Lecture 9

Theories of Quantum Mechanics

Study Goal of This Lecture

- Postulate of quantum mechanics
- Dirac notation

9.1 Theories of quantum mechanics

Now we are ready to summerize the fundation of quantum mechanics. Note that this is introduced to provide a set of well defined rules that allows us to calculate and explain experimental observables. Philosophical questions such as why Schrödinger equation is linear and why measurement are probabilistic are out of the scope of our discussions.

9.1.1 Theories of Quantum Mechanics

Quantum mechanics can be formulated in terms of six postulates:

This is Silbey's version, everything here follow "particle are waves".

1. **Wavefunction**
   The state of a qunatum system is fully specified by a wavefunction $\psi(\vec{r}, t)$. The wavefunction has no physical meaning but $|\psi(\vec{r}, t)|^2 dxdydz$ is the probability of finding the system in the volumn $dxdydz$ located at $\vec{r}$ at time t. This also requires:
$$\int \psi^*(\vec{r})\psi(\vec{r})d\tau = 1, \text{ normalization} \tag{9.1}$$

and

$$\psi(\vec{r}) \text{ is a smooth and single value function.} \tag{9.2}$$

2. **Observables**

   For each experimentally measurable property, there exists a corresponding Hermitian operator in quantum mechanics.

$$\hat{x} \to x\cdot, \ \hat{p}_x \to -i\hbar\frac{\partial}{\partial x}. \tag{9.3}$$

3. **Measurement**

   In a single measurement, the possible outcome of the observable $\hat{A}$ are the eigenvalues $\{a_i\}$ of $\hat{A}$.

$$\hat{A}\phi_i = a_i\phi_i. \tag{9.4}$$

4. **Expectation value**

   If a quantum system is described by the wave function $\psi(\vec{r}, t)$ and the value of the observable is measured once each on many identical preparations of such system, then the averaged value of all these measurement is given by

$$\langle\hat{A}\rangle = \int \psi^*(\vec{r}, t)\hat{A}\psi(\vec{r}, t)d\tau, \tag{9.5}$$

   note that probability of measured the eigenvalue a_i of $\hat{A}$ is

$$|c_i|^2 = |\int \psi^*(\vec{r})\phi_i(\vec{r})d\tau|^2. \tag{9.6}$$

5. **Time evolution**

   The wavefunction of a system changes with the time according to the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) = \hat{H}\psi(\vec{r}, t), \tag{9.7}$$

   where $\hat{H}$ is the Hamiltonian of the system. Assume that $\hat{H}$ is time-independent, then the above equation can be solved via seperation of variables, define:

$$\psi_(\vec{r}, t) = \phi(\vec{r})f(t), \tag{9.8}$$

   plug into Equ(9.7), we obtain

$$i\hbar\phi(\vec{r})\frac{df(t)}{dt} = \hat{H}\phi(\vec{r})f(t), \tag{9.9}$$

$$i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = \tfrac{1}{\phi(\vec{r})}\hat{H}(\vec{r})\phi(\vec{r}). \tag{9.10}$$

Note that the LHS depends on t and the RHS depends on $\vec{r}$, in order to hold the equal sign, the only solution is that both side equal to a constant.

$$\begin{cases} i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = C, \\ \frac{1}{\phi(\vec{r})}\hat{H}(\vec{r})\phi(\vec{r}) = C. \end{cases} \tag{9.11}$$

Clearly, the second equation is the time-independent Schrödinger equation, so $C = E$, and the first equation yields:

$$\frac{df(t)}{dt} = \frac{-i}{\hbar}E_n f(t), \tag{9.12}$$

$$\therefore f(t) = e^{-\frac{iE_n t}{\hbar}}, \tag{9.13}$$

$$\psi_n(\vec{r},t) = \phi_n(\vec{r})e^{\frac{-iE_n t}{\hbar}}. \tag{9.14}$$

The solution of the time-independent Schrödinger equation provides eigenwavefunctions of a quantum mechanic system. These eigenwavefunctions change in time in a single "phase oscillating" form. Note $|\phi_n(\vec{r},t)|^2 = \phi_n^*(\vec{r},t = 0)\phi_n(\vec{r},t = 0)$, it is independent of time, which means $\phi_n(\vec{r},t)$ are stationary wavefunctions.

We solve time-independent Schrödinger equation in order to have a nice/simple way to describe time-evolution. For an arbitrary wave function(i.e. not necessary be the eigenstate), it can be written as a linear superposition of eigenstate $\{\phi_n\}$ at time $t = 0$.

$$\psi(\vec{r},t=0) = \sum_n C_n\phi_n(\vec{r}), \text{ initial condition.} \tag{9.15}$$

According to Schrödinger equation

$$\psi(\vec{r},t) = \sum_n C_n e^{-\frac{E_n t}{\hbar}}\phi_n(\vec{r}), \longleftarrow \text{wavefunction at later time} \tag{9.16}$$

The wave function at any later time can be fully determined! $\Rightarrow$ quantum dynamics.

