SCPY 323: Quantum Mechanics II — **2^{nd} Semester 2022**

Lecture 2: Wave function and Postulate of Quantum Mechanics

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2.1 Quantum State and Wave Function

The main goal of the wave function in quantum mechanics is to represent the quantum state and we can use the wave function to calculate an experimentally measurable quantity, which in this case is the probability. However, it turns out there can be several ways to write down the wave function depending on what bases you choose to use. For example, our $\phi(x)$ in the previous section is the wave function that is a result of the quantum state projected on the spatial x bases. Therefore, it appears there is a more fundamental object, which we will call a *state* and we can represent this state by choosing a basis we want. I assume here that you all read Chapter 1 of Shankar. So, I will skip to the section about the vector space in infinite dimensions, which will be directly related to the wave function in quantum mechanics.

We will start by considering a discrete approximation of the wave function. Let a ket $|\phi_n\rangle$ represent a vector space of n dimensions in $\mathbb{V}^n(\mathbb{C})$, where $\mathbb{C}$ denotes that the scalar field consists of all complex numbers, that is, $\mathbb{V}^n(\mathbb{C})$ is a complex vector space of n dimensions. We can represent $|\phi_n\rangle$ in terms of matrix as

$$|\phi_n\rangle \leftrightarrow \begin{bmatrix} \phi_n(x_1) \\ \phi_n(x_2) \\ \vdots \\ \phi_n(x_n) \end{bmatrix}$$

Now you can think of $\phi_n(x_1)$ as a probability amplitude at a point x_1 and what we are doing here is to extend the probability amplitude to cover the whole, that is, we transfer ϕ to $\phi(x)$ as we have done in previously. Now to create the wave function from the state $|\phi_n\rangle$, we have to calculate the projection of this state on the basis vector in this space, which is represented by

$$|x_i\rangle \leftrightarrow \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

where 1 is at the i^{th} position. The set of vector bases satisfies the following conditions

$$\langle x_i|x_j\rangle = \delta_{ij} \qquad \text{orthogonality}$$

$$\sum_{i=1}^{n} |x_i\rangle\langle x_i| = \mathrm{I} \qquad \text{completeness}$$

The ket $|\phi_n\rangle$ can be written in terms of the project along the bases as:

$$|\phi_n\rangle = \sum_{i=1}^{n} |x_i\rangle \langle x_i|\phi_n\rangle$$

But we know that the project of the state on the base $|x_i\rangle$, $\langle x_i|\phi_n\rangle$ is equal to $\phi_n(x_i)$. Therefore, we can rewrite the expression above as

$$|\phi_n\rangle = \sum_{i=1}^{n} \phi_n(x_i)\,|x_i\rangle$$

What we are doing here is to expand our state in terms of projection along each direction of the n-dimensional complex vector space; note that $\phi_n(x_i)$ is complex. Now we will let n go to infinity. Then the orthogonality and completeness are modified to

$$\begin{aligned} \langle x|x'\rangle &= \delta(x-x') && \text{orthogonality} \\ \int_{-\infty}^{\infty} |x'\rangle\langle x'|\,dx' &= \mathrm{I} && \text{completeness,} \end{aligned}$$

where x is now a continuous variable and $\delta(x-x')$ is called Dirac delta function. The properties of the Dirac delta function are:

$$\begin{aligned} \delta(x-x') &= 0, && x \neq x' \\ \int_{x-\epsilon}^{x+\epsilon} \delta(x-x')\; dx' &= 1 && \epsilon \to 0 \end{aligned}$$

And $|\phi\rangle$ can be expended in terms of the bases $|x'\rangle$ as:

$$|\phi\rangle = \int_{-\infty}^{\infty} |x'\rangle\langle x'|\phi\rangle\;\; dx' = \int_{-\infty}^{\infty} \phi(x')\,|x'\rangle\;\; dx',$$

where $\langle x'|\phi\rangle = \phi(x')$ is the wave function in the sense that we previously discussed. So now we know the relationship between the state $|\phi\rangle$ that is represented by a ket and the wave function in the space bases $\phi(x)$. We note here that we can use different bases to represent the state $|\phi\rangle$ for example we can project $|\phi\rangle$ onto the momentum bases. Which bases we need to project the state onto depends on what probability we want to calculate at the end. In this case, we want to calculate the probability of finding a particle within some range of space; we, therefore, project the state onto the space bases.

