PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 8, February 23, 2021 (Tuesday)

- Handout: Solutions to Problem Set 3.
- 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.* Introduction to the Uncertainty Principle

2.8 Operators in Infinite Dimensions

Topics for Next Lecture: Mathematical Tools

2.9 Hilbert Space and Fourier Transform

2.10 The Uncertainty Principle

2.11 The Momentum Space or the $p-$basis

2.* 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

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

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 Coordinate Space

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

$$\int |x\rangle\langle x|\, dx = \mathrm{I} \quad \text{(completeness relation)}\,.$$

And the expectation value of Ω becomes

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

2.8 Operators in Infinite Dimensions

Let us consider systems with discrete basis vectors.

- We can expand every vector as a linear combination of a complete set of orthonormal basis

$$
\begin{aligned}
|v\rangle &= \left(\sum_i^N |e_i\rangle\langle e_i|\right)|v\rangle = \sum_i^N \langle e_i|v\rangle|e_i\rangle \\
&= \sum_i^N v_i|e_i\rangle \quad \text{where} \quad v_i \equiv \langle e_i|v\rangle\,.
\end{aligned}
$$

  It is similar to ordinary vector analysis

$$
\vec{v} = \sum_i v_i \hat{x}_i \quad \text{where} \quad v_i \equiv \vec{v}\cdot\hat{x}_i\,.
$$

- And every operator can be represented with matrix elements

$$
\Omega_{ij} = \langle e_i|\Omega|e_j\rangle \quad \text{where} \;\; \Omega = X\,, P\,, L\,, \;\text{ or }\; H\,.
$$

Now let us consider the x-basis with a continuous variable x.

- We can expand every vector in terms of a complete set of orthonormal basis

$$
\begin{aligned}
|f\rangle &= \left(\int |x\rangle\langle x|\, dx \right) |f\rangle \\
&= \int \langle x|f\rangle\, |x\rangle\, dx \\
&= \int f(x)\, |x\rangle\, dx \quad \text{where} \quad f(x) \equiv \langle x|f\rangle\,.
\end{aligned}
$$

- Every operator can be represented with matrix elements

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

where $\Omega = X\,, P\,, L$, or H .

We are now familiar with kets $|f\rangle$ and the basis vectors $|x\rangle$. Let us ask how linear operators act on this space

$$\Omega|f\rangle = |g\rangle$$

Since $|f\rangle$ may be expressed as

$$|f\rangle = \mathrm{I}\cdot|f\rangle = \left(\int |x\rangle\langle x|dx\right)|f\rangle = \int f(x)|x\rangle\, dx\,,$$

we can think of the operators as taking the function $f(x)$ into $g(x)$. Let us consider D as the operator which takes $f(x)$ to df/dx, then

$$\begin{aligned}
D|f\rangle &= |\frac{df}{dx}\rangle = |g\rangle \\
\langle x|D|f\rangle &= \langle x|\frac{df}{dx}\rangle = \frac{df(x)}{dx} \quad \text{and} \\
\langle x|D|f\rangle &= \int \langle x|D|y\rangle\langle y|f\rangle\, dy \;=\; \int \langle x|D|y\rangle f(y)\, dy \;=\; \frac{df(x)}{dx}\,.
\end{aligned}$$

We have found that if $D|f\rangle = |df/fx\rangle$, then

$$\int \langle x|D|y\rangle f(y)\, dy \; = \frac{df(x)}{dx}\,.$$

On the other hand, we have

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

Clearly, that leads to the matrix element of D in the x-basis

$$D_{xy} \equiv \langle x|D|y\rangle = \frac{d}{dx} \delta(x-y)\,.$$

In finite dimensional vector spaces, we know that D is Hermitian if $D^\dagger = D$. However we have

$$(D^\dagger)_{xy} = D^*_{yx} = \langle y|D|x\rangle^* = \left[\frac{d}{dy}\delta(y-x)\right]^* = -\frac{d}{dx}\delta(x-y) = -D_{xy}\,.$$

