PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 9, February 25, 2021 (Thursday)

- 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

2.9 Hilbert Space and Fourier Transform

2.10 Introduction to the Uncertainty Principle

Topics for Next Lecture: Mathematical Tools

2.11 Bonus: The Momentum Space or the $p-$basis

3.1 Postulates of Quantum Mechanics

2.9 Hilbert Space and Fourier Transform

The Hilbert space is a linear vector space where every vector can be normalized either to unity or the Dirac delta function.

Any state vector $|f\rangle$ can be expanded in terms of a complete set of orthonormal basis.

- In the coordinate space with basis vectors $|x\rangle$,

$$|f\rangle = \left(\int |x\rangle\langle x| dx \right) |f\rangle = \int \langle x|f\rangle |x\rangle dx = \int f(x)|x\rangle \, dx \, ,$$

  where $f(x) \equiv \langle x|f\rangle$ is the wave function in the x-basis.

- In the momentum space with k-basis,

$$|f\rangle = \left(\int |k\rangle\langle k| dk \right) |f\rangle = \int \langle k|f\rangle |k\rangle \, dk = \int g(k)|k\rangle \, dk \, ,$$

  where $g(k) \equiv \langle k|f\rangle$ is the wave function in the k-basis.

Applying completeness relations

$$\int |x\rangle\langle x|\, dx = \mathrm{I}$$

we can find the relations between wave functions $g(k)$ and $f(x)$

$$\begin{aligned} g(k) &\equiv \langle k|f\rangle \\ &= \int \langle k|x\rangle\langle x|f\rangle\, dx \\ &= \int \psi_k^*(x) f(x)\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x)\, dx\,. \end{aligned}$$

where $g(k) = \langle k|f\rangle$ and $f(x) = \langle x|f\rangle$.

This is just the Fourier transform.

Similarly we can apply the completeness relations

$$\int |k\rangle\langle k| \, dk = \mathrm{I}$$

and show that

$$\begin{aligned} f(x) &\equiv \langle x|f\rangle \\ &= \int \langle x|k\rangle\langle k|f\rangle \, dk \\ &= \int \psi_k(x) g(k) \, dk \\ &= \frac{1}{\sqrt{2\pi}} \int e^{ikx} g(k) \, dk \end{aligned}$$

where $f(x) = \langle x|f\rangle$ and $g(k) = \langle k|f\rangle$.

This is the inverse Fourier transforms.

Fourier transforms take the state vector from one basis to another.

In the eigenbasis of K (the k-basis), the eigenvalue equation is

$$K|k\rangle = k|k\rangle\,.$$

The normalized eigenvectors form a complete set of orthonormal basis

$$\begin{aligned}\langle k|q\rangle &= \delta(k-q) \quad \text{(orthonormal relation)}\,,\\ \int |k\rangle\langle k|\,dk &= \mathrm{I} \quad \text{(completeness relation)}\,.\end{aligned}$$

In the k-basis,

- a state vector $|\psi\rangle$ is represented by a wave function $\phi(k) \equiv \langle k|\psi\rangle$,
- an operator is represented with matrix elements

$$\Omega_{kq} = \langle k|\Omega|q\rangle\,.$$

For example,

$$\begin{aligned}\langle k|K|q\rangle &= q\langle k|q\rangle = q\delta(k-q)\\ &= k\langle k|q\rangle = k\delta(k-q)\,.\end{aligned}$$

In the eigenbasis of X (the x-basis), the eigenvalue equation is

$$X|x\rangle = x|x\rangle \,.$$

The normalized eigenvectors form a complete set of orthonormal basis

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

In the x-basis,

- a state vector $|\psi\rangle$ is represented by a wave function $\psi(x) \equiv \langle x|\psi\rangle$,
- an operator is represented with matrix elements

$$\Omega_{xy} = \langle x|\Omega|y\rangle \,.$$

For example,

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

The operator X usually takes a state vector $|f\rangle$ to a different state vector $|h\rangle$ (transformation)

$$X|f\rangle = |h\rangle\,.$$

Multiplying both sides with a dual basis vector $\langle x|$, we obtain

$$\begin{aligned}\langle x|X|f\rangle &= \int \langle x|X|y\rangle\langle y|f\rangle\,dy \\ &= \int y\delta(x-y)f(y)\,dy \\ &= xf(x) = h(x)\,.\end{aligned}$$

Thus the effect of X on a vector $|f\rangle$ is to multiply it by x.

