PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 7, February 18, 2021 (Thursday)

- Handout: Solutions to Problem Set 2.
- Reading: Mathematical Tools (Chapter 3 in Griffiths)
- Assignment: Problem Set 4 due February 26 (Friday).
  Submit your homework assignments to Canvas.

Topics for Today: Mathematical Tools

2.6 Expectation Value

2.7 Representations of Dirac Delta Function

2.8 Operators in Infinite Dimensions

Topics for Next Lecture: Mathematical Tools

2.9 Hilbert Space and Fourier Transform

2.10 The Momentum Space or the $p-$basis

2.11 The Uncertainty Principle

2.6 Expectation Value

Let us consider a physics system described by a state vector $|\psi\rangle$.

- The outcome of a measurement corresponding to operator Ω is an eigenvalue ω_i with probability $P(\omega_i)$

$$P(\omega_i) = \frac{|\langle \omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle}\,.$$

- Now suppose an infinite number of such experiments are performed. Then we obtain a variety of values with different probabilities.

- The statistical mean of this measurement is and define an average of the operator to be

$$\langle\Omega\rangle = \sum_i P(\omega_i)\omega_i\,.$$

Clearly, therefore,

$$
\begin{aligned}
\langle \Omega \rangle &= \sum_i P(\omega_i)\omega_i \\
&= \sum_i |\langle \omega_i|\psi\rangle|^2 \omega_i \quad (|z|^2 = z^* z) \\
&= \sum_i \langle \psi|\omega_i\rangle\langle \omega_i|\psi\rangle \omega_i \quad (\langle \psi|\omega_i\rangle = \langle \omega_i|\psi\rangle^*) \\
&= \sum_i \langle \psi|\Omega|\omega_i\rangle\langle \omega_i|\psi\rangle \quad \text{(eigenvalue equation)} \\
&= \langle \psi|\Omega| \left(\sum_i |\omega_i\rangle\langle \omega_i| \right) |\psi\rangle \\
&= \langle \psi|\Omega|\psi\rangle \quad \text{with} \quad \sum_i |\omega_i\rangle\langle \omega_i| = \mathrm{I}
\end{aligned}
$$

where we have applied the completeness relation and have assumed that the state vector $|\psi\rangle$ is normalized.

This is the **expectation value** of the operator Ω in the state $|\psi\rangle$.

In the coordinate space, the state vector becomes a wave function $\psi(x)$

$$\psi(x) \equiv \langle x|\psi\rangle \quad \text{(similar to} \quad v_i = \langle e_i|v\rangle)$$

that is the inner product of $|\psi\rangle$ with the normalized basis vector $|x\rangle$.

The vectors $|x\rangle$ and $|y\rangle$ form a complete set of orthonormal basis

$$\begin{aligned} \langle x|y\rangle &= \delta(x-y) \quad \text{(orthonormal relation)} \quad \langle e_i|e_j\rangle = \delta_{ij} \\ \int |x\rangle\langle x|\, dx &= \mathrm{I} \quad \text{(completeness relation)} \quad \sum_i |e_i\rangle\langle e_i| = \mathrm{I}\,. \end{aligned}$$

And the expectation value of Ω becomes

$$\begin{aligned} \langle\psi|\Omega|\psi\rangle &= \langle\psi|\left(\int |x\rangle\langle x|\, dx\right)|\Omega|\left(\int |y\rangle|\langle y|\, dy\right)|\psi\rangle \\ &= \int dx \int dy\, \delta(x-y)\, \langle\psi|x\rangle\langle x|\Omega|y\rangle\langle y|\psi\rangle \\ &= \int \psi^*(x)\langle x|\Omega|x\rangle\psi(x)\, dx\,. \end{aligned}$$

In the same way, we can define the expectation value of the operator Ω^2 in the state $|\psi\rangle$. Thus

$$
\begin{aligned}
\langle\Omega^2\rangle &= \langle\psi|\Omega^2|\psi\rangle \\
&= \langle\psi|\Omega^2(\sum_i |\omega_i\rangle\langle\omega_i|)|\psi\rangle \\
&= \sum_i \langle\psi|\Omega^2|\omega_i\rangle\langle\omega_i|\psi\rangle \\
&= \sum_i \langle\psi|\Omega|\omega_i\rangle\langle\omega_i|\psi\rangle\omega_i \\
&= \sum_i \langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle\omega_i^2 \\
&= \sum_i P(\omega_i)\omega_i^2
\end{aligned}
$$

Thus these are like the familiar quantities in statistical mechanics.

Wave Function and Matrix Elements

In the Hilbert space, a physics system is described with a state vector $|\psi\rangle$ and an observable ω becomes a quantum operator Ω.

