1.2: Recap- Position and Momentum States

Before proceeding, let us review the properties of quantum particles in free space. In a d-dimensional space, a coordinate vector $\mathbf{r}$ is a real vector of d components. A quantum particle can be described by the position basis—a set of quantum states $\{|\mathbf{r}\rangle\}$, one for each possible $\mathbf{r}$. If we are studying a particle trapped in a finite region (e.g., a particle in a box), $\mathbf{r}$ is restricted to that region; otherwise, $\mathbf{r}$ is any real d-dimensional vector. In either case, the $\mathbf{r}$'s are continuous, so the position eigenstates form an uncountably infinite set.

The position eigenstates are assumed to span the state space, so the identity operator can be resolved as

$$\hat{I} = \int d^d r \, |\mathbf{r}\rangle \langle\mathbf{r}|, \tag{1.2.1}$$

where the integral is taken over all allowed $\mathbf{r}$. It follows that

$$\langle\mathbf{r}|\mathbf{r}'\rangle = \delta^d(\mathbf{r}-\mathbf{r}'). \tag{1.2.2}$$

The position eigenstates are thus said to be "delta-function normalized", rather than being normalized to unity. In the above equation, $\delta^d(\cdots)$ denotes the d-dimensional delta function; for example, in 2D,

$$\langle x, y \,|\, x', y'\rangle = \delta(x-x')\,\delta(y-y'). \tag{1.2.3}$$

The position operator $\hat{\mathbf{r}}$ is defined by taking $|\mathbf{r}\rangle$ and $\mathbf{r}$ as its eigenstates and eigenvalues:

$$\hat{\mathbf{r}}|\mathbf{r}\rangle \;=\; \mathbf{r}\,|\mathbf{r}\rangle. \tag{1.2.4}$$

Momentum eigenstates are constructed from position eigenstates via Fourier transforms. First, suppose the allowed region of space is a box of length L on each side, with periodic boundary conditions in every direction. Define the set of wave-vectors $\mathbf{k}$ corresponding to plane waves satisfying the periodic boundary conditions at the box boundaries:

$$\Big\{\mathbf{k} \;\Big|\; k_j = 2\pi m/L \;\text{ for } m\in\mathbb{Z},\; j=1,\ldots,d\Big\}.$$

So long as L is finite, the $\mathbf{k}$ vectors are discrete. Now define

$$|\mathbf{k}\rangle = \frac{1}{L^{d/2}} \int d^d r \; e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle, \tag{1.2.5}$$

where the integral is taken over the box. These can be shown to satisfy

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k},\mathbf{k}'}, \quad \langle\mathbf{r}|\mathbf{k}'\rangle = \frac{1}{L^{d/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad I = \sum_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}|. \tag{1.2.6}$$

The momentum operator is defined so that its eigenstates are $\{|\mathbf{k}\rangle\}$, with $\hbar\mathbf{k}$ as the corresponding eigenvalues:

$$\hat{\mathbf{p}}|\mathbf{k}\rangle \;=\; \hbar\mathbf{k}\,|\mathbf{k}\rangle. \tag{1.2.7}$$

Thus, for finite L, the momentum eigenstates are discrete and normalizable to unity. The momentum component in each direction is quantized to a multiple of $\Delta p = 2\pi\hbar/L$.

We then take the limit of an infinite box, $L\to\infty$. In this limit, $\Delta p \to 0$, so the momentum eigenvalues coalesce into a continuum. It is convenient to re-normalize the momentum eigenstates by taking

$$|\mathbf{k}\rangle \to \left(\frac{L}{2\pi}\right)^{d/2} |\mathbf{k}\rangle. \tag{1.2.8}$$

In the $L\to\infty$ limit, the re-normalized momentum eigenstates satisfy

Definition: Re-normalized momentum eigenstates

$$|\mathbf{k}\rangle = \frac{1}{(2\pi)^{d/2}} \int d^d r \; e^{i\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle, \tag{1.2.9}$$

$$|\mathbf{r}\rangle = \frac{1}{(2\pi)^{d/2}} \int d^d k \; e^{-i\mathbf{k}\cdot\mathbf{r}} |\mathbf{k}\rangle, \tag{1.2.10}$$

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \delta^d(\mathbf{k}-\mathbf{k}'), \quad \langle \mathbf{r}|\mathbf{k}\rangle = \frac{1}{(2\pi)^{d/2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad I = \int d^d k \; |\mathbf{k}\rangle\,\langle\mathbf{k}|. \tag{1.2.11}$$

The above integrals are taken over infinite space, and the position and momentum eigenstates are now on a similar footing: both are delta-function normalized. In deriving the above equations, it is helpful to use the formula

$$\int_{-\infty}^{\infty} dx \;\; \exp(ikx) \;=\; 2\pi\,\delta(k). \tag{1.2.12}$$

For an arbitrary quantum state $|\psi\rangle$, a wavefunction is defined as the projection onto the position basis: $\psi(\mathbf{r}) = \langle \mathbf{r}|\psi\rangle$. Using the momentum eigenstates, we can show that

$$\begin{aligned}\langle \mathbf{r}|\hat{\mathbf{p}}|\psi\rangle &= \int d^d k \; \langle \mathbf{r}|\mathbf{k}\rangle \; \hbar\mathbf{k} \; \langle \mathbf{k}|\psi\rangle \\ &= \int \frac{d^d k}{(2\pi)^{d/2}} \; \hbar\mathbf{k} \; e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\psi\rangle \\ &= -i\hbar\nabla \int \frac{d^d k}{(2\pi)^{d/2}} \;\; e^{i\mathbf{k}\cdot\mathbf{r}} \langle \mathbf{k}|\psi\rangle \\ &= -i\hbar\nabla\psi(\mathbf{r}).\end{aligned} \tag{1.2.13}$$

This result can also be used to prove Heisenberg’s commutation relation $[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$.