B.1. Position and Momentum Eigenstates

B.1.1. Free Particle

Let $|\,\boldsymbol{r}\rangle$ & $|\,\boldsymbol{p}\rangle$ be the eigenstates of the position $\hat{\boldsymbol{q}}$ & momentum $\hat{\boldsymbol{p}}$ operators, respectively, i.e.,

$$\hat{\boldsymbol{q}}\,|\,\boldsymbol{r}\rangle = \boldsymbol{r}\,|\,\boldsymbol{r}\rangle \qquad \& \qquad \hat{\boldsymbol{p}}\,|\,\boldsymbol{p}\rangle = \boldsymbol{p}\,|\,\boldsymbol{p}\rangle \tag{B.2a}$$

With $\boldsymbol{p} = \hbar\boldsymbol{k}$, we also have

$$\hat{\boldsymbol{p}}\,|\,\boldsymbol{k}\rangle = \hbar\boldsymbol{k}\,|\,\boldsymbol{k}\rangle \tag{B.2b}$$

Since $\hat{\boldsymbol{q}}$ & $\hat{\boldsymbol{p}}$ are Hermitian, taking the Hermitian conjugate of (B.2a) gives

$$\langle\,\boldsymbol{r}\,|\,\hat{\boldsymbol{q}} = \langle\,\boldsymbol{r}\,|\,\boldsymbol{r} \qquad \langle\,\boldsymbol{p}\,|\,\hat{\boldsymbol{p}} = \langle\,\boldsymbol{p}\,|\,\boldsymbol{p} \qquad \langle\,\boldsymbol{k}\,|\,\hat{\boldsymbol{p}} = \langle\,\boldsymbol{k}\,|\,\hbar\boldsymbol{k} \tag{B.2b}$$

For unbounded systems, the spectra of both $\hat{\boldsymbol{q}}$ & $\hat{\boldsymbol{p}}$ are continuous. The orthonormal and completeness conditions thus take the form

$$\langle\,\boldsymbol{r}\,|\,\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}') \qquad \langle\,\boldsymbol{p}\,|\,\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}') \qquad \langle\,\boldsymbol{k}\,|\,\boldsymbol{k}'\rangle = \delta(\boldsymbol{k}-\boldsymbol{k}') \tag{B.2c}$$

$$\int d^3r\,|\,\boldsymbol{r}\,\rangle\langle\,\boldsymbol{r}\,| = \hat{1} \qquad \int d^3p\,|\,\boldsymbol{p}\,\rangle\langle\,\boldsymbol{p}\,| = \hat{1} \qquad \int d^3k\,|\,\boldsymbol{k}\,\rangle\langle\,\boldsymbol{k}\,| = \hat{1} \tag{B.2}$$

To recover the quantization rule

$$\hat{\boldsymbol{p}} = \frac{\hbar}{i}\nabla_{\boldsymbol{r}} \tag{B.3a}$$

associated with wave functions, consider the matrix element

$$\langle\,\psi\,|\,\hat{\boldsymbol{p}}\,|\,\phi\,\rangle = \int d^3r\int d^3r'\,\langle\,\psi\,|\,\boldsymbol{r}\,\rangle\langle\,\boldsymbol{r}\,|\,\hat{\boldsymbol{p}}\,|\,\boldsymbol{r}'\rangle\langle\,\boldsymbol{r}'\,|\,\phi\,\rangle \qquad \text{[(B.2) used.]}$$

where ψ & ϕ are arbitrary states in the Hilbert space.

Defining the wave functions as the components of the states in the r-representation (or position basis), i.e.,

$$\phi(\boldsymbol{r}) \equiv \langle\,\boldsymbol{r}\,|\,\phi\,\rangle \qquad \to \qquad \phi^*(\boldsymbol{r}) = \langle\,\phi\,|\,\boldsymbol{r}\,\rangle$$

we have

$$\langle\,\psi\,|\,\hat{\boldsymbol{p}}\,|\,\phi\,\rangle = \int d^3r\int d^3r'\,\psi^*(\boldsymbol{r})\,\langle\,\boldsymbol{r}\,|\,\hat{\boldsymbol{p}}\,|\,\boldsymbol{r}'\rangle\,\phi(\boldsymbol{r}') \tag{B.3b}$$

On the other hand, (B.3a) means

$$\langle\,\psi\,|\,\hat{\boldsymbol{p}}\,|\,\phi\,\rangle = \int d^3r\,\psi^*(\boldsymbol{r})\,\frac{\hbar}{i}\nabla_{\boldsymbol{r}}\,\phi(\boldsymbol{r}) \tag{B.3c}$$

