1.4 Dirac's Bra-Ket Formalism

To emphasize the fact that the wave function $\Psi(\mathbf{x}, t)$ is a vector in the Hilbert space $\mathcal{H}$, we can write it as

$$\Psi(\mathbf{x}, t) = \Psi_{\mathbf{x}}(t) \qquad (1.108)$$

where $\mathbf{x}$ serves as a triply infinite and continuous index for the components of Ψ.

The norm of a complex vector is defined as

$$|\,\mathbf{v}\,| = \sqrt{\sum_i v_i^* v_i} \qquad (1.109)$$

The continuous version is obviously

$$|\,\Psi(t)\,|^2 = \int d^3x\, \Psi_{\mathbf{x}}^*(t)\, \Psi_{\mathbf{x}}(t)$$

$$= \int d^3x\, \Psi^*(\mathbf{x}, t)\, \Psi(\mathbf{x}, t) \qquad (1.110)$$

1.4.1. Basis Transformations

Let $\{ \mathbf{b}^a \mid a = 1, \ldots, D \}$ be a set of orthonormal basis of a finite dimensional complex vector space $\mathcal{V}$. In terms of the original orthonormal basis $\{ \mathbf{e}^i \mid i = 1, \ldots, D \}$, we have

$$\mathbf{b}^a = \sum_i \mathbf{e}^i\, b_i{}^a$$

where $b_i{}^a$ is the i^{th} component of $\mathbf{b}^a$ with respect to the $\{ \mathbf{e}^i \}$ basis. It is common practice to use $b_i{}^a$ to denote the transformation matrix.

For any vector in $\mathcal{V}$,

$$\mathbf{v} = \sum_i \mathbf{e}^i\, v_i$$

$$= \sum_a \mathbf{b}^a\, v_a = \sum_{i,a} \mathbf{e}^i\, b_i{}^a\, v_a$$

$$\rightarrow \qquad v_i = \sum_a b_i{}^a\, v_a \qquad (1.111)$$

Orthonormality of the bases implies the inner products

$$(\mathbf{e}^i, \mathbf{e}^j) = \delta^{ij} \qquad\qquad (\mathbf{b}^a, \mathbf{b}^{a'}) = \delta^{a\,a'}$$

Hence,

$$(\mathbf{b}^a, \mathbf{b}^{a'}) = \sum_{i,j} (\mathbf{e}^i\, b_i{}^a, \mathbf{e}^j\, b_j{}^{a'})$$

$$= \sum_{i,j} b_i{}^{a\,*}\, b_j{}^{a'}\, (\mathbf{e}^i, \mathbf{e}^j)$$

$$= \sum_i b_i{}^{a\,*}\, b_i{}^{a'} = \delta^{a\,a'} \qquad (1.113)$$

which means the transformation matrix $b_i{}^a$ is unitary.

Using (1.113) on (1.111) gives

$$\sum_i b_i{}^{a'\,*}\, v_i = \sum_{a,i} b_i{}^{a'\,*}\, b_i{}^a\, v_a = \sum_a \delta^{a'\,a}\, v_a = v_{a'}$$

i.e.,

$$v_a = \sum_i b_i{}^{a\,*}\, v_i \qquad (1.112)$$

Putting (1.112) into (1.111) gives

$$v_i = \sum_{a,j} b_i^a \, b_j^{a*} \, v_j$$

$$\rightarrow \qquad \sum_a b_i^a \, b_j^{a*} = \delta_{ij} \qquad (1.114)$$

Since (1.114) gaurantees (1.111), it is called the completeness relation (or criterion) for the $\{ \boldsymbol{b}^a \}$ basis.

The Hilbert space is simply the generalization of the vector space to the case of infinite dimensions and bases with continuous indexing.

From (1.108), we see that the Hilbert space $\mathcal{H}$ of wave functions showcases a basis with continuous indexing $\boldsymbol{x}$. An approximate discretized version can be obtained using a set of local basis functions defined by

$$h^{\boldsymbol{n}}(\boldsymbol{x}) = \begin{cases} \epsilon^{-3/2} & \text{for } \left| x_i - x_{\boldsymbol{n}\,i} \right| \le \frac{\epsilon}{2}, \quad i = 1, 2, 3 \\ 0 & \text{otherwise} \end{cases} \qquad (1.116)$$

where

$$\boldsymbol{x}_{\boldsymbol{n}} = (n_1, n_2, n_3)\, \epsilon \qquad n_i = 0, \pm 1, \pm 2, \ \ldots \qquad (1.115)$$

These local basis functions are orthonormal since

$$\left(h^{\boldsymbol{n}}, h^{\boldsymbol{n}'} \right) = \int d^3 x \, h^{\boldsymbol{n}}(\boldsymbol{x})^* \, h^{\boldsymbol{n}'}(\boldsymbol{x})$$

$$= \begin{cases} \epsilon^3 \left(\epsilon^{-3/2} \right)^2 = 1 & \text{if } \boldsymbol{n} = \boldsymbol{n}' \\ 0 & \text{if } \boldsymbol{n} \neq \boldsymbol{n}' \end{cases}$$

$$= \delta^{\boldsymbol{n}\,\boldsymbol{n}'} \qquad (1.117)$$

In terms of this basis, any state in $\mathcal{H}$ is written as

$$\Psi(t) \approx \sum_{\boldsymbol{n}} h^{\boldsymbol{n}} \, \Psi_{\boldsymbol{n}}(t) \qquad (1.118a)$$

where $\Psi_{\boldsymbol{n}}(t)$ is the component of $\Psi(t)$ along $h^{\boldsymbol{n}}$.

