PHYS 3803: Quantum Mechanics I, Spring 2021

Lecture 10, March 02, 2021 (Tuesday)

- Handout: Solutions to Problem Set 4.
- Reading:
  Postulates of Quantum Mechanics and Schrödinger Equation
  [Griffiths 1 and 2]
- Assignment: Problem Set 5 due March 05 (Friday).
  Submit your homework assignments to Canvas.

Topics for Today: Postulates of Quantum Mechanics

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

3.1 The Postulates of Quantum Mechanics

3.2 Implications of the Postulates

3.3 Expectation Value

3.4 The Uncertainty Principle

Topics for Next Lecture: Schrödinger Equation [Griffiths 1 and 2]

3.5 Ehrenfest's Theorem

3.6 Stationary State Solutions

3.7 Equation of continuity

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 $\Delta\Omega \to \sigma_\Omega$.

2.11 Bonus: The Momentum Space or the p−basis

The eigenvalue equation of the momentum operator P is

$$P|p\rangle = p|p\rangle \, .$$

In the x-basis, we have

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

That leads to

$$\begin{aligned} -i\hbar\frac{d}{dx}\psi_p(x) &= p\psi_p(x) \quad \text{or} \\ \frac{d}{dx}\psi_p(x) - \frac{ip}{\hbar}\psi_p(x) &= 0 \, , \end{aligned}$$

with the solution

$$\langle x|p\rangle = \psi_p(x) = Ae^{(\frac{i}{\hbar})p\cdot x} \, .$$

Requiring that the basis vector $|p\rangle$ should be normalized

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

we have

$$\begin{aligned}
\langle p|q\rangle &= \langle p| \left(\int |x\rangle\langle x| dx \right) |q\rangle \\
&= \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|q\rangle \, dx \\
&= \int_{-\infty}^{\infty} A^* A e^{-\left(\frac{i}{\hbar}\right)(p-q)x} \, dx \\
&= |A|^2 \int e^{-i(p-q)u} \, \hbar \, du \\
&= |A|^2 (2\pi\hbar)\delta(p-q) \; = \; \delta(p-q)
\end{aligned}$$

where $u = x/\hbar$ and $dx = \hbar du$.

Choosing $A \in \mathcal{R}$ and $A > 0$, we obtain

$$A = \frac{1}{\sqrt{2\pi\hbar}}$$

and

$$\langle x|p\rangle = \psi_p(x) = \frac{1}{(2\pi\hbar)^{1/2}} e^{\left(\frac{i}{\hbar}\right)p\cdot x} \; .$$

It is the bridge between the coordinate space and the momentum space.

Let us consider a state vector $|\psi\rangle$. The state wave function in the $x-$basis is

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

And the state wave function in the $p-$basis becomes

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

Then, we have a simple relation between $\psi(x)$ and $\phi(p)$

$$\begin{aligned}
\psi(x) &= \langle x|\psi\rangle \\
&= \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|\psi\rangle \; dp \\
&= \int_{-\infty}^{\infty} \psi_p(x)\phi(p) \; dp \\
&= \frac{1}{(2\pi\hbar)^{1/2}} \int_{-\infty}^{\infty} e^{\left(\frac{i}{\hbar}\right)p\cdot x}\phi(p) \; dp
\end{aligned}$$

where $\phi(p)$ is the wave function in the $p-$basis and it is the Fourier transform of $\psi(x)$ multiplied by a constant $1/\sqrt{\hbar}$.

In the k-basis, the wave function becomes

$$\begin{aligned}
\phi(k) &\equiv \langle k|\psi\rangle \\
&= \int_{-\infty}^{\infty} \langle k|x\rangle\langle x|\psi\rangle \, dx \;=\; \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{-ik\cdot x}\psi(x)\, dx \;,
\end{aligned}$$

which is the Fourier transform of the wave function in the $x-$basis

$$\begin{aligned}
\psi(x) &\equiv \langle x|\psi\rangle \\
&= \int_{-\infty}^{\infty} \langle x|k\rangle\langle k|\psi\rangle \, dk \\
&= \int_{-\infty}^{\infty} \psi_k(x)\phi(k)\, dk \\
&= \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} e^{ik\cdot x}\phi(k)\, dk \;.
\end{aligned}$$

It is clear that $\psi(x)$ is the inverse Fourier transform of $\phi(k)$.