The matrix element of the operator X in the $|k\rangle$ basis is

$$
\begin{aligned}
\langle k|X|q\rangle &= \int dx \int dy \, \langle k|x\rangle\langle x|X|y\rangle\langle y|q\rangle \\
&= \int dx \int dy \, \psi_k^*(x) y \delta(x-y) \psi_q(y) \\
&= \frac{1}{2\pi} \int x e^{-i(k-q)x} \, dx \\
&= \frac{1}{2\pi} i \frac{d}{dk} \int e^{-i(k-q)x} \, dx \\
&= i \frac{d}{dk} \delta(k-q) \, .
\end{aligned}
$$

- In the x-basis, X acts as x and K acts as $-id/dx$ on functions.
- In the k-basis, K acts as k and X acts as id/dk on functions.
- Operators with such reciprocity are called conjugate operators.

Clearly, conjugate operators do not commute.

In the x-basis, we have

$$
\begin{aligned}
X|f(x)\rangle &\rightarrow xf(x) \quad \text{and} \quad K|f(x)\rangle \rightarrow -i\frac{df(x)}{dx} \\
XK|f(x)\rangle &\rightarrow -ix\frac{df(x)}{dx} \\
KX|f(x)\rangle &\rightarrow -i\frac{d}{dx}\left[xf(x)\right] .
\end{aligned}
$$

Thus

$$
(XK - KX)|f(x)\rangle \rightarrow -ix\frac{df(x)}{dx} + if(x) + ix\frac{df}{dx} = if(x) \rightarrow i|f\rangle .
$$

Thus

$$
[X, K]|f\rangle = i|f\rangle \quad \text{or} \quad [X, K] = iI ,
$$

and

$$
[X, P]|f\rangle = i\hbar|f\rangle \quad \text{or} \quad [X, P] = i\hbar I .
$$

X is the position operator and $P = \hbar K$ is the momentum operator.

2.10 Introduction to the Uncertainty Principle

Let A and B be two non-commuting operators with

$$[A, B] = i\hbar$$

As we have seen before, these are conjugate operators. Let ΔA be the root mean square deviation of the operator A. Thus

$$(\Delta A)^2 \quad \equiv \quad \langle A^2 \rangle - \langle A \rangle^2$$

Similarly let ΔB be the root mean square deviation of the operator B. Thus

$$(\Delta B)^2 = \langle B^2 \rangle - \langle B \rangle^2$$

then

$$\Delta A \Delta B \geq \frac{\hbar}{2} \ \ (\mathrm{Heisenberg's \ \ uncertainty \ \ principle})$$

First of all notice that

$$
\begin{aligned}
(\Delta\Omega)^2 &= \langle\Omega^2\rangle - \langle\Omega\rangle^2 \\
&= \langle\Omega^2 - 2\Omega\langle\Omega\rangle + \langle\Omega\rangle^2\rangle \\
&= \langle(\Omega - \langle\Omega\rangle)^2\rangle \\
\Delta\Omega &\equiv \langle(\Omega - \langle\Omega\rangle)^2\rangle^{1/2} \;=\; \left[\Omega^2\rangle - \langle\Omega\rangle^2\right]^{1/2}
\end{aligned}
$$

where (i) $\Delta\Omega$ is the standard deviation which measures the average fluctuation around the mean.

