Lecture 1

The Quantum World

Study Goal of This Lecture

- Particles are waves
- Heisenberg uncertainty principle and superposition of waves
- The Schrödinger equation

1.1 Introduction

Quantum mechanics, after all, is the fundation of our everday life. It is often projected as something unusual and sometimes even un-understandable. However, I think that is very wrong. Quantum Mechanics could be very intuitive, actually quite straightforward, once you learn to look at it from the right perspective.

The very key of quantum mechanics is that:

- There is no "quantum" vs. "classical"!
  $\Rightarrow$Newtonian mechanics is a limiting case of quantum mechanics. (high-T, heavy, large numbers, large size ...)
- "Particle-wave duality" should be understood as "particles are waves", i.e. any "particle-like" properties can be explained by wave-like nature of the "things".

So, now the key question becomes, **what happen if we see strictly "particles are waves" ?**

1.2 Particle are Waves

1.2.1 Specifying a physical system

In classical mechanics, the state of a particle is described by

$$\vec{x} : position$$

$$\vec{v} : velocity \ (or \ momentum \ \vec{p})$$

If also the potential V($\vec{x}$) is specified, then the whole (before now and after now) trajectory of the particle is "determined" by classical mechanics.
However, for waves, this description is not valid $\Longrightarrow$ you can't specify $\vec{x}$ and $\vec{p}$ for waves. So how do we describe a wave? A few example:

- string waves

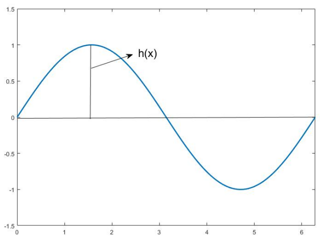

Figure 1.1: String wave, $h(x)$

- water waves

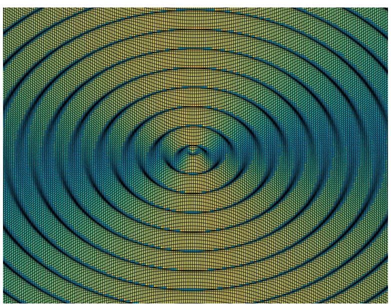

Figure 1.2: Water wave, $h(x, y)$

We use a function in space to describe a wave. The function gives the "displacement from equilibrium"

For simplicity, we use 1-D wavefunction for discussion below.

$$\Longrightarrow \psi(x),\ \psi(x,y),\ \psi(x,y,z).$$

A wave must be described by a wavefunction. Note that $\psi(x)$ in nature is non-local. i.e. a wave appears everywhere, not just at a single point.

1.2.2 De Broglie's Matter Wave

$h = 6.626 \times 10^{-34}$
Unit of h: energy∗time or length∗momentum

De Broglie's expression $\lambda = \frac{h}{p}$ actually specifies the wavelength of a particle in free space, that is, a plane wave.

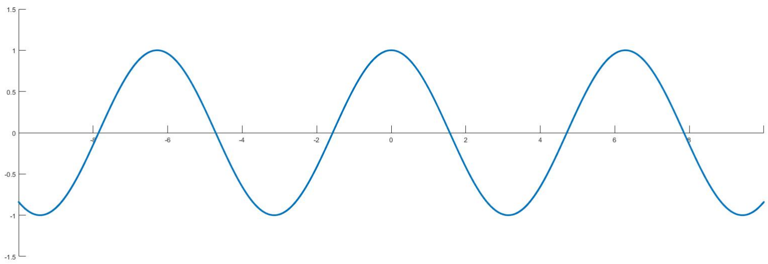

Figure 1.3: Wavefunction of free particle.

Can you write down the wave function for this one?

The wave function of the above wave can be written as:

$$\psi(x,t) = Ae^{2\pi i(\frac{x}{\lambda} - \nu t)} \tag{1.1}$$

$$\Rightarrow \psi(x,t) = A \underbrace{e^{2\pi i \frac{x}{\lambda}}}_{\substack{\text{spatial part} \\ \text{time-independent}}} \overbrace{e^{-2\pi i \nu t.}}^{\substack{\text{temporal part} \\ \text{time-dependent}}} \tag{1.2}$$

1.2.3 Expression of Matter Wave Length

The conservation of energy should still hold and the total energy should also be divided into kinetic part and potential part.

$$\therefore E = \frac{1}{2}mv^2 + V. \tag{1.3}$$

Now if total energy is conserved, then kinetic energy depends on V.

$$\therefore \frac{p^2}{2m} = E - V, \tag{1.4}$$

$$p = \sqrt{2m(E - V)}. \tag{1.5}$$

$$\therefore \lambda = \frac{h}{\sqrt{[2m(E - V)]}}. \tag{1.6}$$

Higher V, longer λ. We will come back to this later

1.2.4 Superposition of Waves

Unlike particles, waves can occupy the same space. Multiple waves can combine to form a new wave. i.e. superposition (interference) of waves. Mathematically, this means waves can form "linear combination"

$$\psi_3(x) = \psi_1(x) + \psi_2(x), \tag{1.7}$$

⟸ "constructive interference"

$$\psi_4(x) = \psi_1(x) - \psi_2(x). \tag{1.8}$$

$$\text{Actually } \psi'(x) = c_1\psi_1(x) + c_2\psi_2(x), c_1 \text{ and } c_2 \text{ are coefficients.} \tag{1.9}$$

$$\text{More generally, } \psi'(x) = \sum_i c_i\psi_i(x). \tag{1.10}$$

1.2.5 Heisenberg Uncertainty Principle

Heisenberg uncertainty principle is also a consequence of wave nature. Consider a wave which its momentum is precisely determined, this means that the particle is described by a perfect, periodic cosine or sine wave. Mathematically, it can be written as the general form:

$$\psi(x, t) = A \cos 2\pi(\frac{x}{\lambda} - \nu t). \tag{1.11}$$

The component $\frac{x}{\lambda}$ in exponentail represent a standing wave with periodicity given by λ and νt represent the wave is oscillating in time, i.e. "propagating wave".