In the coordinate space with x-basis, the eigenvalue equation is

$$X|x\rangle = x|x\rangle \quad \text{or} \quad X|y\rangle = y|y\rangle$$

with the orthonormal relation $\langle x|y\rangle = \delta(x-y)$.

The state vector becomes a wave function

$$\psi(x) \equiv \langle x|\psi\rangle$$

and the operator is represented by a matrix element

$$\langle x|\Omega|y\rangle\,.$$

What are $\langle x|X|y\rangle$ and $\langle x|P|y\rangle$ in the x-basis?

In the x-basis, the matrix element for the operator X becomes

$$\begin{aligned}\langle x|X|y\rangle &= y\langle x|y\rangle = y\delta(x-y) \quad \text{or} \\ \langle x|X|y\rangle &= x\langle x|y\rangle = x\delta(x-y) \quad \text{(eigenvalue equations)}\,.\end{aligned}$$

The operator P is the conjugate momentum w.r.t. X, such that

$$[X,P] \equiv XP - PX = i\hbar \quad \text{(commutation relation)}$$

and

$$\Delta X \Delta P \geq \frac{\hbar}{2}\,\text{(uncertainty relation)}.$$

In the x-basis, the matrix element of P becomes

$$\langle x|P|y\rangle = -i\hbar\frac{d}{dx}\delta(x-y)\,.$$

In the p-basis, the eigenvalue equations are

$$P|p\rangle = p|p\rangle \quad \text{or} \quad P|q\rangle = q|q\rangle$$

with the orthonormal relation $\langle p|q\rangle = \delta(p-q)$.

The state vector becomes a wave function

$$\phi(p) \equiv \langle p|\psi\rangle$$

and an operator Ω is represented by a matrix element

$$\langle p|\Omega|q\rangle \, .$$

The matrix elements for P and X in the p-basis become

- for $\Omega = P$, $\langle p|P|q\rangle = q\delta(p-q) = p\delta(p-q)$ (eigenvalue equations),
- for $\Omega = X$,

$$\langle p|X|q\rangle = i\hbar \frac{d}{dp}\delta(p-q) \, .$$

Example 1: $\Omega = X$

In the coordinate space with x-basis, let us choose the normalized eigenvectors as $|x\rangle$ and $|y\rangle$ that are eigenvectors of the operator X or $\hat{X}$.

The state vector becomes a wave function $\psi(x)$

$$\psi(x) \equiv \langle x|\psi\rangle \quad \text{or} \quad \psi(y) \equiv \langle y|\psi\rangle \,.$$

The eigenvalue equation for the operator X is

$$X|x\rangle = x|x\rangle \quad \text{or} \quad X|y\rangle = y|y\rangle \,.$$

The normalized eigenvectors from a complete set of orthonormal basis.

- What is the orthonormal relation for $|x\rangle$ and $|y\rangle$?
- What is the completeness relation for $|x\rangle$ or $|y\rangle$?

Applying the eigenvalue equation $X|x\rangle = x|x\rangle$ or $X|y\rangle = y|y\rangle$, the completenes relations of basis vectors $|x\rangle$ and $|y\rangle$

$$\int |x\rangle\langle x|\, dx = I \quad \text{and} \quad \int |y\rangle\langle y|\, dy = I\,,$$

and the orthonormal relation

$$\langle x|y\rangle = \delta(x-y)$$

we obtain the expectation value of X

$$\begin{aligned}
\langle\psi|X|\psi\rangle &= \langle\psi|\mathrm{I}|X|\mathrm{I}|\psi\rangle \;=\; \langle\psi|\left(\int x\rangle\langle x|\, dx\right)|X|\left(\int |y\rangle|\langle y|\, dy\right)|\psi\rangle \\
&= \int dx \int dy\, \langle\psi|x\rangle\langle x|X|y\rangle\langle y|\psi\rangle \;\text{ with }\; \langle x|X|y\rangle = y\delta(x-y) \\
&= \int dx \int dy\, \psi^*(x)\,[y\delta(y-x)]\,\psi(y) \;\text{ with }\; \langle\psi|x\rangle = \psi^*(x) \\
&= \int \psi^*(x)\,[x\,\psi(x)]\; dx\,.
\end{aligned}$$

Example 2: $\Omega = P$

In the momentum space with p-basis, let us choose the normalized eigenvectors as $|p\rangle$ and $|q\rangle$ that are eigenvectors of the operator P or $\hat{P}$.