In order to obtain $\phi(x)$ from $|\phi\rangle$, all we have to do is to project $|\phi\rangle$ onto the base $|x\rangle$, that is,

$$\begin{aligned} \langle x|\phi\rangle &= \int_{-\infty}^{\infty} \phi(x')\,\langle x|x'\rangle\;\; dx' \\ &= \int_{-\infty}^{\infty} \phi(x')\delta(x-x')\; dx' \\ &= \phi(x) \end{aligned}$$

One convenient thing of writing the state in the form of a ket is that we can calculate the probability of finding a particle between x_1 and x_2 by taking the inner product of the ket $|\phi\rangle$ in the space bases

$$\begin{aligned} P_{[x_1,x_2]} &= \int_{x_1}^{x_2} \langle\phi|x\rangle\langle x|\phi\rangle\;\; dx \\ &= \int_{x_1}^{x_2} \phi^*(x)\phi(x)\; dx \\ &= \int_{x_1}^{x_2} |\phi(x)|^2\; dx, \end{aligned}$$

where we use the facts that $\langle\phi|x\rangle = \phi^*(x)$ and $\langle x|\phi\rangle = \phi(x)$. We will end the discussion of the state in quantum mechanics and the wave function here. We will come back to this point later when we work with the wave function again later in the course. Now I would like to switch gears and talk about the uncertainty principle, which is the other conclusion that we get from the double-slit experiment.

Here we note that for the infinite-dimensional Hilbert space, we can define the inner product as

$$\langle\phi_1|\phi_2\rangle = \int_a^b \langle\phi_1|x\rangle\langle x|\phi_2\rangle\ dx = \int_a^b \phi_1^*(x)\phi_2(x)\ dx,$$

where we assume that $a \leqslant x \leqslant b$. We require that this inner product is $\langle\phi_1|\phi_2\rangle$ is finite, that is, $\phi_1^*(x)\phi_2(x)$ is integrable in this range.

2.2 Position and Momentum Operators

I assume that you know how to solve the eigenvalue problem of matrices. I believe you have already learned that in linear algebra. If not, do not worry. You will get reminded later in this class. In fact, one of the problems in this week's problem set asks you to solve for eigenvalues and eigenvectors for finite-dimensional operators. Therefore, here, we will discuss the case where the vector is of infinite dimensions and continuous, where we cannot represent it in a form of a conventional matrix. We already know those vectors and their corresponding operators, those are $|x\rangle$ and $|p\rangle$, and the operators X and P.

For the position operator X in the position eigenstate $|x\rangle$, we have

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

We can think of "momentum" as a generator of translation. So let us consider a translational operator. Therefore, in order to describe the momentum operator, let us first define a translation operator. A translation operation $T(\epsilon)$ in one dimension is defined as

$$T(\epsilon)|x\rangle = |x+\epsilon\rangle,$$

where ϵ is infinitesimally small. Now if $\epsilon \to 0$, then $T(\epsilon \to 0) = \mathbb{1}$. Therefore, to first order in ϵ, we can write

$$T(\epsilon) = \mathbb{1} - \frac{i\epsilon}{\hbar}P,$$

where P is a Hermitian operator, which is a "generator of translation" or a momentum operator. Next, we will consider the action of $T(\epsilon)$ on a vector $|\psi\rangle$:

$$|\psi_\epsilon\rangle = T(\epsilon)\mathbb{1}|\psi\rangle = \int_{-\infty}^{\infty} dx\ T(\epsilon)|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\ \ |x+\epsilon\rangle\,\psi(x),$$

where $\langle x|\psi\rangle = \psi(x)$. Let $x' = x+\epsilon$,

$$\Rightarrow |\psi_\epsilon\rangle = \int_{-\infty}^{\infty} dx'\ \ |x'\rangle\,\psi(x'-\epsilon).$$

