Chapter 3: Representation in continuous basis

The observables considered so far have been assumed to exhibits discrete eigenvalue spectra. In quantum mechanics, however, there are observables with continuous eigenvalues, for instance the eigenvalues of p_z can take any real value between ∞ and -∞. In this chapter we are going to consider the representation of state vectors, bras, and operators in continuous bases. After presenting the general formalism, we will consider two important applications: representations in the position and momentum spaces.

3.1. General treatment

The orthonormality condition of the continuous basis $|\xi_k\rangle$ is expressed by Dirac's continuous delta function:

$$\langle \xi_k | \xi_{k'} \rangle = \delta(k - k') \quad \text{.....(3-1-1)}$$

Where k and k' are continuous indices.

The Dirac delta function $\delta(k-k')$ is the continuous generalization of the familiar δ_{ij} used in discrete bases with the following properties:

- $$\delta(k-k') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(k-k')x}dx \quad \text{.....(3-1-2)}$$
- It is zero everywhere except at $k = k'$, i.e.,
  $$\langle \xi_k | \xi_{k'} \rangle = \delta(k-k') = \begin{cases} \text{diverges} & \text{for } k = k' \\ 0 & \text{for } k \neq k' \end{cases} \quad \text{.....(3-1-3)}$$
- $$\int_{-\infty}^{\infty} \delta(k-k') f(k) dk = f(k') \quad \text{.....(3-1-4)}$$
- $$\int_{-\infty}^{\infty} \delta(k-k') dk = 1 \quad \text{.....(3-1-5)}$$

The norm of the discrete base kets is finite ($\langle \chi_n | \chi_m \rangle = \delta_{nm}$), but the norm of the continuous base kets is infinite; a combination of (3-1-1) and (3-1-2) leads to

$$\langle \xi_k | \xi_k \rangle = \delta(0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx \to \infty \quad \text{.....(3-1-6)}$$

The completeness relation is not given by a discrete sum as in (2-1-3), but by an integral over the continuous variable is given by:

$$\int_{-\infty}^{\infty} dk \left|\xi_k\right\rangle\left\langle\xi_k\right| = \hat{I} \qquad \text{.....(3-1-7)}$$

Where $\hat{I}$ is the identity (unit) operator.

Any admissible ket state vector $\left|\psi\right\rangle$ can be expanded in terms of continuous complete set of basis kets

$$\left|\psi\right\rangle = \hat{I}\left|\psi\right\rangle = \int_{-\infty}^{\infty} dk \left|\xi_k\right\rangle\left\langle\xi_k\middle|\psi\right\rangle = \int_{-\infty}^{\infty} dk\, b(k)\left|\xi_k\right\rangle \qquad \text{.....(3-1-8)}$$

where $b(k) = \left\langle\xi_k\middle|\psi\right\rangle$ represents the projection of $\left|\psi\right\rangle$ on $\left|\xi_k\right\rangle$.

Similarly, the bra state $\left\langle\psi\right|$ is represented by:

$$\left\langle\psi\right| = \left\langle\psi\right| I = \int_{-\infty}^{\infty} dk \left\langle\psi\middle|\xi_k\right\rangle\left\langle\xi_k\right| = \int_{-\infty}^{\infty} dk\, b^*(k)\left\langle\xi_k\right| \qquad \text{.....(3-1-9)}$$

The scalar product of two state vectors $\left\langle\psi\middle|\phi\right\rangle$ expanded in terms of infinite noncountable continuous basis set $\left|\xi_k\right\rangle$,

$$\left\langle\phi\middle|\psi\right\rangle = \int_{-\infty}^{\infty} dk\; b^*(k)\; c(k) \qquad \textbf{Prove} \qquad \text{.....(3-1-10)}$$

Where $b^*(k) = \left\langle\xi_k\middle|\phi\right\rangle^*$ and $c(k) = \left\langle\xi_{k'}\middle|\psi\right\rangle$

Finally, an operator $\hat{A}$ can be represented by continuous basis:

$$\hat{A} = \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \left|\xi_k\right\rangle A_{kk'} \left\langle\xi_{k'}\right| \qquad \text{.....(3-1-11)}$$

where,

$$A_{kk'} = \left\langle\xi_k\middle|\hat{A}\middle|\xi_{k'}\right\rangle \qquad \text{.....(3-1-12)}$$