The state vector $\psi\rangle$ becomes a wave function $\phi(p)$

$$\phi(p) \equiv \langle p|\psi\rangle \quad \text{or} \quad \phi(q) \equiv \langle q|\psi\rangle\,.$$

The eigenvalue equation for the operator P is

$$P|p\rangle = p|p\rangle \quad \text{or} \quad P|q\rangle = q|q\rangle\,.$$

The normalized eigenvectors from a complete set of orthonormal basis with the completeness relation

$$\int |p\rangle\langle p|\,dp = I \quad \text{and} \quad \int |q\rangle\langle q|\,dq = I\,,$$

as well as the orthonormal relation

$$\langle p|q\rangle = \delta(p-q)\,.$$

In the x-basis, let us apply the completeness relation

$$\int |x\rangle\langle x|\, dx = I \quad \text{or} \quad \int |y\rangle\langle y|\, dy = I$$

and the matirx element of P

$$\langle x|P|y\rangle = -i\hbar \frac{d}{dx}\delta(x-y)\,.$$

The expectation value of P becomes

$$\begin{aligned}
\langle\psi|P|\psi\rangle &= \langle\psi|\mathrm{I}|P|\mathrm{I}|\psi\rangle \;=\; \langle\psi|\left(\int x\rangle\langle x|\, dx\right)|P|\left(\int |y\rangle|\langle y|\, dy\right)|\psi\rangle \\
&= \int dx \int dy\, \langle\psi|x\rangle\langle x|P|y\rangle\langle y|\psi\rangle \\
&= \int dx \int dy\; \psi^*(x)\left[-i\hbar\frac{d}{dx}\delta(x-y)\right]\psi(y) \\
&= -i\hbar \int \psi^*(x)\left[\frac{d}{dx}\,\psi(x)\right] dx\,.
\end{aligned}$$

2.7 Representations of Dirac Delta Function

Infinite Dimensional Vector Spaces

Let us consider a string fixed at two end points: $x = 0$ and $x = L$. In the limit with N discrete points and $N - 1$ equal intervals, we can think of an ordered $N-$tuple describing the displacement at these N points. Let us denote that by $f_N(x_i)$. This, of course, will not be the true displacement $f(x)$, but as N is made larger and larger, would become closer to the true description. We can consider the ordered $N-$tuple, $f_N(x_1), f_N(x_2), \cdots, f_N(x_N$ to be an $N-$dimensional vector denoted by

$$|f_N\rangle = \begin{pmatrix} f_N(x_1) \\ f_N(x_2) \\ \vdots \\ f_N(x_N) \end{pmatrix} = \sum_{i=1}^{N} f_N(x_i)|x_i\rangle$$

in terms of the basis vectors

$$|x_i\rangle = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

where 1 appears only at the $i-$th place and $f_N(x_i) = \langle x_i | f_N \rangle$.

The vectors $|x_i\rangle$ form a set of complete and orthonormal basis vectors

$$\begin{aligned} \langle x_i | x_j \rangle &= \delta_{ij}, \\ \sum_{i=1}^{N} |x_i\rangle\langle x_i| &= \mathrm{I} = \text{ Identity operator}. \end{aligned}$$

Let us consider the limit $N \to \infty$ with the length of each interval becoming infinitesimal such that the positions become continuous variables and the displacement $f_\infty(x)$ approaches the true displacement. We can pass from finite dimensions to infinite dimensions by making $N \to \infty$

$$
\begin{aligned}
\langle f_N | g_N \rangle &= \sum_{i,j=1}^{N} \langle x_j | f_N^*(x_j) g_N(x_i) | x_i \rangle \\
&= \sum_{i,j=1}^{N} f_N^*(x_j) g_N(x_i) \langle x_j | x_i \rangle \\
&= \sum_{i,j=1}^{N} f_N^*(x_i) g_N(x_j) \delta_{ij} \\
&= \sum_{i}^{N} f_N^*(x_i) g_N(x_i).
\end{aligned}
$$

And in particular

$$\langle f_N | f_N \rangle = \sum_i^N f_N(x_i) f_N^*(x_i) = \sum_i^N |f_N(x_i)|^2 \,.$$

This diverges as $N \to \infty$. Therefore, we need a redefinition of the inner product such that a finite limit is obtained as $N \to \infty$. This can be done by defining

$$\begin{aligned} \langle f_N | g_N \rangle &\equiv \sum_i^N f_N^*(x_i) g_N^*(x_i) (\frac{L}{N-1}) \\ &\to \int_0^L f_N^*(x) g_N(x) dx, \text{ as } N \to \infty. \end{aligned}$$

Thus for vectors defined within the interval $a \le x \le b$, we have

$$\langle f_N | g_N \rangle \to \int_a^b f_N^*(x) g_N(x) dx = \int_a^b f^*(x) g(x)\, dx \text{ as } N \to \infty.$$

The completeness relation still holds,

$$\int_a^b |x\rangle\langle x| dx = I = \text{the identity operator.}$$

Multiplying the above equation on the left by $\langle y|$ and on the right by $|f\rangle$, we obtain

$$\begin{aligned} \int_a^b \langle y|x\rangle\langle x|f\rangle dx &= \langle y|f\rangle, \text{ or} \\ \int_a^b \langle y|x\rangle f(x) dx &= f(y) \end{aligned}$$

From the orthogonality relation, we know that

$$\langle y|x\rangle = 0, \text{ if } y \neq x.$$

Therefore, we can limit the range of integration to an infinitesimal region

$$\int_{x_0-\epsilon}^{x_0+\epsilon} f(x)\langle x|x_0\rangle dx = f(x_0).$$

If $\langle x|x_0\rangle$ is finite at $x = x_0$, then the left hand side would vanish.