*We will spend some time on next lecture to discuss about quantum dynamics, but they are beyond our scope and the materials will not show up in the exam.

6. **Pauli exclusion principle**

   Wave functions describing a many-electron system must change sign(i.e. anti-symmetry) under the exchange of any two electrons.

This part will be discussed later when we dealing with many-electron wave functions.

Think that these rules were verified by experiments but not "proved" through logical deductions. These theories form the fundation of quantum mechanic. We have applied these rules, either explicitly or implicitly, to study several quantum systems. Later when we encounter more complicated systems, you will see these again and again. These principles provide satisfactory explanation of physical experiments!

Now we are in position to introduce a compact notation for the description of quantum mechanical systems $\rightarrow$ The Dirac notation.

9.2 The Dirac Bracket Notation

Dirac notation is a compact notation to describe quantum mechanical phenomena, most useful when formulating the "matrix formalation" of quantum mechanics. Here, we will only introduce the notation without going into the detailed formulation of "Matrix mechanics". The goal is to introduce this common notation that we will be using later in the course. The quantum mechanics can be formulated into two mechanics:

- Schrödinger $\rightarrow$ wave mechanics
- Heisenberg $\rightarrow$ matrix mechanics

These are two approaches to quantum mechanics. Heisenberg's approach came out after Schrödinger's wave mechanics had been well accepted by the community. Heisenberg's approach puzzled the physicist then. There even a intense debate on which formalism is correct. At the end, Von Neumann proves that two approches are equivalent and Dirac proposed a whole new mechanics which unified these two mechanics. Dirac's idea is the mechanics we use nowaday.

Recall, the key in qunatum mechanics is the superposition principle. It states that any wavefunction can be written as linear combination of eigenfunctions of an operator $\hat{A}$

$$\psi = \sum_n C_n \phi_n, \text{ where } \hat{A}\phi_n = a_n \phi_n. \tag{9.17}$$

Let's expand this summation:

$$
\begin{aligned}
\psi &= \sum_n C_n \phi_n \\
&= C_1\phi_1 + C_2\phi_2 + \cdots + C_n\phi_n
\end{aligned}
$$

$$
= \begin{matrix} C_1\phi_1 + \\ C_2\phi_2 + \\ C_3\phi_3 + \\ \vdots \\ C_n\phi_n \end{matrix} = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_n \end{pmatrix}.
$$

We find that we can write a wavefunction as a column vector and the basis is the eigenfunction of $\hat{A}$. Also, we can define a operators as a matrix. Now the problem becomes: How can one write down the expectation value with these fomulation? We define "dual" kets and bras.

Definition 1. Kets and Bras

$$
\text{Quantum state } \psi \longrightarrow \text{a ket } \ |\psi\rangle \ \text{ (column vector)}
$$

Each ket has a complimentary "bra"

$$
\longrightarrow \ \text{a bra } \ \langle\psi| \equiv (|\psi\rangle)^\dagger \therefore \ \text{row vector}
$$

$$
|\psi\rangle = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_n \end{pmatrix}, \ \langle\psi| = \begin{pmatrix} C_1^* & C_2^* & C_3^* & \cdots & C_n^* \end{pmatrix}.
$$

Kets and bras can also be written as superposition form

$$
\begin{cases}
|\psi\rangle & = C_1 |\phi_1\rangle + C_2 |\phi_2\rangle + \cdots, \\
\langle\psi| & = C_1^* \langle\phi_1| + C_2^* \langle\phi_2| + \cdots.
\end{cases}
$$

Definition 2. Inner product

The inner product is defined as:

$$
\langle\psi_1|\psi_2\rangle = \int \psi_1^* \psi_2 d\tau. \tag{9.18}
$$

Then for eigenstates of $\hat{A}$, $\{|\phi_n\rangle\}$ ($\hat{A}$ is Hermitian)

$$\langle\phi_n|\phi_m\rangle = \delta_{nm}, \tag{9.19}$$

so

$$\begin{aligned}\langle\psi|\psi\rangle &= (\sum_n C_n^* \langle\phi_n|)(\sum_m C_m |\phi_m\rangle) \\ &= \sum_{n,m} C_n^* C_m \langle\phi_n|\phi_m\rangle = \sum_{n,m} C_n^* C_m \delta_{n,m} \\ &= \sum_n |C_n|^2 = 1 \ \leftarrow \text{normalization condition.}\end{aligned} \tag{9.20}$$