3.2. Position representation

In the position representation, the basis consists of an infinite set of vectors $\{\left|\vec{r}\right\rangle\}$ which are eigenkets to the position operator $\hat{\vec{R}}$:

$$\hat{\vec{R}}\left|\vec{r}\right\rangle = \vec{r}\left|\vec{r}\right\rangle \qquad \text{.....(3-2-1)}$$

Where $\vec{r}$ is the eigenvalue of the operator $\hat{\vec{R}}$. The orthonormality and completeness conditions are, respectively, given by:

$$\left\langle\vec{r}\middle|\vec{r}'\right\rangle = \delta(\vec{r}-\vec{r}') = \delta(x-x')\delta(y-y')\delta(z-z') \qquad \text{.....(3-2-2)}$$

$$\int d^3r\left|\vec{r}\right\rangle\left\langle\vec{r}\right| = \hat{I} \qquad \text{.....(3-2-3)}$$

Where, the three-dimensional delta function is given by:

$$\delta(\vec{r}-\vec{r}') = \frac{1}{(2\pi)^3}\int e^{ik(\vec{r}-\vec{r}')}d^3k \qquad \text{.....(3-2-4)}$$

So, every state vector $\left|\psi\right\rangle$ can be expanded as follows

$$\left|\psi\right\rangle = \int d^3r\left|\vec{r}\right\rangle\left\langle\vec{r}\middle|\psi\right\rangle = \int d^3r\,\psi(\vec{r})\left|\vec{r}\right\rangle \qquad \text{.....(3-2-5)}$$

where $\psi(\vec{r})$ denotes the components of $\left|\psi\right\rangle$ in the $\left|\vec{r}\right\rangle$ basis:

$$\left\langle\vec{r}\middle|\psi\right\rangle = \psi(\vec{r}) \qquad \text{.....(3-2-6)}$$

This is known as the (position space) wave function for the state vector $\left|\psi\right\rangle$. A universally accepted interpretation of $\psi(\vec{r})$ was suggested by Born in 1926. He interpreted $\left|\left\langle\vec{r}\middle|\psi\right\rangle\right|^2 = \left|\psi(\vec{r})\right|^2$ as the position probability density.

The scalar product between two state vectors, $\left|\psi\right\rangle$ and $\left|\phi\right\rangle$, can be expressed in this form:

$$\left\langle\phi\middle|\psi\right\rangle = \left\langle\phi\right|\left(\int d^3r\left|\vec{r}\right\rangle\left\langle\vec{r}\right|\right)\left|\psi\right\rangle = \int d^3r\left\langle\phi\middle|\vec{r}\right\rangle\left\langle\vec{r}\middle|\psi\right\rangle = \int d^3r\,\phi^*(\vec{r})\psi(\vec{r}) \qquad \text{.....(3-2-7)}$$

So, $\left\langle\phi\middle|\psi\right\rangle$ characterize the overlap between the two wavefunction $\phi(\vec{r})$ and $\psi(\vec{r})$.

The quantity $\left\langle\phi\middle|\psi\right\rangle$ is independent of representation and represents the probability amplitude for state $\left|\psi\right\rangle$ to be found in the state $\left|\phi\right\rangle$.

Since $\hat{\vec{R}}\left|\vec{r}\right\rangle = \vec{r}\left|\vec{r}\right\rangle$, we have:

$$\langle \vec{r}|\hat{\vec{R}}^n|\vec{r}'\rangle = \vec{r}^n \delta(\vec{r}-\vec{r}') \qquad \text{…..(3-2-8)}$$

3.3. Momentum representation

The basis $\{|\vec{p}\rangle\}$ of the momentum representation is obtained from the eigenkets of the momentum operator $\hat{\vec{p}}$:

$$\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle \qquad \text{…..(3-3-1)}$$

Where $\vec{p}$ is the momentum vector. The orthonormality and completeness conditions of the momentum space basis $|\vec{p}\rangle$ are given by:

$$\langle \vec{p}|\vec{p}'\rangle = \delta(\vec{p}-\vec{p}') \qquad \text{…..(3-3-2)}$$

$$\int d^3p|\vec{p}\rangle\langle\vec{p}| = \hat{I} \qquad \text{…..(3-3-3)}$$

Expanding $|\psi\rangle$ in this basis, we obtain

$$|\psi\rangle = \int d^3p|p\rangle\langle p|\psi\rangle = \int d^3p\,\psi(\vec{p})|\vec{p}\rangle \qquad \text{…..(3-3-4)}$$

where the expansion coefficient $\psi(\vec{p})$ represents the momentum space wave function. The quantity $d^3p|\psi(\vec{p})|^2$ is the probability of finding the system's momentum in the volume element d^3p located between $\vec{p}$ and $\vec{p}+d\vec{p}$.

