Notes for Lectures on Quantum Mechanics *

Coordinate Representation

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1 A useful result

The canonical commutation relation $[\widehat{x},\widehat{p}] = i\hbar$ can be used to show that if x_0 is an eigenvalue of $\widehat{x}$, $x_0 + a$, $a \in \mathbb{R}$, is also an eigenvalue. This is most easily seen by making use of the identity GBox-01 GBox-02

$$\widehat{x}\exp(-ia\widehat{p}/\hbar) = exp(-ia\widehat{p}/\hbar)(\widehat{x} + a). \tag{1}$$

here a is a real number. To see this note that $U(a) \equiv \exp(-ia\widehat{p}/\hbar)$ is a unitary operator. If $|x_0\rangle$ is an eigenvector of $\widehat{x}$ with eigenvalue x_0, $U(a)|x_0\rangle$ is an eigenvector of $\widehat{x}$ with eigenvalue $x_0 + a$. Using Eq.(1) we get

$$\widehat{x}\Big(U(a)|x_0\rangle\Big) = \exp(-ia\widehat{p}/\hbar)(\widehat{x} + a)ketx_0, \tag{2}$$

$$= (x_0 + a)\Big(U(a)|x_0\rangle\Big). \tag{3}$$

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This shows that $(x_0 + a)$ is an eigenvalue of $\widehat{x}$ with $U(a)|x_0\rangle$ as the eigenvector. Since a is any real number, all real numbers are eigenvalues of the position operator $\widehat{x}$. A similar argument shows that all real values are allowed as eigenvalues of the momentum operator $\widehat{p}$.

2 Coordinate representation — One dimension

We shall first consider a particle in one dimension. To set up the coordinate representation, we use the eigenvectors of position operator $\widehat{x}$ as o.n. basis. We have seen that the eigenvalues of $\widehat{x}$ are all real values in range $(-\infty, \infty)$. Let x be one such eigenvalue and $|x\rangle$ be the corresponding eigenvector, *i.e.*,

$$\widehat{x}|x\rangle = x|x\rangle. \tag{4}$$

The orthogonality property of the eigenvectors now assumes the form

$$\langle x''|x'\rangle = \delta(x'' - x'), \tag{5}$$

and the completeness relation $\sum_n |n\rangle\langle n| = \widehat{I}$ takes the form

$$\int_{-\infty}^{\infty} |x\rangle\langle x|\, dx = \widehat{I}. \tag{6}$$

where $\widehat{I}$ denotes the identity operator. Everywhere the sum $\sum_n$ over all eigenvalues is replaced by integration, $\int dx$, as the eigenvalues are now continuous. This choice of the eigenvectors $\{|x\rangle\}$ as a basis leads to the **coordinate representation** or the *position representation*, also known as the *Schrödinger representation.*

Thus an expansion of abstract vector $|\psi\rangle$ in the basis $\big\{|x\rangle\big\}$ becomes

$$|\psi\rangle = \int dx |x\rangle\langle x|\psi\rangle, \tag{7}$$

and the abstract vector $|\psi\rangle$ is represented by the numbers $\langle x|\psi\rangle$, with x having values in real numbers. Instead of arranging all the components of $|\psi\rangle$ in form of a column, we regard them as values of a function of x:

$$\langle x|\psi\rangle = \psi(x). \tag{8}$$

✍ *Due to the fact that the eigenvalues of x are continuous, it is not meaningful to ask for probability that the position has a single value x_0; instead we must ask for probability position has a value in the specified range, such as x and $x + dx$.*

The third postulate tells us that this probability is given by

$$|\langle x|\psi\rangle|^2 dx = |\psi(x)|^2 dx. \tag{9}$$

Thus the function $\psi(x)$, to be called the **wave function**, gives the probability density of position. The Parseval relation GBox-03

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx \tag{10}$$

ensures that, for normalized state vector $|\psi\rangle$, the total probability will be one.

Every operator $\widehat{T}$ is represented as a infinite dimensional matrix with continuous row and column indices $\{(\mathsf{T})_{x,x'} = \langle x|\widehat{T}|x'\rangle\}$. The action of operator $\widehat{T}$ on wave function $\psi(x)$ is then given by

$$\widehat{T}\psi(x) = \sum_{x'} (\mathsf{T})_{x,x'} \, \psi(x') = \int_{-\infty}^{\infty} \langle x|\widehat{T}|x'\rangle \, \psi(x') \, dx'. \tag{11}$$

The operator $\widehat{x}$ will be represented by an infinite dimensional *diagonal matrix* having rows and columns labelled by continuous indices x', x'' and the matrix elements of x are

$$\langle x'|\widehat{x}|x''\rangle = x'\delta(x'' - x'). \tag{12}$$

Using the canonical commutation relation, $[\widehat{x}, \widehat{p}] = i\hbar$, the matrix elements of the momentum operator can be worked out and is given by GBox-04

$$\langle x'|\widehat{p}|x''\rangle = -i\hbar \frac{d}{dx'}\delta(x'' - x'). \tag{13}$$