If we take the inner product of $|x\rangle$ and $|\psi_\epsilon\rangle$, we will obtain a translated wave function $\langle x|\psi_\epsilon(x)\rangle \equiv \psi_\epsilon(x)$:

$$\psi_\epsilon(x) \equiv \langle x|\psi_\epsilon(x)\rangle = \int_{-\infty}^{\infty} dx'\ \ \langle x|x'\rangle\,\psi(x'-\epsilon) = \int_{-\infty}^{\infty} dx'\ \delta(x-x')\psi(x'-\epsilon) = \psi(x-\epsilon).$$

The translated wave function is translated in the opposite direction to the translation of the axis $|x\rangle$. Next we will derive the relation between $T(\epsilon)$ and P. From,

$$T(\epsilon) = \mathbb{1} - \frac{i\epsilon}{\hbar}P,$$

we will write the operator P in the position basis $|x\rangle$ up to first order in ϵ, that is,

$$\begin{aligned}
\langle x|T(\epsilon)|\psi\rangle &= \psi(x-\epsilon) \\
\langle x|\mathbb{1} - \frac{i\epsilon}{\hbar}P|\psi\rangle &= \psi(x) - \epsilon\frac{d\psi}{dx} \\
\langle x|\psi\rangle - \frac{i\epsilon}{\hbar}\langle x|P|\psi\rangle &= \psi(x) - \epsilon\frac{d\psi}{dx} \\
\Rightarrow \langle x|P|\psi\rangle &= -i\hbar\frac{d\psi}{dx}.
\end{aligned}$$

Therefore, in the position basis,

$$P \to -i\hbar\frac{d}{dx}.$$

To generalize the operator P into three dimensions, we have

$$\begin{aligned}
P_x &\to -i\hbar\frac{\partial}{\partial x} \\
P_y &\to -i\hbar\frac{\partial}{\partial y} \\
P_z &\to -i\hbar\frac{\partial}{\partial z}.
\end{aligned}$$

The *matrix elements* of operator X and P in the $|x\rangle$ basis is:

$$\langle x|X|x'\rangle = x\delta(x-x')$$

Similarly, we can express the matrix elements of the momentum operator P in the position eigenstate $|x\rangle$:

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

We can derive the wave function that is an eigenfunction of the momentum operator in the position basis, that is, $\psi_p(x) = \langle x|p\rangle$. In the momentum basis, the state $|p\rangle$ is an eigenstate of the operator P with the corresponding eigenvalue p, that is,

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

We can determine $\langle x|p\rangle$ by the expansion of $P\,|p\rangle$ in the x basis

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

For the left hand side, we have

$$\begin{aligned}
\langle x|P|p\rangle &= \int_{-\infty}^{\infty} dx' \, \langle x|P|x'\rangle \, \langle x'|p\rangle \\
&= \int_{-\infty}^{\infty} dx' \left[-i\hbar \frac{d}{dx}\delta(x-x')\right] \langle x'|p\rangle \\
&= -i\hbar \frac{d}{dx} \int_{-\infty}^{\infty} dx' \delta(x-x') \, \langle x'|p\rangle \\
&= -i\hbar \frac{d}{dx} \, \langle x|p\rangle \\
&= -i\hbar \frac{d}{dx} \psi_p(x) \\
\Rightarrow \quad -i\hbar \frac{d}{dx}\psi_p(x) &= p \, \langle x|p\rangle = p\psi_p(x).
\end{aligned}$$