3.1 The Postulates of Quantum Mechanics

There are four most important postulates in quantum mechanics.

(i) In quantum mechanics the state of a system at a fixed time is denoted by the state vector $|\Psi(t)\rangle$ that belongs to a Hilbert space.

(ii) The observables x and p are replaced by operators X and P with the commutation relation $[X, P] = i\hbar$. The matrix elements of operators X and P in the x-basis become

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

Any operator Ω corresponding to the observable ω is obtained as the same function of the operators X and P. We usually symmetrize products of two operators. Thus we have

$$\begin{aligned} \omega(x,p) &\rightarrow \Omega(X,P) \quad \text{and} \\ xp &\rightarrow \frac{1}{2}(XP+PX)\,. \end{aligned}$$

(iii) Quantum mechanics gives probabilistic results. If a system is in a state $|\psi\rangle$, then a measurement corresponding to Ω yields one of the eigenvalues ω_i of Ω with a probability

$$\begin{aligned} P(\omega_i) &= \frac{|\langle\omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle}, \\ \sum_i P(\omega_i) &= 1\,. \end{aligned}$$

The result of the measurement would be to change the state of the system to the eigenstate $|\omega_i\rangle$ of the operator Ω.

(iv) In quantum mechanics the state vector evolve with time according to Schrödinger equation

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

where $H = H(X, P) =$ the Hamiltonian operator.

In relativistic mechanics, we know that the energy and momentum form a four vector denoted by

$$p^\mu = (E/c, +\vec{p}) \;\; \text{(contravariant)} \quad \text{and} \quad p_\mu = (E/c, -\vec{p}) \;\; \text{(covariant)}.$$

The relative negative sign is a consequence of the Lorentz group structure. Recall that the P operator in the x-basis becomes

$$P_{xy} \equiv \langle x|P|y\rangle = -i\hbar\frac{d}{dx}\delta(x-y) \quad \text{or} \quad P_x \rightarrow -i\hbar\frac{d}{dx}\,.$$

This suggests that

$$E \rightarrow i\hbar\frac{d}{dt} \quad \text{and} \quad H|\Psi(t)\rangle = i\hbar\frac{d}{dt}|\Psi(t)\rangle\,,$$

which is the Schrödinger equation.

Since $H(X,P)$ is the operator corresponding to the total energy of the system, if $|\psi\rangle$ is an eigenstate with energy E, we can write

$$H|\psi\rangle = E|\psi\rangle \quad \text{(eigenvalue equation)}\,.$$

3.2 Implications of the Postulates

In quantum mechanics, a physics system is described with a state vector $|\Psi(t)\rangle$ belonging to a Hilbert space.

In the x basis,

- a state vector is represented by a wave function $\psi(x) \equiv \langle x|\psi\rangle$, and
- an operator $(X, P, L$ or $H)$ is represented with matrix elements $\Omega_{xy} \equiv \langle x|\Omega|y\rangle$.

The state vector is expanded with the basis vector $|x\rangle$

$$|\Psi(t)\rangle = \int |x\rangle\langle x|\Psi(t)\rangle \, dx \quad \text{(completeness relation)},$$

and

$$\langle x|\Psi(t)\rangle = \Psi(x, t)$$

is the coefficient of expansion. This is also the wave function.

- The particles in microscopic systems spread out and the spread can be infinite.
- The quantity $|\Psi(x,t)|^2$ is the probability density at position x and at time t.
- The quantity $|\Psi(x,t)|^2 dx$ not only measures the probability of finding a particle between x and $x + dx$, but also how the probability changes with time.
- Since the state vectors define a Hilbert space, if $|\psi\rangle$ and $|\phi\rangle$ define two states of the system, then so does $\alpha|\psi\rangle + \beta|\phi\rangle$. This is called the principle of superposition.