3 Action of position and momentum operators

The action of position and momentum operators is given as matrix multiplication by considering these operators as matrices with continuous row and column indices:

$$\begin{aligned} \widehat{x}\psi(x) &= \int_{-\infty}^{\infty} \langle x|\widehat{x}|x'\rangle\psi(x') \, dx' & (14)\\ &= \int_{-\infty}^{\infty} x\delta(x - x')\psi(x') \, dx' & (15)\\ &= x\psi(x) & (16) \end{aligned}$$

and

$$\widehat{p}\psi(x) = \int_{-\infty}^{\infty} \langle x|\widehat{p}|x'\rangle\psi(x')\,dx' \tag{17}$$

$$= \int_{-\infty}^{\infty} -i\hbar\delta(x-x')\psi(x')\,dx' \tag{18}$$

$$= -i\hbar\frac{d\psi(x)}{dx}. \tag{19}$$

Thus, in the position representation we have $\widehat{p} \to -i\hbar\frac{d}{dx}$. An operator corresponding to a dynamical variable can be obtained by making a replacement

$$\widehat{x} \to x, \qquad \widehat{p} \to -i\hbar\frac{d}{dx}. \tag{20}$$

4 Hamiltonian in coordinate representation

The most important variable for a system is the Hamiltonian

$$H = \frac{p^2}{2m} + V(x). \tag{21}$$

and the corresponding operator is

$$\widehat{H} = \frac{\widehat{p}}{2m} + V(\widehat{x}) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{22}$$

5 Wave function as position probability density

Let $|\psi\rangle$ denote the state vector of a particle and $\psi(x) = \langle x|\psi\rangle$ be the corresponding wave function. We now come to the physical interpretation of the coordinate space wave function $\psi(x)$. Note that $\psi(x)$ is the coefficient of $|x\rangle$ in the expansion of the state vector $|\psi\rangle$:

$$|\psi\rangle = \int |x\rangle\langle x|\psi\rangle\,dx = \int \psi(x)|x\rangle\,dx. \tag{23}$$

The third postulate tells us that the expansion coefficient will give the probability amplitude for position and the the absolute square $|\psi(x)|^2$ gives the probability density for position. Thus the probability of finding position in the range $x, x+dx$ is $|\psi(x)|^2dx$. The integral $\int_a^b |\psi(x)|^2\,dx$ is the probability that the particle will be found in the interval (a, b).

6 Several degrees of freedom

Generalization to a particle in three dimensions is straightforward. The basis vectors $|\vec{r}\rangle$ in this case are simultaneous eigenvectors of position operators $\widehat{x}, \widehat{y}, \widehat{z}$:

$$\widehat{x}|\vec{r}\rangle = x|\vec{r}\rangle, \qquad \widehat{y}|\vec{r}\rangle = y|\vec{r}\rangle, \qquad \widehat{z}|\vec{r}\rangle = z|\vec{r}\rangle. \tag{24}$$

The orthogonality and completeness relations assume the form

$$\langle \vec{r}\,''|\vec{r}\,'\rangle = \delta(\vec{r}\,'' - \vec{r}\,'), \qquad \int d^3\vec{r}\,|\vec{r}\rangle\langle\vec{r}| = \widehat{I}. \tag{25}$$

Expansion of an arbitrary $|\psi\rangle$ in the basis $|\vec{r}\rangle$ assumes the form

$$|\psi\rangle = \int |\vec{r}\rangle\,\langle\vec{r}|\psi\rangle d^3r. \tag{26}$$

We call the function $\langle\vec{r}|\psi\rangle$ the wave function and also denote it by $\psi(\vec{r})$. The absolute square of wave function gives the probability density; $|\psi(\vec{r})|^2 dV$ is the probability density for the particle to be a small volume dV at position $\vec{r}$. The corresponding probability for a a particle to be in a finite volume V is obtained integrating over the volume V and is given by

$$\iiint\limits_V |\langle\psi|\vec{r}\rangle|^2\, d^3r = \iiint\limits_V |\psi(\vec{r})|^2\, d^3r. \tag{27}$$

The action of position operators $\widehat{\vec{r}}$ is to multiply by $\vec{r}$ and that of momentum operators is given by $\widehat{\vec{p}} \to -i\hbar\nabla$. Thus

$$\widehat{\vec{r}}\,\psi(\vec{r}) = \vec{r}\,\psi(\vec{r}), \qquad \widehat{\vec{p}}\,\psi(\vec{r}) = -i\hbar\nabla\psi(\vec{r}). \tag{28}$$