N.B. (i) $\Delta\Omega$ is often called the root mean squared deviation or the uncertainty in Ω.
(ii) $(\Delta\Omega)^2$ is called the mean square deviation or the variance.

Expectation Value in the x-Basis

In the x-basis with $|x\rangle$, the state vector can be expanded as

$$|\psi\rangle = \left(\int |x\rangle\langle x\right) |\psi\rangle\, dx = \int \psi(x)|x\rangle dx\,, \quad \text{where} \quad \psi(x) \equiv \langle x|\psi\rangle\,.$$

And the expectation value of Ω becomes

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

For example, the matrix elements of X and P are

$$\begin{aligned} \langle x|X|y\rangle &= y\delta(x-y) = x\delta(x-y)\,, \quad \text{and} \\ \langle x|P|y\rangle &= -i\hbar\frac{d}{dx}\delta(x-y)\,. \end{aligned}$$

Examples: (a) $\Omega = X$ and (b) $\Omega = P$

In the coordinate space we have a complete set of orthonormal basis

$$\langle x|y\rangle = \delta(x-y) \quad \text{(orthonormal)}\,, \qquad \int |x\rangle\langle x|\, dx = \mathrm{I} \quad \text{(completeness)}\,.$$

The state vector $|\psi\rangle$ and operators (Ω) are represented with

$$\psi(x) \equiv \langle x|\psi\rangle \quad \text{(wave function)}\,, \qquad \Omega_{xy} \equiv \langle x|\Omega|y\rangle \quad \text{(matrix element)}\,.$$

(a) The expectation value of X becomes

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

(b) The expectation value of P becomes

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

where

$$\langle x|P|y\rangle = -i\hbar\frac{d}{dx}\delta(x-y) \quad \text{where} \quad P = \hbar K = -i\hbar D$$

in the x-basis.

Useful formulas:

(a) $$\int_0^\infty \frac{1}{(x^2+\alpha^2)^2}\,dx = \left(\frac{1}{2\alpha^2}\right)\left[\frac{x}{x^2+\alpha^2}+\frac{1}{\alpha}\tan^{-1}\left(\frac{x}{\alpha}\right)\right]_0^\infty$$

(b) $$\int_0^\infty \frac{x^{m-1}}{(1+x)^{m+n}}\,dx = \frac{\Gamma(m)\Gamma(n)}{\Gamma(m+n)}\,.$$

(c) To apply Gaussian Integrals, you might need to complete the square for a quadratic function

$$\begin{aligned}
ax^2+bx+c &= a\left(x^2+\frac{b}{a}x\right)+c \\
&= a\left[x^2+\frac{b}{a}x+\left(\frac{b}{2a}\right)^2\right]-a\cdot\left(\frac{b}{2a}\right)^2+c \\
&= a\left[x+\left(\frac{b}{2a}\right)\right]^2-\frac{b^2}{4a}+c \\
&= a\left[x+\left(\frac{b}{2a}\right)\right]^2+c-\frac{b^2}{4a}\,.
\end{aligned}$$

A Brief Dictionary for Notations

Here are some helpful relations between two sets of notations when you read the textbook:

- State vector: $|\Psi(t)\rangle \to |S(t)\rangle$
- Operators: $\Omega \to \hat{Q}$
- Basis vectors: $|e_1\rangle \to |1\rangle$ and $|e_2\rangle \to |2\rangle$
- Orthonormal relations: $\langle x|y\rangle = \delta(x-y) \;\to\; \langle g_x|g_y\rangle = \delta(x-y)$ and $\langle p|q\rangle = \delta(p-q) \;\to\; \langle f_p|f_q\rangle = \delta(p-q)$.
- Special wave functions: $\psi_k(x) = \langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} \to f_k(x)$ and $\psi_p(x) = \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{(i/\hbar)px} \to f_p(x)$.
- Uncertainty or root mean square deviation $\Delta\Omega \to \sigma_\Omega$.