The wave function $\Psi(\boldsymbol{x}, t)$, which is just the component of $\Psi(t)$ along $\boldsymbol{x}$, is therefore

$$\Psi(\boldsymbol{x}, t) \approx \sum_{\boldsymbol{n}} h^{\boldsymbol{n}}(\boldsymbol{x}) \, \Psi_{\boldsymbol{n}}(t) \qquad (1.118)$$

$\Psi_{\boldsymbol{n}}(t)$ can be calculated using (1.117) on (1.118):

$$\left(h^{\boldsymbol{n}}, \Psi(t) \right) = \int d^3 x \, h^{\boldsymbol{n}}(\boldsymbol{x})^* \, \Psi(\boldsymbol{x}, t) = \sum_{\boldsymbol{n}'} \int d^3 x \, h^{\boldsymbol{n}}(\boldsymbol{x})^* \, h^{\boldsymbol{n}'}(\boldsymbol{x}) \, \Psi_{\boldsymbol{n}'}(t)$$

$$= \sum_{\boldsymbol{n}'} \delta^{\boldsymbol{n}\,\boldsymbol{n}'} \, \Psi_{\boldsymbol{n}'}(t) = \Psi_{\boldsymbol{n}}(t)$$

By (1.116), we also have

$$\int d^3 x \, h^{\boldsymbol{n}}(\boldsymbol{x})^* \, \Psi(\boldsymbol{x}, t) \approx \epsilon^3 \, \epsilon^{-3/2} \, \Psi(\boldsymbol{x}_{\boldsymbol{n}}, t) \ = \epsilon^{3/2} \, \Psi(\boldsymbol{x}_{\boldsymbol{n}}, t)$$

so that

$$\Psi_{\boldsymbol{n}}(t) \approx \epsilon^{3/2} \, \Psi(\boldsymbol{x}_{\boldsymbol{n}}, t) \qquad (1.119)$$

In general, given a set of complete, orthonormal basis functions $\{ f^a(\boldsymbol{x}) \}$ so that

$$\left(f^a, f^{a'} \right) = \int d^3 x \, f^a(\boldsymbol{x})^* \, f^{a'}(\boldsymbol{x}) = \delta^{a\,a'} \qquad (1.120)$$

any state or wave function that can be expanded as

$$\Psi(t) = \sum_a f^a \, \Psi_a(t)$$

$$\Psi(\boldsymbol{x}, t) = \sum_a f^a(\boldsymbol{x})\, \Psi_a(t) \tag{1.121}$$

has components

$$\Psi_a(t) = (\, f^a, \Psi(t)\,)$$
$$= \int d^3 x\, f^a(\boldsymbol{x})^* \, \Psi(\boldsymbol{x}, t) \tag{1.122}$$

Given another set of orthonormal basis functions $\left\{ \tilde{f}^{\,b}(\boldsymbol{x}) \right\}$ so that

$$\int d^3 x\, \tilde{f}^{\,b}(\boldsymbol{x})^* \, \tilde{f}^{\,b'}(\boldsymbol{x}) = \delta^{b\, b'} \tag{1.123}$$

any wave function that can be expanded as

$$\Psi(\boldsymbol{x}, t) = \sum_a \tilde{f}^{\,b}(\boldsymbol{x})\, \tilde{\Psi}_b(t) \tag{1.124}$$

has components

$$\tilde{\Psi}_b(t) = \int d^3 x\, \tilde{f}^{\,b}(\boldsymbol{x})^* \, \Psi(\boldsymbol{x}, t) \tag{1.125}$$

Inserting (1.121) into (1.125) gives

$$\tilde{\Psi}_b(t) = \sum_a \int d^3 x\, \tilde{f}^{\,b}(\boldsymbol{x})^* \, f^a(\boldsymbol{x})\, \Psi_a(t) \tag{1.126}$$

1.4.2. Bracket Notation

Dirac's bracket notation:

$$\left\langle \tilde{b} \mid a \right\rangle \equiv \int d^3 x\, \tilde{f}^{\,b}(\boldsymbol{x})^* \, f^a(\boldsymbol{x}) \tag{1.127}$$

Note: Strictly speaking, (1.127) should be written as

$$\left\langle \tilde{f}^{\,b} \mid f^a \right\rangle \equiv \int d^3 x\, \tilde{f}^{\,b}(\boldsymbol{x})^* \, f^a(\boldsymbol{x}) \tag{1.127a}$$

However, the simplified notation of (1.127) is preferred.

Using

$$f^a(\boldsymbol{x}) = \langle \boldsymbol{x} \mid f^a \rangle = \langle \boldsymbol{x} \mid a \rangle$$
$$\tilde{f}^{\,b}(\boldsymbol{x})^* = \left\langle \boldsymbol{x} \mid \tilde{f}^{\,b} \right\rangle^* = \left\langle \boldsymbol{x} \mid \tilde{b} \right\rangle^*$$
$$= \left\langle \tilde{f}^{\,b} \mid \boldsymbol{x} \right\rangle = \left\langle \tilde{b} \mid \boldsymbol{x} \right\rangle$$

we can write (1.27) & (1.127a) as

$$\left\langle \tilde{b} \mid a \right\rangle \equiv \int d^3 x \left\langle \tilde{b} \mid \boldsymbol{x} \right\rangle \langle \boldsymbol{x} \mid a \rangle$$

$$\left\langle \tilde{f}^{\,b} \mid f^a \right\rangle \equiv \int d^3 x \left\langle \tilde{f}^{\,b} \mid \boldsymbol{x} \right\rangle \langle \boldsymbol{x} \mid f^a \rangle$$

which are identities by virtue of the completeness relation

$$\int d^3 x \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid = 1 \tag{1.127b}$$

of the basis $\mid \boldsymbol{x} \rangle$. In other words, in writing (1.127), we've already assumed (1.127b).

