m} |E_n\rangle\langle E_n|\Psi(t)\rangle\langle\Psi(t)|E_m\rangle\langle E_m|$$

$$= \sum_{n,m} |E_n\rangle\langle E_n|\hat{\rho}(t)|E_m\rangle\langle E_m|$$

$$= \sum_{n,m} |E_n\rangle \rho_{nm}(t) \langle E_m| \tag{1.223}$$

Let

$$\boldsymbol{X} = \frac{1}{2}(\boldsymbol{x}_1 + \boldsymbol{x}_2) \qquad \Delta\boldsymbol{x} = \boldsymbol{x}_1 - \boldsymbol{x}_2$$

$$\rightarrow \qquad \boldsymbol{x}_1 = \boldsymbol{X} + \frac{1}{2}\Delta\boldsymbol{x} \qquad \boldsymbol{x}_2 = \boldsymbol{X} - \frac{1}{2}\Delta\boldsymbol{x}$$

$$\therefore \qquad \rho(\boldsymbol{x}_1, \boldsymbol{x}_2; t) = \rho\left(\boldsymbol{X} + \frac{1}{2}\Delta\boldsymbol{x}, \boldsymbol{X} - \frac{1}{2}\Delta\boldsymbol{x}; t\right)$$

The Wigner function is the Fourier transform on the relative coordinates $\Delta\boldsymbol{x}$,

$$W(\boldsymbol{X}, \boldsymbol{p}; t) = \int \frac{d^3\Delta x}{(2\pi\hbar)^3} e^{i\boldsymbol{p}\cdot\Delta\boldsymbol{x}/\hbar} \rho\left(\boldsymbol{X} + \frac{1}{2}\Delta\boldsymbol{x}, \boldsymbol{X} - \frac{1}{2}\Delta\boldsymbol{x}; t\right) \tag{1.224}$$

For a particle of mass M in a potential $V(\boldsymbol{x})$, it can be shown that W satisfies the Wigner-Liouville eq.
[see §7.G of L.E.Reichl, "A Modern Course in Statistical Physics" for proof]

$$\left(\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{X}}\right) W(\boldsymbol{X}, \boldsymbol{p}; t) = W_t(\boldsymbol{X}, \boldsymbol{p}; t) \tag{1.225}$$

where

$$\boldsymbol{v} = \frac{\boldsymbol{p}}{M}$$

$$W_t(\boldsymbol{X}, \boldsymbol{p}; t) = \frac{i}{\hbar} \int \frac{d^3 q}{(2\pi\hbar)^3} W(\boldsymbol{X}, \boldsymbol{p} - \boldsymbol{q}; t) \tag{1.226}$$

$$\times \int d^3\Delta x \left[V\left(\boldsymbol{X} + \frac{1}{2}\Delta\boldsymbol{x}\right) - V\left(\boldsymbol{X} - \frac{1}{2}\Delta\boldsymbol{x}\right)\right] e^{i\boldsymbol{q}\cdot\Delta\boldsymbol{x}/\hbar}$$

In the limit $\hbar \to 0$, only terms small in both $|\boldsymbol{q}|$ and $|\Delta\boldsymbol{x}|$ can avoid rapid fluctuations in $e^{i\boldsymbol{q}\cdot\Delta\boldsymbol{x}/\hbar}$.
Keeping the lowest order terms only, we get

$$\Delta V = V\left(\boldsymbol{X} + \frac{1}{2}\Delta\boldsymbol{x}\right) - V\left(\boldsymbol{X} - \frac{1}{2}\Delta\boldsymbol{x}\right) \approx \Delta\boldsymbol{x}\cdot\nabla_{\boldsymbol{X}} V(\boldsymbol{X})$$

$$\rightarrow \qquad \int d^3\Delta x\,(\Delta V)\, e^{i\boldsymbol{q}\cdot\Delta\boldsymbol{x}/\hbar} \approx \frac{\hbar}{i}[\nabla_{\boldsymbol{X}} V(\boldsymbol{X})]\cdot\nabla_{\boldsymbol{q}} \int d^3\Delta x\, e^{i\boldsymbol{q}\cdot\Delta\boldsymbol{x}/\hbar}$$

$$= \frac{\hbar}{i}(2\pi\hbar)^3 [\nabla_{\boldsymbol{X}} V(\boldsymbol{X})]\cdot\nabla_{\boldsymbol{q}}\delta(\boldsymbol{q})$$

$$\therefore \qquad W_t(\boldsymbol{X}, \boldsymbol{p}; t) \approx \int d^3 q\, W(\boldsymbol{X}, \boldsymbol{p} - \boldsymbol{q}; t)\, [\nabla_{\boldsymbol{X}} V(\boldsymbol{X})]\cdot\nabla_{\boldsymbol{q}}\delta(\boldsymbol{q})$$

$$= [\nabla_{\boldsymbol{X}} V(\boldsymbol{X})] \cdot \nabla_{\boldsymbol{p}} W(\boldsymbol{X}, \boldsymbol{p}; t)$$
$$= -\boldsymbol{F}(\boldsymbol{X}) \cdot \nabla_{\boldsymbol{p}} W(\boldsymbol{X}, \boldsymbol{p}; t)$$

where

$$\boldsymbol{F}(\boldsymbol{X}) = -\nabla_{\boldsymbol{X}} V(\boldsymbol{X})$$

is the force due to V.

(1.225) thus becomes the classical Liouville equation

$$\left(\frac{\partial}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{X}} \right) W(\boldsymbol{X}, \boldsymbol{p}; t) = -\boldsymbol{F}(\boldsymbol{X}) \cdot \nabla_{\boldsymbol{p}} W(\boldsymbol{X}, \boldsymbol{p}; t) \qquad (1.227)$$

1.5.3. Generalization to Many Particles

Generalization to a system of N distinguishable particles with Cartesian coordinates $\boldsymbol{x} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$ is straightforward. With $\boldsymbol{p} = (\boldsymbol{p}_1, \ldots, \boldsymbol{p}_N)$, the Schrodinger eq. is

$$i \hbar \frac{\partial}{\partial t} | \Psi(t) \rangle = H\left(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}, t\right) | \Psi(t) \rangle \qquad (1.228)$$

In the x-representation, the basis vectors are direct products of the 1-particle states

$$| \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \rangle \equiv | \boldsymbol{x}_1 \rangle \otimes \ldots \otimes | x_N \rangle$$

with orthonormality

$$\langle \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N | \boldsymbol{x}_1', \ldots, \boldsymbol{x}_N' \rangle = \delta(\boldsymbol{x}_1 - \boldsymbol{x}_1') \ldots \delta(\boldsymbol{x}_N - \boldsymbol{x}_N') \qquad (1.229)$$

and completeness

$$\int d^3 x_1 \ldots \int d^3 x_N \, | \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \rangle \langle x_1, \ldots, \boldsymbol{x}_N | = 1 \qquad (1.229a)$$

The analog of (1.166) is

$$\left\langle \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \,|\, \hat{\boldsymbol{p}}_\nu \,|\, \Psi \right\rangle = \frac{\hbar}{i} \nabla_{\boldsymbol{x}_\nu} \langle \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N | \Psi \rangle \qquad (1.230)$$