Let us denote

$$\langle x|y\rangle = \delta(x-y)\,.$$

- Thus $\delta(x-y) = 0$ if $x \neq y$.
- For $x = y$ it diverges in such a way that the integral is unity:

$$\int f(x)\delta(x-y)dx = f(y)\,, \ \text{ and } \int \delta(x-y)dx = 1, \ \text{ with } \ f(x) = 1\,.$$

This is called the Dirac delta function and it is used to normalize continuous basis vectors

$$\langle x|y\rangle = \delta(x-y)\,.$$

Properties of the Dirac delta function:

(i) $\int \delta(x-y)f(x)dx = f(y)$.

(ii) $\delta(x-y) = \langle x|y\rangle = \langle x|y\rangle^\dagger = \langle y|x\rangle = \delta(y-x)$. It is an even function.

(iii) $\int \delta'(x-y)f(x)dx = -f'(y)$.

Proof:

$$\begin{aligned}\int [\frac{d}{dx}\delta(x-y)]f(x)dx &= \int_a^b \{\frac{d}{dx}[\delta(x-y)f(x)] - \delta(x-y)\frac{d}{dx}f(x)\} \\ &= \delta(x-y)f(x)|_a^b - \int_a^b \delta(x-y)\frac{d}{dx}f(x)\,dx \\ &= -\frac{d}{dx}f(x)|_{x=y} = -f'(y)\,.\end{aligned}$$

It is clear that

$$\frac{d}{dx}\delta(x-y) = -\frac{d}{dy}\delta(x-y)\,.$$

More general properties:

$$\begin{aligned}
\delta'(x) &= -\delta'(-x) \\
x\delta(x) &= 0 \\
x\delta'(x) &= -\delta(-x) \\
\delta(ax) &= \frac{1}{|a|}\delta(x) \\
\delta(x^2 - a^2) &= \frac{1}{2a}[\delta(x-a) + \delta(x+a)] \quad \text{for} a > 0 \\
f(x)\delta(x-a) &= f(a)\delta(x-a) \\
\int \delta(x-a)\delta(x-b)dx &= \delta(a-b)
\end{aligned}$$

One more very useful property:

$$\delta(f(x)) = \sum_i \frac{\delta(x - x_i)}{|df(x)/dx_i|}|_{x=x_i}$$

where x_i is chosen so that $f(x_i) = 0$, i.e. the roots of $f(x_i) = 0$.

Gaussian Representation of the Dirac delta function

In quantum mechanics, we often express the Dirac delta function as an integral

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-x_0)}\,dk = \delta(x-x_0)$$

or

$$\int_{-\infty}^{\infty} e^{ik(x-x_0)}\,dk = 2\pi\delta(x-x_0)$$

This is known as the Gaussian Representations of the Dirac delta function.

Let us consider

$$\begin{aligned} I = \int_{-\epsilon}^{\epsilon} f(x)\lim_{q\to\infty}\frac{1}{2\pi}\int_{-q}^{q} e^{ikx}dk &= \lim_{q\to\infty}\frac{1}{2\pi}\int_{-\epsilon}^{\epsilon} f(x)\frac{2\sin qx}{x} \\ &= \lim_{q\to\infty}\frac{1}{\pi}Im[\int_{-\epsilon}^{\epsilon} f(x)\frac{e^{iqx}}{x}] \end{aligned}$$

Let $z = qx$, then

$$\begin{aligned} z &= -\epsilon \rightarrow z = -q\epsilon \\ z &= \epsilon \rightarrow z = q\epsilon \end{aligned}$$

Therefore, the integral becomes

$$I = \lim_{q\to\infty} Im[\int_{-q\epsilon}^{q\epsilon} f(z/q)\frac{e^{iz}}{z}]$$

In the limit of $q \rightarrow \infty$, we can use contour integral. There is a pole at $z = 0$. Therefore, the value of the integral is

$$I = Im[\frac{1}{\pi} \cdot i\pi f(0)] = f(0)$$

Thus

$$\begin{aligned} \int_{-\epsilon}^{\epsilon} f(x) \lim_{q\to\infty} \frac{1}{2\pi} \int_{-q}^{q} e^{ikx} dk &= f(0), \\ \Longrightarrow \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk &= \delta(x)\,. \end{aligned}$$