(1.122), (1.125) & (1.126) become

$$\Psi_a(t) = \langle\, a \mid \Psi(t)\, \rangle$$
$$\tilde{\Psi}_b(t) = \left\langle\, \tilde{b} \mid \Psi(t)\, \right\rangle \tag{1.128}$$
$$= \sum_a \left\langle \tilde{b} \mid a \right\rangle \langle\, a \mid \Psi(t)\, \rangle \tag{1.129}$$

which implies the completeness relation

$$\sum_a |\, a \rangle \langle a \,| = 1 \tag{1.130}$$

Orthonormality relations (1.120) & (1.123) become

$$\langle a \mid a' \rangle = \int d^3x\, f^a(\boldsymbol{x})^* f^{a'}(\boldsymbol{x}) = \delta^{a\,a'}$$

$$\langle \tilde{b} \mid b' \rangle = \int d^3x\, \tilde{f}^b(\boldsymbol{x})^* \tilde{f}^{b'}(\boldsymbol{x}) = \delta^{b\,b'} \tag{1.132}$$

For (1.117), we set

$$h^{\boldsymbol{n}}(\boldsymbol{x}) = \langle \boldsymbol{x} \mid h^{\boldsymbol{n}} \rangle = \langle \boldsymbol{x} \mid \boldsymbol{x}_{\boldsymbol{n}} \rangle$$

$$\rightarrow \qquad h^{\boldsymbol{n}}(\boldsymbol{x})^* = \langle h^{\boldsymbol{n}} \mid \boldsymbol{x} \rangle = \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \boldsymbol{x} \rangle \tag{1.132a}$$

By (1.127), we have

$$\langle h^{\boldsymbol{n}} \mid h^{\boldsymbol{n}'} \rangle = \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \boldsymbol{x}_{\boldsymbol{n}'} \rangle = \int d^3x\, \langle h^{\boldsymbol{n}} \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid h^{\boldsymbol{n}'} \rangle$$

$$= \int d^3x\, h^{\boldsymbol{n}}(\boldsymbol{x})^* h^{\boldsymbol{n}'}(\boldsymbol{x}) = \delta^{\boldsymbol{n}\,\boldsymbol{n}'} \tag{1.133}$$

where the last equality comes from (1.117).

For (1.119),

$$\Psi_{\boldsymbol{n}}(t) = \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \Psi(t) \rangle \approx \epsilon^{3/2}\, \Psi(\boldsymbol{x}_{\boldsymbol{n}}, t) \tag{1.134}$$

$$= \sum_a \langle \boldsymbol{x}_{\boldsymbol{n}} \mid a \rangle \langle a \mid \Psi(t) \rangle \tag{1.135}$$

where the completeness relation (1.130) was used.

Alternatively, using the completeness relation of $|\, \boldsymbol{x} \rangle$, we have

$$\langle \boldsymbol{x}_{\boldsymbol{n}} \mid \Psi(t) \rangle = \int d^3x\, \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid \Psi(t) \rangle$$

$$= \int d^3x\, h^{\boldsymbol{n}}(\boldsymbol{x})^* \langle \boldsymbol{x} \mid \Psi(t) \rangle \tag{1.137}$$

$$= \int d^3x\, h^{\boldsymbol{n}}(\boldsymbol{x})^*\, \Psi(\boldsymbol{x}, t)$$

Writing (1.118) as

$$\langle \boldsymbol{x} \mid \Psi(t) \rangle \approx \sum_{\boldsymbol{n}} \langle \boldsymbol{x} \mid \boldsymbol{x}_{\boldsymbol{n}} \rangle \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \Psi(t) \rangle \tag{1.136}$$

gives us the approximate completeness relation

$$\sum_{\boldsymbol{n}} |\, \boldsymbol{x}_{\boldsymbol{n}} \rangle \langle \boldsymbol{x}_{\boldsymbol{n}} \,| \approx 1 \tag{1.138}$$

which is the bracket version of (1.118a).

1.4.3. Continuum Limit

Using (1.116) on (1.137) gives

$$\langle \boldsymbol{x}_{\boldsymbol{n}} \mid \Psi(t) \rangle \approx \epsilon^3\, \epsilon^{-3/2} \langle \boldsymbol{x} \mid \Psi(t) \rangle \text{with} \qquad \left| \boldsymbol{x} - \boldsymbol{x}_n \right| < \frac{\epsilon}{2}$$

$$\rightarrow \qquad \langle \boldsymbol{x} \mid \Psi(t) \rangle \approx \epsilon^{-3/2} \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \Psi(t) \rangle \tag{1.139}$$

Using the completeness relation (1.138), we can write

$$\langle a \mid \Psi(t) \rangle \approx \sum_{\boldsymbol{n}} \langle a \mid \boldsymbol{x}_{\boldsymbol{n}} \rangle \langle \boldsymbol{x}_{\boldsymbol{n}} \mid \Psi(t) \rangle$$

$$\approx \sum_{n} \epsilon^3 \langle a \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid \Psi(t) \rangle \Big|_{\boldsymbol{x}=\boldsymbol{x}_n} \tag{1.141}$$

As $\epsilon \to 0$, the sum goes into an integral and we have

$$\langle a \mid \Psi(t) \rangle = \int d^3 x \langle a \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid \Psi(t) \rangle \tag{1.142}$$

which agrees with the completeness relation

$$\int d^3 x \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid = 1 \tag{1.143}$$

Taking $\mid \Psi(t) \rangle$ as a vector in the Hilbert space, (1.142) can also be viewed as the transformation of the components of $\mid \Psi(t) \rangle$ from the $\mid \boldsymbol{x} \rangle$ basis to the $\mid a \rangle$ basis.