Comparing (B.3b & c) then gives

$$\langle\,\boldsymbol{r}\,|\,\hat{\boldsymbol{p}}\,|\,\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')\,\frac{\hbar}{i}\nabla_{\boldsymbol{r}'} \tag{B.3}$$

Applying the foregoing procedure to $\langle\,\psi\,|\,f(\hat{\boldsymbol{p}})\,|\,\phi\,\rangle$ then gives

$$\langle\,\boldsymbol{r}\,|\,f(\hat{\boldsymbol{p}})\,|\,\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')\,f\!\left(\frac{\hbar}{i}\nabla_{\boldsymbol{r}'}\right) \tag{B.4}$$

Now, the quantization rule (B.3a) may be taken as the solution to the uncertainty principle as expressed in terms of the commutation relation

$$[\,\hat{\boldsymbol{r}},\hat{\boldsymbol{p}}\,] = i\,\hbar\,\hat{I} \tag{B.4a}$$

in the r-representation. Indeed,

$$\left(\boldsymbol{r} \frac{\hbar}{i} \nabla_{\boldsymbol{r}} - \frac{\hbar}{i} \nabla_{\boldsymbol{r}}\, \boldsymbol{r} \right) \psi(\boldsymbol{r}) = i\, \hbar\, \psi(\boldsymbol{r})$$

for arbitrary ψ. The solution to (B.4a) in the p-representation then gives

$$\hat{\boldsymbol{q}} = -\frac{\hbar}{i} \nabla_{\boldsymbol{p}} \qquad \text{(B.4b)}$$

which leads to the counterparts of (B.3-4)

$$\langle\, \boldsymbol{p} \mid \hat{\boldsymbol{q}} \mid \boldsymbol{p}' \,\rangle = -\delta(\boldsymbol{p} - \boldsymbol{p}')\, \frac{\hbar}{i} \nabla_{\boldsymbol{p}'} \qquad \text{(B.5)}$$

$$\langle\, \boldsymbol{p} \mid f(\hat{\boldsymbol{q}}) \mid \boldsymbol{p}' \,\rangle = \delta(\boldsymbol{p} - \boldsymbol{p}')\, f\!\left(-\frac{\hbar}{i} \nabla_{\boldsymbol{p}'} \right) \qquad \text{(B.6)}$$

The momentum eigenstates in the r-representation satisfy the eigen-equation

$$\begin{aligned}
\langle\, \boldsymbol{r} \mid \hat{\boldsymbol{p}} \mid \boldsymbol{p} \,\rangle &= \boldsymbol{p}\, \langle\, \boldsymbol{r} \mid \boldsymbol{p} \,\rangle \\
&= \int d^3 r' \langle\, \boldsymbol{r} \mid \hat{\boldsymbol{p}} \mid \boldsymbol{r}' \,\rangle \langle\, \boldsymbol{r}' \mid \boldsymbol{p} \,\rangle \qquad \text{[(B.2) used.]} \\
&= \int d^3 r'\, \delta(\boldsymbol{r} - \boldsymbol{r}')\, \frac{\hbar}{i} \nabla_{\boldsymbol{r}'} \langle\, \boldsymbol{r}' \mid \boldsymbol{p} \,\rangle \\
&= \frac{\hbar}{i} \nabla_{\boldsymbol{r}} \langle\, \boldsymbol{r} \mid \boldsymbol{p} \,\rangle \qquad \text{(B.7)}
\end{aligned}$$

$$\rightarrow \quad \langle\, \boldsymbol{r} \mid \boldsymbol{p} \,\rangle = c\, \exp\!\left(\frac{i}{\hbar} \boldsymbol{p} \cdot \boldsymbol{r} \right) \qquad \text{(B.8a)}$$

where c is a normalization constant. For the normalization (B.2c), we have

$$\begin{aligned}
\delta(\boldsymbol{p} - \boldsymbol{p}') = \langle\, \boldsymbol{p} \mid \boldsymbol{p}' \,\rangle &= \int d^3 r \langle\, \boldsymbol{p} \mid \boldsymbol{r} \,\rangle \langle\, \boldsymbol{r} \mid \boldsymbol{p}' \,\rangle \qquad \text{[(B.2) used.]} \\
&= c^* c \int d^3 r\, \exp\!\left(-\frac{i}{\hbar} \boldsymbol{p} \cdot \boldsymbol{r} \right) \exp\!\left(\frac{i}{\hbar} \boldsymbol{p}' \cdot \boldsymbol{r} \right) \qquad \text{[(B.8a) used.]} \\
&= c^* c\, (2\pi\hbar)^3\, \delta(\boldsymbol{p} - \boldsymbol{p}')
\end{aligned}$$