We can easily solve this equation and obtain:

$$\psi_p(x) = Ce^{ipx/\hbar}$$

The constant C can be obtained by using the definition of the Fourier transform, which we will encounter later, and requiring that $|p\rangle$ is normalized to unity, that is, $\langle p|p'\rangle = \delta(p-p')$:

$$\delta(p-p') = \langle p|p'\rangle = \int_{-\infty}^{\infty} \langle p|x\rangle \, \langle x|p'\rangle \, dx = C^2 \int_{-\infty}^{\infty} e^{-i(p-p')x/\hbar} dx,$$

which implies that

$$C = \frac{1}{\sqrt{2\pi\hbar}} \tag{2.1}$$

We can also expand an arbitrary state vector $|\psi\rangle$ as a sum of momentum eigenstates, that is,

$$|\psi\rangle = \int_{-\infty}^{\infty} dp \, |p\rangle \, \langle p|\psi\rangle = \int_{-\infty}^{\infty} dp \, |p\rangle \, \tilde{\psi}(p)$$

We can then calculate $\tilde{\psi}(p)$ by expanding it in the x basis.

$$\begin{aligned}
\tilde{\psi}(p) &= \langle p|\psi\rangle = \int_{-\infty}^{\infty} dx \, \langle p|x\rangle \, \langle x|\psi\rangle \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \; e^{-ipx/\hbar}\psi(x).
\end{aligned}$$

This is basically a Fourier transform, which transforms our wave function from the x basis to the p basis. You might have well written the Fourier transformation in terms of $k = p/\hbar$. Note that the constant $\frac{1}{\sqrt{2\pi\hbar}}$ (or $\frac{1}{\sqrt{2\pi}}$ if it is defined in terms of k) is thereby the convention of how people define the Fourier transform.

Inversely, it is also true that we can transform the wave function $\tilde{\psi}(p)$ in the p basis to the wave function $\psi(x)$ in the x basis:

$$\begin{aligned}
\psi(x) &= \langle x|\psi\rangle = \int_{-\infty}^{\infty} dp \, \langle x|p\rangle \, \langle p|\psi\rangle \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \; e^{ipx/\hbar}\tilde{\psi}(p).
\end{aligned}$$

You might as well prove and it should be clear to you that if you perform the Fourier transform twice then you will get back the wave function you start with. And that is the reason why we obtain the constant C in Eq. 2.1.

The momentum operator can also act on an arbitrary state vector ψ, in which case, we obtain:

$$\begin{aligned}
\langle x|P|\psi\rangle &= \int_{-\infty}^{\infty} dx' \ \langle x|P|x'\rangle \langle x'|\psi\rangle \\
&= \int_{-\infty}^{\infty} dx' \left(-i\hbar\frac{d}{dx}\delta(x-x')\right)\psi(x') \\
&= -i\hbar\frac{d}{dx}\int_{-\infty}^{\infty} dx \ \delta(x-x')\psi(x') \\
&= -i\hbar\frac{d\psi(x)}{dx}.
\end{aligned}$$

Therefore, when acting on a wave function in the x basis,

$$P \to -i\hbar\frac{d}{dx}$$

And as expected, the position operator when acting on a wave function in the x basis, will give

$$X \to x$$

This can be easily shown.

$$\begin{aligned}
\langle x|X|\psi\rangle &= \int_{-\infty}^{\infty} dx' \ \langle x|X|x'\rangle \langle x'|\psi\rangle \\
&= \int_{-\infty}^{\infty} dx' \ x\,\langle x|x'\rangle \langle x'|\psi\rangle \\
&= x\int_{-\infty}^{\infty} dx' \ \delta(x-x')\psi(x') \\
&= x\psi(x) \\
\Rightarrow \quad X &\to x
\end{aligned}$$

Now, let's consider the operator g(P), which we obtain from a corresponding classical dependent variable $g(p)$ by changing $p \to P$, acting on a wave function in the x basis.

$$g(P) \to g(-i\hbar\frac{d}{dx})$$

For example, a kinetic energy $g(p) = \frac{p^2}{2m}$ becomes the Hermitian operator:

$$\frac{P^2}{2m} \to -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Similarly for the potential energy, we have

$$V(X) \to V(x),$$

when it acts on the wave function in the x basis.