In summary, given a basis satisfying the completeness relation

$$\sum_a \mid a \rangle \langle a \mid = 1 \tag{1.145}$$

any vector $\mid \Psi(t) \rangle$ can be written as

$$\mid \Psi(t) \rangle = \sum_a \mid a \rangle \langle a \mid \Psi(t) \rangle \tag{1.146}$$

which implies

$$\langle b \mid \Psi(t) \rangle = \sum_a \langle b \mid a \rangle \langle a \mid \Psi(t) \rangle \tag{1.147}$$

so that $\langle b \mid a \rangle$ is the transformation matrix between the $\mid a \rangle$ & $\mid b \rangle$ bases.

Using the completeness relation

$$\int d^3 x \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid = 1 \tag{1.148}$$

we can write

$$\mid \Psi(t) \rangle = \int d^3 x \mid \boldsymbol{x} \rangle \langle \boldsymbol{x} \mid \Psi(t) \rangle \tag{1.149}$$

in which the wave function $\Psi(\boldsymbol{x}, t) = \langle \boldsymbol{x} \mid \Psi(t) \rangle$ plays the role of the component of $\mid \Psi(t) \rangle$ in the local basis $\mid \boldsymbol{x} \rangle$ basis, which in turn, is the continuum limit of the discrete local basis

$$\mid \boldsymbol{x} \rangle \approx \epsilon^{-3/2} \mid \boldsymbol{x}_n \rangle \tag{1.150}$$

Since

$$\langle \tilde{b} \mid a \rangle = \int d^3 x \, \tilde{f}^b(\boldsymbol{x})^* f^a(\boldsymbol{x})$$

$$\langle a \mid \tilde{b} \rangle = \int d^3 x \, f^a(\boldsymbol{x})^* \tilde{f}^b(\boldsymbol{x}) \tag{1.151}$$

we have

$$\langle \tilde{b} \mid a \rangle = \langle a \mid \tilde{b} \rangle^* \tag{1.152}$$

Using the completeness relation (1.145), we can expand $\Psi(t)$ as a ket vector

$$\mid \Psi(t) \rangle = \sum_a \mid a \rangle \langle a \mid \Psi(t) \rangle \tag{1.153}$$

or a bra vector

$$\langle \Psi(t) \mid = \sum_a \langle \Psi(t) \mid a \rangle \langle a \mid \tag{1.154}$$

1.4.4. Generalized Functions

A Hilbert space was loosely defined [see (1.109)] as a set of vectors with finite norms. Using (1.150) and (1.133), we have

$$\langle \boldsymbol{x} \mid \boldsymbol{x}' \rangle \approx \epsilon^{-3} \langle \boldsymbol{x}_n \mid \boldsymbol{x}_n' \rangle = \epsilon^{-3} \delta_{n n'} \tag{1.155}$$

where

$$\left| \boldsymbol{x} - \boldsymbol{x}_n \right| < \frac{\epsilon}{2} \text{ and } \qquad \left| \boldsymbol{x}' - \boldsymbol{x}_n' \right| < \frac{\epsilon}{2}$$

Thus, for $\boldsymbol{x} \neq \boldsymbol{x}'$, the states $| \boldsymbol{x} \rangle$ and $| \boldsymbol{x}' \rangle$ are orthogonal. However, as $\epsilon \to 0$, the norm $\langle \boldsymbol{x} \mid \boldsymbol{x} \rangle$ becomes inifinite so that $| \boldsymbol{x} \rangle$ is not a member of the Hilbert space.

Note that

$$\epsilon^3 \sum_{n'} \epsilon^{-3} \delta_{n n'} = \sum_{n'} \delta_{n n'} = 1 \tag{1.156}$$

In the limit $\epsilon \to 0$, (1.155) becomes

$$\langle \boldsymbol{x} \mid \boldsymbol{x}' \rangle = \delta(\boldsymbol{x} - \boldsymbol{x}') \tag{1.157}$$

where

$$\delta(\boldsymbol{x} - \boldsymbol{x}') = 0 \qquad \text{for } \boldsymbol{x} \neq \boldsymbol{x}' \tag{1.158}$$

$$\int d^3 x' \, \delta(\boldsymbol{x} - \boldsymbol{x}') = 1 \tag{1.159}$$

As $\epsilon \to 0$, we can treat $\boldsymbol{x}_n$, $\boldsymbol{x}_{n'}$ as continuous variables and the sum becomes an integral

$$\epsilon^3 \sum_{n'} \epsilon^{-3} \delta_{n n'} \approx \int d^3 x_{n'} \, \delta(\boldsymbol{x}_{n'} - \boldsymbol{x}_n) = 1$$

where we have set

$$\delta(\boldsymbol{x}_n - \boldsymbol{x}_{n'}) = \lim_{\epsilon \to 0} \epsilon^{-3} \delta_{n n'}$$

$\delta(\boldsymbol{x}_n - \boldsymbol{x}_{n'})$ is the 3-D version of a Dirac delta-function $\delta(x)$ defined as a distribution (or generalized function) satisfying

$$\delta(x - a) = 0 \qquad \text{for } x \neq a$$

and

$$\int_\Omega d x \, \delta(x - a) f(x) = f(a) \tag{1.162}$$

where f is any function and Ω is any positively oriented interval that includes the point $x = a$. Thus, the δ-function is called a generalized function or distribution which picks out the value of any smooth test function f at some chosen point.