9.2.1 Expectation value

So far, we have learned: Given a hermitian operator $\hat{A}$, the expectation value:

$$\langle\hat{A}\rangle = \int \psi^* \hat{A}\psi d\tau. \tag{9.21}$$

How do we express this in Dirac notation? Note that if ψ is a "ket" $\rightarrow |\psi\rangle$, then $\hat{A}\psi$ is also a "ket" $\rightarrow \left|\hat{A}\psi\right\rangle$. Therefore

$$\langle\hat{A}\rangle = \int \phi^*(\hat{A}\psi)d\tau = \left\langle\psi\middle|\hat{A}\psi\right\rangle. \tag{9.22}$$

Because of the Hermitian properties:

$$\int \psi^* \hat{A}\psi d\tau = \int \psi(\hat{A}^\dagger\psi)^* d\tau = \int (\hat{A}\psi)^*\psi d\tau = \left\langle\hat{A}\psi\middle|\psi\right\rangle. \tag{9.23}$$

We conclude that we can write

$$\langle\hat{A}\rangle = \left\langle\psi\middle|\hat{A}\psi\right\rangle = \left\langle\hat{A}\psi\middle|\psi\right\rangle = \langle\psi|\hat{A}|\psi\rangle, \tag{9.24}$$

and this gives us:

$$\langle\phi_n|\hat{A}|\phi_n\rangle = a_n \langle\phi_n|\phi_n\rangle = a_n. \tag{9.25}$$

Now we back to the algebra in Dirac notation:

$$|\psi\rangle = \sum_n C_n |\phi_n\rangle,$$

$$
\begin{aligned}
\left\langle \hat{A} \right\rangle &= \langle\psi|\hat{A}|\psi\rangle \\
&= (\sum_n C_n^* \langle\phi_n|)\hat{A}(\sum_m C_m |\phi_m\rangle) \\
&= (\sum_n C_n^* \langle\phi_n|) \sum_m C_m \hat{A} |\phi_m\rangle \\
&= \sum_{n,m} C_n^* C_m \langle\phi_n|\hat{A}|\phi_n\rangle \\
&= \sum_{n,m} C_n^* C_m a_n \langle\phi_n|\phi_n\rangle = \sum_{n,m} C_n^* C_m a_n \delta n, m \\
&= \sum_n |C_n|^2 a_n.
\end{aligned}
$$

$\uparrow$ This is the definition of measurement we mentioned in previous lecture!

Comparision	
Wave mechanics	Dirac notation
$\psi(x)$	$\|\psi\rangle$
$\psi^*(x)$	$\langle\psi\|$
$\int \psi_1^*(x)\psi_2(x)dx$	$\langle\psi_1\|\psi_2\rangle$
$\left\langle \hat{A} \right\rangle = \int \psi^*(x)\hat{A}\psi(x)dx$	$\langle\psi\|\hat{A}\|\psi\rangle$

9.3 Example of Utilizing Dirac Notation

Here we demostrate the using of Dirac notation in harmonic oscillator. The solution of Schrödinger equation can be written as:

$$\hat{H} |n\rangle = (n + \frac{1}{2})\hbar\omega |n\rangle , \tag{9.26}$$

and for ladder operator, the identities:

$$\hat{N} = \hat{a}^\dagger \hat{a}, \tag{9.27}$$

$$\hat{N} |n\rangle = n |n\rangle , \tag{9.28}$$

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle , \tag{9.29}$$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle . \tag{9.30}$$

Now we consider the expecation value of $\hat{x}^2$ and $\hat{p}^2$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}}(\hat{a}^\dagger + \hat{a}),\ \hat{p} = i\sqrt{\frac{\hbar m\omega_0}{2}}(\hat{a}^\dagger - \hat{a}), \tag{9.31}$$

$$
\begin{aligned}
\left\langle x^2 \right\rangle_n &= \langle n| \frac{\hbar}{2m\omega_0} (\hat{a}^\dagger + \hat{a})(\hat{a}^\dagger + \hat{a})|n\rangle \\
&= \frac{\hbar}{2m\omega_0} \langle n|\hat{a}^\dagger\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}\hat{a}|n\rangle \\
&= \frac{\hbar}{2m\omega_0} \langle n|\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger|n\rangle \\
&= \frac{\hbar}{2m\omega_0} \langle n|n + n + 1|n\rangle \\
&= (n + \frac{1}{2})\frac{\hbar}{m\omega}.
\end{aligned} \tag{9.32}
$$

$$
\langle \hat{p}^2 \rangle_n = (n + \frac{1}{2})\hbar m\omega. \tag{9.33}
$$

For the eigenstate:

$$
\Delta x \Delta p = \sqrt{(n + \frac{1}{2})\frac{\hbar}{m\omega}}\sqrt{(n + \frac{1}{2})\hbar m\omega} = (n + \frac{1}{2})\hbar \geq \frac{\hbar}{2}. \tag{9.34}
$$

Dirac notation makes the algebra more concise and easy to read.