The probabilistic nature of quantum mechanics of course implies two states $|\psi\rangle$ and $\alpha|\psi\rangle$ give the same probability of a particular measurement. Thus corresponding to each physical state $|\psi\rangle$, there exists a set of states $\alpha|\psi\rangle$ for all possible values of α which define a ray in the Hilbert space. Clearly for a physical state we assume

$$\langle\psi|\psi\rangle = 1 \text{ or a Dirac delta function.}$$

This still allows a ray of the form $e^{i\theta}|\psi\rangle$.

If a state is an eigenstate $|\omega_i\rangle$ of some operator Ω, then the corresponding measurement would definitely yield the value ω_i. This follows immediately from the fact that

$$P(\omega_i) = \frac{|\langle\omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle} = 1\,.$$

Let us consider the state formed by superposing two eigenstates $|\omega_1\rangle$ and $|\omega_2\rangle$ of the operator Ω.
The normalized state vector is

$$|\psi\rangle = \frac{\alpha|\omega_1\rangle + \beta|\omega_2\rangle}{(|\alpha|^2 + |\beta|^2)^{1/2}} \,.$$

- If we make a measurement corresponding to Ω then the measurement would yield a value ω_1 with a probability $|\alpha|^2/(|\alpha|^2 + |\beta|^2)$ and a value ω_2 with a probability $|\beta|^2/(|\alpha|^2 + |\beta|^2)$.
- Thus the measurement on a superposed state sometimes behaves like it is in one of the states and sometimes like in the other.

If an operator is degenerate, for example, Ω is doubly degenerate with eigenstates $|\omega, 1\rangle$ and $|\omega, 2\rangle$, then the probability that a measurement would yield an eigenvalue ω is given by

$$P(\omega) = \frac{1}{\langle\psi|\psi\rangle}\left[|\langle\omega, 1|\psi\rangle|^2 + |\langle\omega, 2|\psi\rangle|^2\right] \,.$$

3.3 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 $|\psi\rangle$.

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.

3.4 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.

Let us define

$$\delta A \equiv A - \langle A \rangle \quad \text{and} \quad \delta B \equiv B - \langle B \rangle.$$

Then we have $[\delta A, \delta B] = [A, B] = i\hbar$. Furthermore,

$$\begin{aligned}
(\Delta A)^2(\Delta B)^2 &= \langle (A - \langle A \rangle)^2 \rangle \langle (B - \langle B \rangle)^2 \rangle \\
&= \langle (\delta A)^2 \rangle \langle (\delta B)^2 \rangle \\
&\geq |\langle \delta A \delta B \rangle|^2 \;\; \text{(Schwartz inequality)} \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) + \frac{1}{2}(\delta A \delta B - \delta B \delta A) \rangle|^2 \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) + \frac{1}{2}[\delta A, \delta B] \rangle|^2 \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) + \frac{1}{2}(i\hbar) \rangle|^2 \\
&= |\langle \frac{1}{2}(\delta A \delta B + \delta B \delta A) \rangle|^2 + \frac{\hbar^2}{4}
\end{aligned}$$

Therefore,

$$\Delta A \Delta B \geq \frac{\hbar}{2}.$$

- This tells us that for any two conjugate variables, there is a minimum of uncertainty associated with their measurements.
- Note that the Schwartz inequality becomes an equality if the vectors are parallel to each other. Thus

  $$\delta A|\psi\rangle = \lambda \delta B|\psi\rangle$$

  and

  $$\begin{aligned}
  \frac{1}{2}\langle\psi|(\delta A\delta B + \delta B\delta A)|\psi\rangle &= \frac{1}{2}\langle\psi|\lambda^*\delta B\delta B + \lambda\delta B\delta B)|\psi\rangle \\
  &= \frac{1}{2}(\lambda^* + \lambda)\langle\psi|\delta B\delta B|\psi\rangle \\
  &= \frac{1}{2}(\lambda^* + \lambda)\langle\delta B\psi|\delta B\psi\rangle\,.
  \end{aligned}$$