Setting $f(x) = 1$ in (1.162) gives

$$\int_\Omega d x \, \delta(x - a) = 1 \tag{1.162a}$$

For α, $\Delta > 0$, we set $y = \alpha x$ to get

$$\int_{a-\Delta}^{a+\Delta} d x \, \delta[\alpha (x - a)] f(x) = \frac{1}{\alpha} \int_{\alpha a - \alpha \Delta}^{\alpha a + \alpha \Delta} d y \, \delta(y - \alpha a) f\left(\frac{y}{\alpha}\right) = \frac{1}{\alpha} f(a)$$

$$= \frac{1}{\alpha} \int_{a-\Delta}^{a+\Delta} d x \, \delta (x - a) f(x)$$

$$\to \qquad \delta[\alpha (x - a)] = \frac{1}{\alpha} \delta (x - a)$$

For $\alpha < 0$, we set $y = -\alpha x = | \alpha | x$ to get

$$\int_{a-\Delta}^{a+\Delta} d x \, \delta[\alpha (x - a)] f(x) = -\frac{1}{\alpha} \int_{-\alpha a + \alpha \Delta}^{-\alpha a - \alpha \Delta} d y \, \delta(-y - \alpha a) f\left(-\frac{y}{\alpha}\right)$$

$$= \frac{1}{| \alpha |} \int_{| \alpha | a - | \alpha | \Delta}^{| \alpha | a + | \alpha | \Delta} d y \, \delta (-y + | \alpha | a) f\left(\frac{y}{| \alpha |}\right)$$

$$= \frac{1}{|\alpha|} f(a) = \frac{1}{|\alpha|} \int_{a-\Delta}^{a+\Delta} dx\, \delta(x-a) f(x)$$

$$\rightarrow \quad \delta[\alpha(x-a)] = \frac{1}{|\alpha|} \delta(x-a) \qquad (1.160)$$

which is applicable for all α. Note that (1.160) assumes the domains of integration are always positively oriented.

For $\alpha = -1$, we have

$$\delta[-(x-a)] = \delta(x-a) \qquad (1.160a)$$

so that δ is an even function.

Setting $y = f(x)$, we have

$$\mathcal{I} = \int dx\, \delta[f(x)]\, g(x)$$

$$= \int dy \frac{1}{|f'(x)|} \delta(y)\, g(x)$$

where the absolute value of $f' = \frac{df}{dx}$ was used for the same reason that led to (1.160). This includes the implicit assumption that the domain of both integrals are positively oriented. Since $y = 0$ for all roots x_i of $f(x)$, we have

$$\mathcal{I} = \sum_i \frac{1}{|f'(x_i)|} g(x_i)$$

$$= \sum_i \frac{1}{|f'(x_i)|} \int dx\, \delta(x - x_i)\, g(x)$$

where we've assumed that the domain of integration covers all x_i. Comparing both expressions of $\mathcal{I}$, we have

$$\delta[f(x)] = \sum_i \frac{1}{|f'(x_i)|} \delta(x - x_i) \qquad (1.161)$$

1.4.5. Schrodinger Equation in Dirac Notation

In terms of the bra-ket notation, the Schrodinger eq. can be written as

$$i\hbar \frac{\partial}{\partial t} \left| \Psi(t) \right\rangle = \hat{H} \left| \Psi(t) \right\rangle \qquad (1.163)$$

which is basis independent.

In the x-representation, one uses the eigenstates $\{ | \boldsymbol{x} \rangle \}$ of the Cartesian position operator $\hat{\boldsymbol{x}}$ as basis. By definition,

$$\hat{\boldsymbol{x}} \,|\, \boldsymbol{x} \rangle = \boldsymbol{x} \,|\, \boldsymbol{x} \rangle \qquad (1.164a)$$

It is easy to show that $\hat{\boldsymbol{x}}$ is self-adjoint (hermitian) in the x-representation. Since hermiticity is independent of basis, $\hat{\boldsymbol{x}}$ is hermitian. Taking the adjoint on (1.164a), we get

$$\langle \boldsymbol{x} \,|\, \hat{\boldsymbol{x}} = \boldsymbol{x} \langle \boldsymbol{x} \,| \qquad (1.165)$$

$$\langle \boldsymbol{x} \,|\, \hat{\boldsymbol{x}} \,|\, \boldsymbol{x}' \rangle = \boldsymbol{x} \langle \boldsymbol{x} \,|\, \boldsymbol{x}' \rangle = \boldsymbol{x}\, \delta(\boldsymbol{x} - \boldsymbol{x}') \qquad (1.167)$$

The canonical commutator

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

implies

$$\langle \boldsymbol{x} \,|\, [\hat{x}_i, \hat{p}_i] \,|\, \boldsymbol{x}' \rangle = i\hbar \langle \boldsymbol{x} \,|\, \boldsymbol{x}' \rangle$$

$$\therefore \quad \langle \boldsymbol{x} \mid (x_i \hat{p}_i - \hat{p}_i x_i'] \mid \boldsymbol{x}' \rangle = i\hbar\, \delta(\boldsymbol{x} - \boldsymbol{x}')$$
$$= (x_i - x_i') \langle \boldsymbol{x} \mid \hat{p}_i \mid \boldsymbol{x}' \rangle$$

$$\rightarrow \quad (x_i - x_i') \langle x_i \mid \hat{p}_i \mid x_i' \rangle = i\hbar\, \delta(x_i - x_i') \qquad (1.164b)$$