The scalar product between two state vectors, $|\psi\rangle$ and $|\phi\rangle$, is given in the momentum space by:

$$\langle\phi|\psi\rangle = \langle\phi|\left(\int d^3p|\vec{p}\rangle\langle\vec{p}|\right)|\psi\rangle = \int d^3p\langle\phi|\vec{p}\rangle\langle\vec{p}|\psi\rangle = \int d^3p\,\phi^*(\vec{p})\psi(\vec{p}) \qquad \text{…..(3-3-5)}$$

Since $\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle$, we have

$$\langle\vec{p}|\hat{\vec{p}}^n|\vec{p}'\rangle = \vec{p}^n\delta(\vec{p}-\vec{p}') \qquad \text{…..(3-3-6)}$$

3.4. Connecting the position and momentum representations

Let us now study how to establish a connection between the position and the momentum representations. By analogy with the foregoing study, when changing from the $\{|\vec{r}\rangle\}$ basis to the $\{|\vec{p}\rangle\}$ basis, we encounter the transformation function $\langle\vec{r}|\vec{p}\rangle$. To find the expression for the transformation function $\langle\vec{r}|\vec{p}\rangle$, let us establish a connection between the position and momentum representations of the state vector $|\psi\rangle$:

$$\langle\vec{r}|\psi\rangle = \langle\vec{r}|\hat{I}|\psi\rangle = \langle\vec{r}|\left(\int d^3p|\vec{p}\rangle\langle\vec{p}|\right)|\psi\rangle = \int d^3p\langle\vec{r}|\vec{p}\rangle\psi(\vec{p})$$

That is

$$\psi(\vec{r}) = \int d^3p\langle\vec{r}|\vec{p}\rangle\psi(\vec{p}) \qquad \text{…..(3-4-1)}$$

Similarly, we can write:

$$\psi(\vec{p}) = \int d^3r\langle\vec{p}|\vec{r}\rangle\psi(\vec{r}) \qquad \textbf{Prove} \qquad \text{…..(3-4-2)}$$

The two relations (3-4-1) and (3-4-2) imply that $\psi(\vec{r})$ and $\psi(\vec{p})$ are to be viewed as Fourier transforms of each other. In quantum mechanics the Fourier transform of a function $f(\vec{r})$ is given by:

$$f(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3p e^{i\vec{p}.\vec{r}/\hbar}g(\vec{p}) \qquad \text{…..(3-4-3)}$$

Hence the function $\langle\vec{r}|\vec{p}\rangle$ is given by

$$\langle\vec{r}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{p}.\vec{r}/\hbar} \qquad \text{…..(3-4-4)}$$

This function transforms from the momentum to the position representation. The function corresponding to the inverse transformation, $\langle\vec{p}|\vec{r}\rangle$, is given by

$$\langle\vec{p}|\vec{r}\rangle = \langle\vec{r}|\vec{p}\rangle^* = \frac{1}{(2\pi\hbar)^{3/2}}e^{-i\vec{p}.\vec{r}/\hbar} \qquad \text{…..(3-4-5)}$$

The quantity $|\langle\vec{p}|\vec{r}\rangle|^2$ represents the probability density of finding the particle in a region around $\vec{r}$ where its momentum is equal to $\vec{p}$.

HW. Prove that if the position space wavefunction is normalized then its Fourier transform (the momentum space wavefunction) must also normalize.

HW. Prove that if the momentum space wavefunction is normalized then its Fourier transform (the position wavefunction) must also normalize.