Note that for Hermitian or anti-Hermitian operator Ω, Ω^2 is always Hermitian due to the square. In this case, both P and P^2 are Hermitian. Can you show in one line that P is Hermitian? (Hint: consider the matrix element of P in the x basis.)

As mentioned before, we can express the Hermitian operator on a momentum basis. In that case, when the momentum and position operators act on the wave function in the momentum basis $\tilde{\psi}(p)$, we will have

$$P \to p$$

and

$$X \to i\hbar \frac{d}{dp}$$

In some case, it is more convenient to write the Hamiltonian in the momentum basis, so this could become useful.

For example, for the "energy" operator of Hamiltonian in one dimension, we can write as

$$\mathcal{H} \to \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

in the x basis, or

$$\mathcal{H} \to \frac{p^2}{2m} + V\left(i\hbar \frac{d}{dp}\right)$$

in the p basis.

2.3 Measurements and Expectation Value

Testing the theory of quantum mechanics means that we have to compare predictions of the theory with experimental data. However, as we have discussed quantum mechanics is an indeterministic theory, that is, it does not give a unique answer given an initial state. The theory predicts possible outcomes and the probability of getting all those outcomes. We can use the postulates we discussed at the beginning of this lecture to obtain the possible outcomes and their probability by following these steps:

1. Construct the corresponding quantum operator $\Omega = \omega(x \to X, p \to P)$, where X and P are the operators defined in Postulate II.

2. Find the orthonormal eigenvectors $|\omega_i\rangle$ and eigenvalues ω_i of Ω

3. Expand ψ (an initial wave function) in this basis:

$$|\psi\rangle = \sum_i |\omega_i\rangle \langle\omega_i|\psi\rangle$$

4. The probability $P(\omega_i)$ of obtaining ω_i as a result of the measurement is proportional to the modulus squared of the projection of ψ along the eigenvector ω_i, that is,

$$P(\omega) \propto |\langle\omega|\psi\rangle|^2.$$

The $\propto$ sign becomes the equal sign ($=$) if $|\psi\rangle$ is normalized to unity. In terms of the projection operator $\mathbb{P}_{\omega_i} = |\omega_i\rangle \langle\omega_i|$, we can write

$$P(\omega_i) \propto \langle\omega|\psi\rangle|^2 = \langle\psi|\omega_i\rangle \langle\omega|\psi\rangle = \langle\psi|\mathbb{P}_{\omega_i}|\psi\rangle = \langle\psi|\mathbb{P}_{\omega_i}\mathbb{P}_{\omega_i}|\psi\rangle = \langle\mathbb{P}_{\omega_i}\psi|\mathbb{P}_{\omega_i}\psi\rangle$$

In a general case where $|\psi\rangle$ is not normalized to unity, we can calculate a constant of the proportionality C by requiring that $\sum_i P(\omega_i) = 1$; hence $C = [\sum_i |\langle\omega_i|\psi\rangle|^2]^{-1} = [\langle\psi|\psi\rangle]^{-1}$. Therefore, we have

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

Since the outcome of each measurement is determined by the probability, it can be different when the same measurement on the exact same state is repeated. Therefore, to compare with the theory, we need to do many measurements and compare the distribution of the outcomes. One quantity we can use to compare the theory and experiment is the expectation value or weighted average. For the operator Ω, its expectation value $\langle\Omega\rangle$ is

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

or we can rewrite as

$$\begin{aligned}
\langle\Omega\rangle &= \sum_i \omega_i \frac{|\langle\omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle} \\
&= \sum_i \frac{\omega_i \langle\psi|\omega_i\rangle \langle\omega_i|\psi\rangle}{\langle\psi|\psi\rangle} \\
&= \sum_i \frac{\langle\psi|\omega_i\rangle \,\Omega\, \langle\omega_i|\psi\rangle}{\langle\psi|\psi\rangle} \\
&= \frac{\langle\psi|\Omega|\psi\rangle}{\langle\psi|\psi\rangle}
\end{aligned}$$