Integrating by part gives

$$\int d\,x\, \delta'(x-a)\, f(x) = -\int d\,x\, \delta(x-a)\, f'(x) = f'(a)$$

Setting $f(x) = x - a$, we have

$$\int d\,x\, \delta'(x-a)\,(x-a) = -\int d\,x\, \delta(x-a)$$

or

$$\delta'(x-a)\,(x-a) = -\delta(x-a)$$

(1.164b) thus implies

$$\langle x_i \mid \hat{p}_i \mid x_i' \rangle = -i\hbar \frac{d}{d\,x} \delta(x_i - x_i')$$

$$\rightarrow \quad \langle \boldsymbol{x} \mid \hat{\boldsymbol{p}} \mid \boldsymbol{x}' \rangle = -i\hbar \nabla \delta(\boldsymbol{x} - \boldsymbol{x}') = -i\hbar \nabla \langle \boldsymbol{x} \mid \boldsymbol{x}' \rangle \qquad (1.166)$$

Since this is valid for all $\mid \boldsymbol{x}' \rangle$, we have

$$\therefore \quad \langle \boldsymbol{x} \mid \hat{\boldsymbol{p}} = \frac{\hbar}{i} \nabla \langle \boldsymbol{x} \mid \qquad (1.164)$$

$$\rightarrow \quad \langle \boldsymbol{x} \mid H(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}, t) \mid \Psi(t) \rangle = H\left(\hat{\boldsymbol{x}}, \frac{\hbar}{i} \nabla, t\right) \langle \boldsymbol{x} \mid \Psi(t) \rangle$$
$$= i\hbar \frac{\partial}{\partial t} \langle \boldsymbol{x} \mid \Psi(t) \rangle \qquad (1.168)$$

where (1.163) was used to get last expression.

Setting $\Psi(\boldsymbol{x}, t) = \langle \boldsymbol{x} \mid \Psi(t) \rangle$, we recover the familiar form

$$i\hbar \frac{\partial}{\partial t} \Psi(\boldsymbol{x}, t) = H\left(\hat{\boldsymbol{x}}, \frac{\hbar}{i} \nabla, t\right) \Psi(\boldsymbol{x}, t)$$

By definition,

$$\langle a \mid \hat{O} \mid b \rangle = \langle a \mid \hat{O}\, b \rangle = \langle \hat{O}^{+} a \mid b \rangle$$
$$= \langle b \mid \hat{O}^{+} a \rangle^{*} = \langle b \mid \hat{O}^{+} \mid a \rangle^{*} \qquad (1.173)$$

for any states a, b, and operator $\hat{O}$.

If $\hat{O}$ is hermitian, then

$$\langle a \mid \hat{O} \mid b \rangle = \langle b \mid \hat{O} \mid a \rangle^{*}$$

The matrix with elements

$$O_{a\,b} = \langle a \mid \hat{O} \mid b \rangle = O_{b\,a}^{*}$$

is therefore a hermitian matrix.

Using (1.164), one can show that $\hat{\boldsymbol{p}}$ is hermitian. Hence,

$$\langle a \mid \hat{\boldsymbol{x}} \mid b \rangle = \langle b \mid \hat{\boldsymbol{x}} \mid a \rangle^{*} \qquad (1.169)$$
$$\langle a \mid \hat{\boldsymbol{p}} \mid b \rangle = \langle b \mid \hat{\boldsymbol{p}} \mid a \rangle^{*} \qquad (1.170)$$

For $\hat{H}$ hermitian,

$$\langle a \mid \hat{H} \mid b \rangle = \langle b \mid \hat{H} \mid a \rangle^{*} \qquad (1.171)$$

All quantities that have classical counterparts can be expressed in operator form

$$\hat{O}(t) = O(\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}, t) \qquad (1.172)$$

The measured values of a physical quantity must be real. Assuming the particle is in some state a, this means

$$\left\langle a \mid \hat{O} \mid a \right\rangle = \left\langle a \mid \hat{O} \mid a \right\rangle^*$$

i.e., $\hat{O}$ must be hermitian.

Let $\mid E_n \rangle$ be the stationary states of (1.94), then they are also the eigenstates of $\hat{H}$ so that

$$\hat{H} \mid E_n \rangle = E_n \mid E_n \rangle \qquad (1.175)$$

1.4.6. Momentum States

Consider the momentum eigenstates satisfying

$$\hat{\boldsymbol{p}} \mid \boldsymbol{p} \rangle = \boldsymbol{p} \mid \boldsymbol{p} \rangle \qquad (1.176)$$

$$\rightarrow \qquad \langle \boldsymbol{x} \mid \hat{\boldsymbol{p}} \mid \boldsymbol{p} \rangle = \boldsymbol{p} \langle \boldsymbol{x} \mid \boldsymbol{p} \rangle$$

Using (1.164), we have

$$\frac{\hbar}{i} \nabla \langle \boldsymbol{x} \mid \boldsymbol{p} \rangle = \boldsymbol{p} \langle \boldsymbol{x} \mid \boldsymbol{p} \rangle \qquad (1.177)$$

Hence,

$$\langle \boldsymbol{x} \mid \boldsymbol{p} \rangle = C e^{i \boldsymbol{p} \cdot \boldsymbol{x} / \hbar} \qquad (1.178)$$

where C is some normalization constant. Comparing with (1.75), we see that the wave function of a free particle with momentum $\boldsymbol{p}$ is also the eigenstate of $\hat{\boldsymbol{p}}$.