3.5. Momentum Operator in the Position Representation

To determine the form of the momentum operator $\hat{\vec{p}}$ in the position representation, let us calculate $\langle \vec{r}|\hat{\vec{p}}|\psi\rangle$:

$$\langle \vec{r}|\hat{\vec{p}}|\psi\rangle = \langle \vec{r}|\hat{\vec{p}}I|\psi\rangle = \langle \vec{r}|\hat{\vec{p}}\left(\int d^3p|\vec{p}\rangle\langle\vec{p}|\right)|\psi\rangle = \int d^3p\langle \vec{r}|\hat{\vec{p}}|\vec{p}\rangle\langle\vec{p}|\psi\rangle$$

$$= \int d^3p\ \vec{p}\langle \vec{r}|\vec{p}\rangle\langle\vec{p}|\psi\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\int \vec{p}e^{i\vec{p}.\vec{r}/\hbar}\psi(\vec{p})d^3p$$

Since $\vec{p}e^{\vec{p}.\vec{r}/\hbar} = -i\hbar\vec{\nabla}e^{i\vec{p}.\vec{r}/\hbar}$

$$\langle \vec{r}|\hat{\vec{p}}|\psi\rangle = -i\hbar\vec{\nabla}\left(\frac{1}{(2\pi\hbar)^{3/2}}\int e^{i\vec{p}.\vec{r}/\hbar}\psi(\vec{p})d^3p\right) = -i\hbar\vec{\nabla}\int d^3p\langle\vec{r}|\vec{p}\rangle\langle\vec{p}|\psi\rangle = -i\hbar\vec{\nabla}\left\langle\vec{r}\hat{I}\middle|\psi\right\rangle = -i\hbar\vec{\nabla}\langle\vec{r}|\psi\rangle$$

$$\langle \vec{r}|\hat{\vec{p}}|\psi\rangle = \langle\vec{r}|-i\hbar\vec{\nabla}|\psi\rangle$$

Thus, $\hat{\vec{p}}$ is given in the position representation by

$$\hat{\vec{p}} = -i\hbar\vec{\nabla} \qquad \text{…..(3-5-1)}$$

Its Cartesian components are

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \qquad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}, \qquad \hat{p}_z = -i\hbar\frac{\partial}{\partial z} \qquad \text{…..(3-5-2)}$$

3.6. Position Operator in the momentum Representation

The form of the position operator $\hat{\vec{R}}$ in the momentum representation can be easily found as follows:

$$\hat{R}_j = i\hbar\frac{\partial}{\partial p_j} \qquad (j=x,\ y,\ z) \qquad \textbf{Prove} \qquad \text{…..(3-6-1)}$$

Or

$$\hat{x} = i\hbar\frac{\partial}{\partial p_x}\ , \qquad \hat{y} = i\hbar\frac{\partial}{\partial p_y}\ , \qquad \hat{z} = i\hbar\frac{\partial}{\partial p_z} \qquad .....(3\text{-}6\text{-}2)$$

Ex. Prove that commutation relations for operators are representation independent. In particular, the commutator $\left[\hat{\vec{R}},\hat{\vec{p}}\right]$ in the position and the momentum representations.

Soln.

1- Calculate the action of $\left[\hat{x},\hat{p}_x\right]$ on $\psi(\vec{r})$ in the position representation:

$$\left[\hat{x},\hat{p}_x\right]\psi(\vec{r}) = \left(\hat{x}\hat{p}_x - \hat{p}_x\hat{x}\right)\psi(\vec{r})$$

$$\hat{x}\hat{p}_x\psi(\vec{r}) = -i\hbar x\frac{\partial\psi(\vec{r})}{\partial x} \quad , \quad \hat{p}_x\hat{x}\psi(\vec{r}) = -i\hbar\frac{\partial}{\partial x}\left(\hat{x}\psi(\vec{r})\right) = -i\hbar\psi(\vec{r}) - i\hbar\hat{x}\frac{\partial\psi(\vec{r})}{\partial x}$$

$$\left[\hat{x},\hat{p}_x\right]\psi(\vec{r}) = -i\hbar x\frac{\partial\psi(\vec{r})}{\partial x} + i\hbar\psi(\vec{r}) + x\frac{\partial\psi(\vec{r})}{\partial x} = i\hbar\psi(\vec{r}) \qquad \rightarrow \qquad \left[\hat{x},\hat{p}_x\right] = i\hbar$$