If $|\psi\rangle$ is normalized to unity, that is $\langle\psi|\psi\rangle = 1$, the expression above becomes

$$\langle\Omega\rangle = \langle\psi|\Omega|\psi\rangle \,.$$

2.4 Postulates of nonrelativistic quantum mechanics

Now we know what wave functions are and why we need them to describe a quantum mechanical state. The next question that we have to ask ourselves is how we can measure this state. This question is very important because the only way we can test our theory is to verify its results with experiments, and predicting measurable quantities that are testable is the only way to achieve that goal. That is what we are going to discuss in this lecture. So, what do we want to measure? A mathematical object associated with measurable quantities in quantum mechanics is what we call "an observable", for example the position operator X is associated with measuring the position, the momentum operator P is associated with measuring the momentum, the Hamiltonian operator is associated with measuring the energy and etc.

We will start by stating the postulates of quantum mechanics, which will tell us how to construct those operators and how the measurements work. The following are the postulates of nonrelativistic quantum mechanics:

Quantum Mechanics	**Classical Mechanics**
I. A state of a particle at time t is represented by a vector $\|\psi(t)\rangle$ in a Hilbert space.	I. A state of a particle at time t can be specified by a set of two variables representing its position $x(t)$ and momentum $p(t)$
II. The position x and momentum p are represented by Hermitian operators X and P with the following matrix elements in the eigenbasis of X $$\langle x\|X\|x'\rangle = x\delta(x-x')$$ $$\langle x\|P\|x'\rangle = -i\hbar\frac{d}{dx}\delta(x-x')$$ An operator that corresponds to the dependent variable $\omega(x,p)$ is given by a Hermitian operator $$\Omega(X,P) = \omega(x\to X, p\to P).$$	II. The dependent variable ω, which represents a dynamical property of the particle, such as kinetic or potential energy, is a function of x and p, that is, $\omega = \omega(x,p)$.
III. The measurement, associated with the operator Ω of a system in a state $\|\psi\rangle$ will yield one of the eigenvalues ω with the probability $$P(\omega) \propto \|\langle\omega\|\psi\rangle\|^2.$$ The state of the system will change from the initial state $\|\psi\rangle$ to the final state $\|\omega\rangle$ as a result of the measurement. This phenomenon is called the *collapse of wave function.*	III. If the state is given by x and p, the measurement of the dynamical variable ω will yield $\omega(x,p)$, and the state remains unaffected.
IV. The time-dependent state $\|\psi(t)\rangle$ can be calculated from the *Schrödinger equation* $$i\hbar\frac{d}{dt}\|\psi(t)\rangle = H\|\psi(t)\rangle,$$ where $H(X,P) = \mathcal{H}(x\to X, p\to P)$ is the quantum Hamiltonian operator and $\mathcal{H}$ is the Hamiltonian for the corresponding classical system.	IV. The state variables x and p change with time according to Hamiltonian's equations: $$\dot{x} = \frac{\partial\mathcal{H}}{\partial p}$$ $$\dot{p} = -\frac{\partial\mathcal{H}}{\partial x}$$

Note that for II, we can equally well write the Hermitian operators X and P in the eigenbasis $|p\rangle$ of P, in which case we will get:

$$\langle p|P|p'\rangle = p\delta(p - p')$$

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

At this point, I assume again that you all have read Chapter 1 of Shankar. However, I will go through the math of linear operators quickly to freshen up your memory and to emphasize important points that you need to know about linear operators and that you will be using in this class. For a more complete and coherent treatment of linear operators, I urge you to go back and review Chapter 1 of Shankar or any other linear algebra textbook.