In order for $\mid \boldsymbol{p} \rangle$ to have a finite norm, the particle must be confined to a finite volume, say, a cube of side L and volume L^3. Assuming periodic boundary conditions, we have

$$e^{i p_i L / \hbar} = 1 \qquad i = 1, 2, 3$$

with solutions

$$\frac{p_i^{m_i} L}{\hbar} = 2 \pi m_i \qquad m_i = 0, \pm 1, \pm 2, \ldots$$

In vector form,

$$\boldsymbol{p}^{\boldsymbol{m}} = \frac{2 \pi \hbar}{L} \boldsymbol{m} = \frac{2 \pi \hbar}{L} (m_1, m_2, m_3) \qquad (1.179)$$

Using

$$\int_{L^3} d^3 x \left| \langle \boldsymbol{x} \mid \boldsymbol{p}^{\boldsymbol{m}} \rangle \right|^2 = L^3 \mid C \mid^2 = 1 \qquad (1.181)$$

we have

$$\langle \boldsymbol{x} \mid \boldsymbol{p}^{\boldsymbol{m}} \rangle = \frac{1}{L^{3/2}} e^{i \boldsymbol{p}^{\boldsymbol{m}} \cdot \boldsymbol{x} / \hbar} \qquad (1.180)$$

$$= \frac{1}{L^{3/2}} e^{i 2 \pi \boldsymbol{m} \cdot \boldsymbol{x} / L} \qquad (1.180a)$$

States $\mid \boldsymbol{p}^{\boldsymbol{m}} \rangle$ are orthonormal since

$$\left\langle \boldsymbol{p}^{\boldsymbol{m}'} \mid \boldsymbol{p}^{\boldsymbol{m}} \right\rangle = \int_{L^3} d^3 x \left\langle \boldsymbol{p}^{\boldsymbol{m}'} \mid \boldsymbol{x} \right\rangle \langle \boldsymbol{x} \mid \boldsymbol{p}^{\boldsymbol{m}} \rangle$$

$$= \frac{1}{L^3} \int_{L^3} d^3 x \, e^{i \left(\boldsymbol{p}^{\boldsymbol{m}} - \boldsymbol{p}^{\boldsymbol{m}'} \right) \cdot \boldsymbol{x} / \hbar} = \delta_{\boldsymbol{m}, \boldsymbol{m}'} \qquad (1.180b)$$

where the completeness of $\mid \boldsymbol{x} \rangle$ now reads

$$\int_{L^3} d^3x \; | \, \boldsymbol{x} \rangle \langle \boldsymbol{x} \, | = 1 \qquad (1.192)$$

Completeness of $| \, \boldsymbol{p}^{\boldsymbol{m}} \rangle$

$$\sum_{\boldsymbol{m}} | \, \boldsymbol{p}^{\boldsymbol{m}} \rangle \langle \boldsymbol{p}^{\boldsymbol{m}} \, | = 1 \qquad (1.182)$$

can be deduced from

$$\sum_{\boldsymbol{m}} \langle \boldsymbol{x} \, | \, \boldsymbol{p}^{\boldsymbol{m}} \rangle \langle \boldsymbol{p}^{\boldsymbol{m}} \, | \, \boldsymbol{x}' \rangle = \frac{1}{L^3} \sum_{\boldsymbol{m}} e^{i \boldsymbol{p}^{\boldsymbol{m}} \cdot (\boldsymbol{x} - \boldsymbol{x}')/\hbar} = \delta(\boldsymbol{x} - \boldsymbol{x}') = \langle \boldsymbol{x} \, | \, \boldsymbol{x}' \rangle$$

where we've used the 3-D version of the equality

$$\lim_{N \to \infty} \frac{1}{L} \sum_{m=-N}^{N} e^{i 2\pi m (x - x')/L} = \delta(x - x') \qquad (1.182a)$$

The proof of (1.182a) can be done in 2 steps. First, we discretize x and set $x_n = n\,a$. Since x & p come in pairs, we should have the same number of independent x_n & p^m points. Hence, we set $L = (2N+1)\,a$ so that

$$\frac{1}{L} \sum_{m=-N}^{N} e^{i 2\pi m (x_n - x_{n'})/L} = \frac{1}{(2N+1)\,a} \sum_{m=-N}^{N} e^{i 2\pi m (n - n')/(2N+1)}$$

$$= \frac{1}{(2N+1)\,a} \sum_{m=-N}^{N} e^{i m b} \qquad (1.182b)$$

where $b = \dfrac{2\pi (n - n')}{2N+1}$.

For $n \neq n'$,

$$\sum_{m=-N}^{N} e^{i m b} = \frac{e^{-i N b} - e^{i (N+1) b}}{1 - e^{i b}} = \frac{\sin\left(N + \frac{1}{2}\right) b}{\sin \frac{b}{2}} \xrightarrow[N \to \infty]{} 0 \qquad (1.182c)$$

For $n = n'$,

$$\sum_{m=-N}^{N} e^{i m b} = 2N + 1$$

(1.182c) thus becomes

$$\frac{1}{L} \sum_{m=-N}^{N} e^{i 2\pi m (x_n - x_{n'})/L} = \frac{2N+1}{L} \delta_{n n'} = \frac{1}{a} \delta_{n n'} \qquad (1.182d)$$

which implies

$$a \sum_{n=-N}^{N} \left(\frac{1}{L} \sum_{m=-N}^{N} e^{i 2\pi m (x_n - x_{n'})/L} \right) = 1 \qquad (1.182e)$$

Next, in the continuum limit, we set $a \to 0$ (and hence $N \to \infty$) so that (1.182e) becomes

$$\int_0^L d x \left(\frac{1}{L} \sum_{m=-N}^{N} e^{i 2\pi m (x - x')/L} \right) = 1$$

whereas (1.182d) gives

$$\frac{1}{L} \sum_{m=-N}^{N} e^{i 2\pi m (x - x')/L} = 0 \qquad \text{for } x \neq x'$$

thus proving (1.182a).

Using the completeness (1.182), we can write

$$\Psi(\mathbf{x},t)=\langle \mathbf{x}\mid\Psi(t)\rangle=\sum_{\mathbf{m}}\langle \mathbf{x}\mid \mathbf{p}^{\mathbf{m}}\rangle\langle \mathbf{p}^{\mathbf{m}}\mid\Psi(t)\rangle \qquad (1.183)$$

which is just the Fourier series expansion of Ψ.