In fact we see that the operator D is naively anti-Hermitian. However, we can easily make it Hermitian by defining

$$K = -iD \quad \text{then} \quad K^\dagger = K$$

and would be naively Hermitian. But we also know that for an operator to be Hermitian if must satisfy

$$\begin{aligned}
\langle g|K|f\rangle &= \langle f|K|g\rangle^* \\
\text{L.H.S.} &= \langle g|K|f\rangle \\
&= \int_a^b dx \int_a^b dy\, \langle g|x\rangle\langle x|K|y\rangle\langle y|f\rangle \\
&= \int_a^b dx \int_a^b dy\, g^*(x)(-i\frac{d}{dx}\delta(x-y))f(y) \\
&= \int_a^b g^*(x)(-i)\frac{df(x)}{dx}\, dx \\
&= -i\int_a^b g^*(x)\frac{df(x)}{dx}\, dx\,.
\end{aligned}$$

$$
\begin{aligned}
\text{R.H.S.} \quad &= \quad \langle f|K|g\rangle^* \\
&= \quad [\int_a^b dx \int_a^b \, dy \, \langle f|x\rangle\langle x|K|y\rangle\langle y|g\rangle]^* \\
&= \quad [\int_a^b dx \int_a^b dy f^*(x)(i\frac{d}{dy}\delta(x-y))g(y)]^* \\
&= \quad [\int_a^b dx f^*(x)(-i)\frac{dg(x)}{dx}]^* \\
&= \quad i\int_a^b dx \frac{dg^*(x)}{dx} f(x) dx \\
&= \quad i\int_a^b dx [\frac{d}{dx}(g^*(x)f(x)) - g^*(x)\frac{df(x)}{dx}] \\
&= \quad ig^*(x)f(x)|_a^b - i\int_a^b \, g^*(x)\frac{df(x)}{dx}\, dx \,.
\end{aligned}
$$

Thus we see that only if

$$g^*(x)f(x)|_a^b = 0$$

then the operator K would be Hermitian.

If the functions are like the displacements of a string which is fixed, then of course this product vanishes.

However, we can also think of periodic functions such that

$$\begin{aligned} f(b) &= f(a)\,, \\ g(b) &= g(a)\,, \end{aligned}$$

then also this vanishes and the operator K is Hermitian.

In quantum mechanics, we often work with $-\infty \le x \le \infty$. A function of the form e^{ikx} raises the following question:

$$e^{-ikx} e^{+iqx}|_{-\infty}^{\infty} = 0?$$

We can write

$$\begin{aligned} e^{-i(k-q)x}|_{-\infty}^{\infty} &= -i(k-q) \int_{-\infty}^{\infty} e^{-i(k-q)x}\, dx \\ &= -2\pi i(k-q)\delta(k-q) = 0\,. \end{aligned}$$

N.B. $x\delta(x) = 0$ as a distribution.

This shows that K is Hermitian in this space. Let us now calculate the eigenvalues of K. It would seem formidable since K is an infinite matrix and, therefore, the characteristic equation would involve polynomials of infinite order.

Let us consider the eigenvector of K as $|k\rangle$ with the eigenvalue k

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

In the x-basis, the eigenvalue equation becomes

$$\begin{aligned} \langle x|K|k\rangle &= k\langle x|k\rangle \\ \int \langle x|K|y\rangle\langle y|k\rangle\,dy &= k\langle x|k\rangle \end{aligned}$$

Defining $\langle x|k\rangle = \psi_k(x)$, we have

$$\begin{aligned} \int -i\frac{d}{dx}\delta(x-y)\psi_k(y)\,dy &= k\psi_k(x) \\ \text{or} \quad -i\frac{d}{dx}\psi_k(x) &= k\psi_k(x) \end{aligned}$$

Therefore, $\psi_k(x) = Ae^{ikx}$ and any real number k is an eigenvalue with $\psi_k(x)$ as the eigenfunction.

We have found a differential equation in the standard form

$$\frac{d}{dx}\psi_k(x) - ik\psi_k(x) = 0 \quad \text{where} \quad \psi_k(x) \equiv \langle x|k\rangle \,.$$

The characteristic equation of this linear differential equation is

$$\lambda - ik = 0 \quad \text{with} \quad \lambda = ik \,.$$

Therefore, the solution is $\psi_k(x) = Ae^{\lambda x} = Ae^{ikx}$.

Here A is an arbitrary constant and we can choose $A = 1/\sqrt{2\pi}$ so that the vector $|k\rangle$ is normalized:

$$\begin{aligned}
\langle k|q\rangle &= \int \langle k|x\rangle\langle x|q\rangle\, dx \;=\; \int \psi_k^*(x)\psi_q(x)\, dx \\
&= |A|^2 \int e^{-ikx}e^{iqx}\, dx \;=\; |A|^2 \int e^{-i(k-q)x}\, dx \\
&= |A|^2(2\pi)\delta(k-q) \;=\; \delta(k-q)\,.
\end{aligned}$$

Choosing $A \in \mathcal{R}$, $A > 0$, we obtain $A = 1/\sqrt{2\pi}$.