$$\rightarrow \quad c^* c\, (2\pi\hbar)^3 = 1$$

$$\therefore \quad \langle\, \boldsymbol{r} \mid \boldsymbol{p} \,\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp\!\left(\frac{i}{\hbar} \boldsymbol{p} \cdot \boldsymbol{r} \right) \equiv \phi_{\boldsymbol{p}}(\boldsymbol{r}) \qquad \text{(B.8)}$$

where both $\phi_{\boldsymbol{p}}$ & $\mid \boldsymbol{p} \,\rangle$ denote the momentum eigenstate of eigenvalue $\boldsymbol{p}$. In terms of the wave-vectors,

$$\langle\, \boldsymbol{r} \mid \boldsymbol{k} \,\rangle = \frac{1}{(2\pi)^{3/2}} \exp(i\, \boldsymbol{k} \cdot \boldsymbol{r}) \equiv \phi_{\boldsymbol{k}}(\boldsymbol{r}) \qquad \text{(B.8b)}$$

In the p-representation, we have

$$\langle\, \boldsymbol{p}' \mid \boldsymbol{p} \,\rangle = \phi_{\boldsymbol{p}}(\boldsymbol{p}') = \delta(\boldsymbol{p} - \boldsymbol{p}') \qquad \text{[(B.2c) used.]} \qquad \text{(B.9)}$$

$$\langle\, \boldsymbol{k}' \mid \boldsymbol{k} \,\rangle = \phi_{\boldsymbol{k}}(\boldsymbol{k}') = \delta(\boldsymbol{k} - \boldsymbol{k}')$$

Taking the complex conjugate of (B.8) gives the position eigenstates in the p-representation as

$$\langle\, \boldsymbol{p} \mid \boldsymbol{r} \,\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \exp\!\left(-\frac{i}{\hbar} \boldsymbol{p} \cdot \boldsymbol{r} \right) \equiv \phi_{\boldsymbol{r}}(\boldsymbol{p}) \qquad \text{(B.10)}$$

$$\langle\, \boldsymbol{k} \mid \boldsymbol{r} \,\rangle = \frac{1}{(2\pi)^{3/2}} \exp(-i\, \boldsymbol{k} \cdot \boldsymbol{r}) \equiv \phi_{\boldsymbol{r}}(\boldsymbol{k})$$

which, of course, can also be derived the hard way following the path from (B.7) to (B.8). In the In the r-representation, we have

$$\langle \boldsymbol{r}' \mid \boldsymbol{r} \rangle = \phi_{\boldsymbol{r}}(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \qquad \text{[(B.2c) used.]} \tag{B.11}$$

B.1.2. Particle in a Box

For bounded systems, eigenvalues of $\hat{\boldsymbol{p}}$ become discrete.

Consider a particle in a box of sides L and volume $V = L^3$. Imposing periodic boundary conditions

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}(\boldsymbol{r} + \hat{\boldsymbol{x}} L) = \phi_{\boldsymbol{k}}(\boldsymbol{r} + \hat{\boldsymbol{y}} L) = \phi_{\boldsymbol{k}}(\boldsymbol{r} + \hat{\boldsymbol{z}} L) \tag{B.12a}$$

on (B.8b) gives the constraints

$$\exp(i \boldsymbol{k} \cdot \hat{\boldsymbol{x}} L) = \exp(i \boldsymbol{k} \cdot \hat{\boldsymbol{y}} L) = \exp(i \boldsymbol{k} \cdot \hat{\boldsymbol{z}} L) = 1$$

which can be satisfied if

$$\boldsymbol{k} = \frac{2\pi}{L} \boldsymbol{n} \qquad \boldsymbol{n} = (n_x, n_y, n_z) \qquad \forall\ n_j = 0, \pm 1, \pm 2, \ \ldots \tag{B.12}$$

The orthonormal & completeness relations (B.2c) & (B.2) are likewise discretized

$$\langle \boldsymbol{k} \mid \boldsymbol{k}' \rangle = \delta_{\boldsymbol{k}\boldsymbol{k}'} \qquad \& \qquad \sum_{\boldsymbol{k}} \mid \boldsymbol{k} \rangle \langle \boldsymbol{k} \mid = \hat{1} \tag{B.13}$$

In the r-representation, the normalization condition becomes

$$1 = \langle \boldsymbol{k} \mid \boldsymbol{k} \rangle = \int d^3 r\, \phi_{\boldsymbol{k}}^*(\boldsymbol{r})\, \phi_{\boldsymbol{k}}(\boldsymbol{r}) = L^3 c^* c \qquad \text{[(B.8a) used.]}$$

$$\rightarrow \quad \langle \boldsymbol{r} \mid \boldsymbol{k} \rangle = \phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{L^{3/2}} e^{i \boldsymbol{k} \cdot \boldsymbol{r}} \tag{B.14}$$