For L large, (1.179) gives

$$\sum_{\mathbf{m}}\approx\left(\frac{L}{2\pi\hbar}\right)^3\int d^3p \qquad (1.184)$$

There are numerous ways to define the continuum version of $\mid \mathbf{p}^{\mathbf{m}}\rangle$, depending on the choice of normalization.

If we set the counterpart of the completeness (1.182) as

$$\int\frac{d^3p}{(2\pi\hbar)^3}\mid \mathbf{p}\rangle\langle \mathbf{p}\mid=1 \qquad (1.187)$$

then

$$\mid \mathbf{p}\rangle=L^{3/2}\mid \mathbf{p}^{\mathbf{m}}\rangle \qquad (1.185)$$

$$\langle \mathbf{x}\mid \mathbf{p}\rangle=e^{i\,\mathbf{p}\cdot\mathbf{x}/\hbar} \qquad (1.189)$$

and the orthogonality (1.180b) becomes

$$\langle \mathbf{p}'\mid \mathbf{p}\rangle=\int_{L^3}d^3x\,e^{i\,(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}/\hbar}=(2\pi\hbar)^3\,\delta(\mathbf{p}-\mathbf{p}') \qquad (1.186)$$

The expansion (1.183) becomes

$$\Psi(\mathbf{x},t)=\int\frac{d^3p}{(2\pi\hbar)^3}\langle \mathbf{x}\mid \mathbf{p}\rangle\langle \mathbf{p}\mid\Psi(t)\rangle \qquad (1.188)$$

Using the completeness (1.192), we have

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

$$=\int d^3x\,e^{-i\,\mathbf{p}\cdot\mathbf{x}/\hbar}\,\Psi(\mathbf{x},t) \qquad (1.191)$$

$\langle \mathbf{p}\mid\Psi(t)\rangle$ is therefore the inverse Fourier transform of $\Psi(\mathbf{x},t)$. It is often called the momentum space wave function.

1.4.7. Incompleteness and Poisson's Summation Formula

We wish to find out what happens when only a subset of the basis is used.

For the sake of simplicity, consider the 1-D case with the basis $\{\mid x\rangle\}$ satisfying the completeness

$$\int dx\mid x\rangle\langle x\mid=1 \qquad (1.194)$$

An often used subset of the basis is

$$B_N=\{\mid x_n\rangle;\ n=-N,\ \ldots,\ N\}\quad\text{with}\quad x_n=n\,a \qquad (1.194a)$$

Of particular interest is the sum

$$S_N=\sum_{n=-N}^{N}\mid x_n\rangle\langle x_n\mid \qquad (1.195)$$

To begin,

$$\langle p\mid S_N\mid p'\rangle=\sum_{n=-N}^{N}\langle p\mid x_n\rangle\langle x_n\mid p'\rangle$$

$$= \sum_{n=-N}^{N} e^{i(p'-p)na/\hbar} \tag{1.196}$$

Next, we shall make use of the Poisson summation formula

$$\sum_{n=-\infty}^{\infty} e^{2\pi i\mu n} = \sum_{m=-\infty}^{\infty} \delta(\mu - m) \tag{1.197}$$

which is a generalization of (1.182a) achieved by setting $L = 1$ so that $\mu = \frac{x - x'}{L}$ is no longer restricted to values smaller than 1. Conversely, (1.182a) is just a special case of (1.197) with $m = 0$. Kleinert also provided a similar proof [see eqs(1.199, 201-3) & Fig.2.4].

Thus (1.196) implies

$$\begin{aligned} \langle p \mid S_\infty \mid p' \rangle &= \sum_{m=-\infty}^{\infty} \langle p \mid x_n \rangle \langle x_n \mid p' \rangle \\ &= \sum_{m=-\infty}^{\infty} \delta\left(\frac{(p'-p)a}{2\pi\hbar} - m\right) \\ &= \sum_{m=-\infty}^{\infty} \frac{2\pi\hbar}{a}\, \delta\left(p' - p - \frac{2\pi\hbar}{a} m\right) \end{aligned} \tag{1.198}$$

On the other hand, keeping N finite in (1.182c) allows us to write (1.196) as

$$\begin{aligned} \langle p \mid S_N \mid p' \rangle &= \sum_{n=-N}^{N} \langle p \mid x_n \rangle \langle x_n \mid p' \rangle \\ &= \frac{\sin \frac{(p'-p)(2N+1)a}{2\hbar}}{\sin \frac{(p'-p)a}{2\hbar}} \end{aligned} \tag{1.200}$$

In (1.201-3), Kleinert showed by direct integration that the right hand side of (1.120) was indeed a sum of delta functions as $N \to \infty$. We'll skip this since we've already done it by other means in the proof of (1.182a).

Consider now a smooth function $f(\mu)$ for which the sum

$$S = \sum_{m=-\infty}^{\infty} f(m) \tag{1.204}$$

is convergent. From the Poisson's formula (1.197), we have

$$\sum_{n=-\infty}^{\infty} e^{2\pi i\mu n} f(\mu) = \sum_{m=-\infty}^{\infty} \delta(\mu - m) f(\mu)$$

$$\begin{aligned} \to \quad \int_{-\infty}^{\infty} d\mu \sum_{n=-\infty}^{\infty} e^{2\pi i\mu n} f(\mu) &= \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} d\mu\, \delta(\mu - m) f(\mu) \\ &= \sum_{m=-\infty}^{\infty} f(m) \end{aligned} \tag{1.205}$$