Similar relations can be derived at once for the y and the z components:

$$\left[\hat{y},\hat{p}_y\right] = i\hbar \quad , \quad \left[\hat{z},\hat{p}_z\right] = i\hbar$$

2- Calculate the action of $\left[\hat{x},\hat{p}_x\right]$ on $\psi(\vec{p})$ in the momentum representation:

$$\left[\hat{x},\hat{p}_x\right]\psi(\vec{p}) = \left(\hat{x}\hat{p}_x - \hat{p}_x\hat{x}\right)\psi(\vec{p})$$

$$\hat{x}\hat{p}_x\psi(\vec{p}) = i\hbar\frac{\partial}{\partial p_x}\left(p_x\psi(\vec{p})\right) = i\hbar\psi(\vec{p}) + i\hbar p_x\frac{\partial\psi(\vec{p})}{\partial p_x} \quad , \quad \hat{p}_x\hat{x}\psi(\vec{p}) = i\hbar\frac{\partial}{\partial p_x}\left(p_x\psi(\vec{p})\right) = i\hbar p_x\frac{\partial\psi(\vec{p})}{\partial p_x}$$

$$\left[\hat{x},\hat{p}_x\right]\psi(\vec{p}) = i\hbar\psi(\vec{p}) + i\hbar p_x\frac{\partial\psi(\vec{p})}{\partial p_x} - i\hbar p_x\frac{\partial\psi(\vec{p})}{\partial p_x} = i\hbar\psi(\vec{p}) \quad \rightarrow \quad \left[\hat{x},\hat{p}_x\right] = i\hbar$$

HW. Calculate the matrix element $\langle\vec{r}|\hat{p}_x|\vec{r}'\rangle$.

3.7. Matrix and wave mechanics

So far worked out the mathematics pertaining to quantum mechanics in two different representations: discrete basis systems and continuous basis systems. The theory of quantum mechanics deals in essence with solving the following eigenvalue problem:

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle \qquad n=1,2,\ldots N \qquad .....(3\text{-}7\text{-}1)$$

where $\hat{H}$ is the Hamiltonian of the system. This equation is general and does not depend on any coordinate system or representation. But to solve it, we need to represent it in a given basis system. The complexity associated with solving this eigenvalue equation will then vary from one basis to another.

3.7.1. Matrix Mechanics

Representing the formalism of quantum mechanics in a discrete basis yields a matrix eigenvalue problem. That is, the representation of (3-7-1) in a discrete basis $\{|\chi_i\rangle\}$ yields the following secular equation

$$\begin{vmatrix} H_{11}-E & H_{12} & H_{13} & \cdots & H_{1N} \\ H_{21} & H_{22}-E & H_{23} & \cdots & H_{2N} \\ H_{31} & H_{32} & H_{33}-E & \cdots & H_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ H_{N1} & H_{N2} & H_{N3} & \cdots & H_{NN}-E \end{vmatrix} = 0 \qquad \text{.....(3-7-2)}$$

This is an Nth order equation in E; its solutions yield the energy spectrum of the system: E_1, E_2, E_3, …, E_N. Knowing the set of eigenvalues E_1, E_2, E_3, …, E_N , we can easily determine the corresponding set of eigenvectors $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$, ..., $|\psi_N\rangle$.

i.e., The diagonalization of the Hamiltonian matrix of a system yields the energy spectrum as well as the state vectors of the system. This procedure, which was worked out by Heisenberg, involves only matrix quantities and matrix eigenvalue equations. This formulation of quantum mechanics is known as matrix mechanics.

3.7.2. Wave Mechanics

Representing the formalism of quantum mechanics in a continuous basis yields an eigenvalue problem not in the form of a matrix equation, as in Heisenberg's formulation, but in the form of a differential equation. The representation of the eigenvalue equation (3-7-1) in the position space yields

$$\frac{-\hbar^2\nabla^2}{2m}\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r},) \qquad \textbf{Prove} \qquad \text{.....(3-7-3)}$$

This differential equation is known as Schrödinger equation. Its solutions yield the energy spectrum of the system as well as its wave function. This formulation of quantum mechanics in the position representation is called wave mechanics.

HW. Write the time dependent Schrödinger equation $i\hbar \frac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle$ in the $\left|\vec{r}\right\rangle$ representation, where $\hat{H}$ is the Hamiltonian operator given by: $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\vec{r})$.