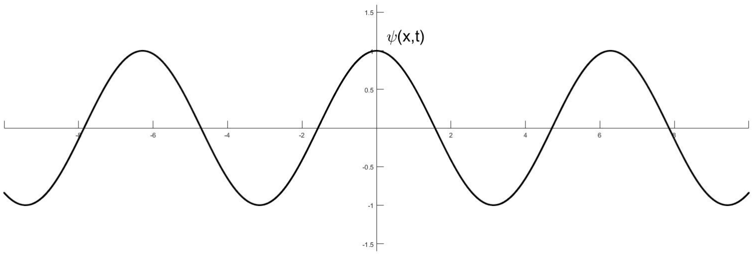

Figure 1.4: Wavefunction of free particle.

A more convenient form is to use complex numbers and the Euler's formula

$$\begin{aligned}\psi(x,t) &= Ae^{i2\pi(\frac{x}{\lambda}-\nu t)} \\ &\equiv A[\cos 2\pi(\frac{x}{\lambda}-\nu t) + i\sin 2\pi(\frac{x}{\lambda}-\nu t)].\end{aligned} \tag{1.12}$$

Equ (1.13) contains both cosine and sine waves ⇐ selecting from real/imaginary part. For the sake of simplicity, we will assume standing wave, $t = 0$. However, in this case, the position of particle is over the whole space, i.e. if one were to measure its position, the standard deviation or uncertainty, Δx will be infinity ⇐ *delocalized*.

Euler's formula: $e^{i\theta} = \cos\theta + i\sin\theta$

To construct a $\psi(x)$ that has finite width, wa have to add several wave of different wavelength:

linear combination, or "superposition" of waves is natural!!

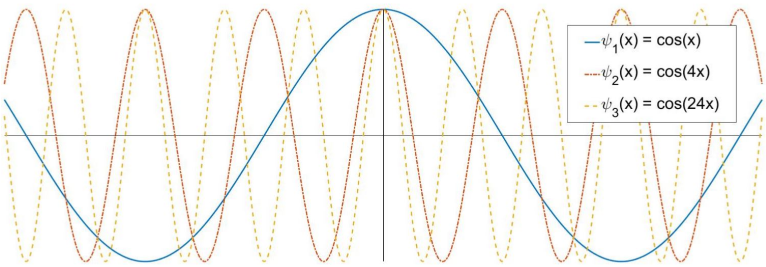

Figure 1.5: Superposition of several wave.

Mathematically:

$$\psi(x) = \sum_i A_i e^{2\pi i \frac{x}{\lambda i}}, \tag{1.13}$$

$$\psi(x) = \int_{\lambda=0}^{\infty} a(\lambda) e^{2\pi i \frac{x}{\lambda i}} d\frac{1}{\lambda} \equiv \int_{k=0}^{\infty} a(k) e^{2\pi i k} dk. \tag{1.14}$$

$k = \frac{1}{\lambda}$, pseudo-momentum

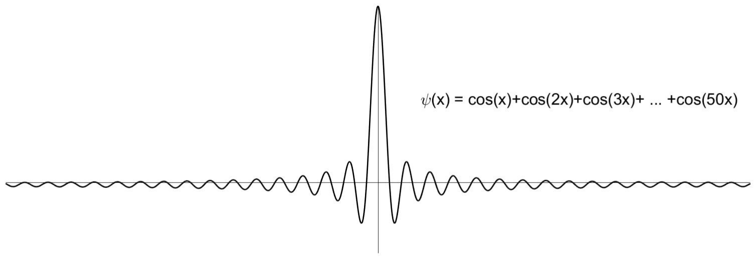

Figure 1.6: A wave packet as a linear superposition of many waves.

This is the definition of "Fourier Transform" and (k, x) are a Fourier tranform pair, which term complementary variables or conjugate variables. $\psi(x)$ is the Fourier transform of $a(k)$.

There is a theorem in the theory of Fourier transform stating that the width of $a(k)$ $(\Delta\frac{1}{\lambda})$ and the width of $\psi(x)$ (Δx) must satisfy the inequality

$$\Delta x \Delta k = \Delta x \Delta \frac{1}{x} \geqslant \frac{1}{4\pi}. \tag{1.15}$$

Note that $\frac{1}{\lambda} = \frac{p}{h}$, we obtain

$$\Delta x \Delta \frac{1}{x} \geqslant \frac{h}{4\pi} = \frac{\hbar}{2}. \tag{1.16}$$

$\hbar = \frac{h}{2\pi}$, reduced Planck constant

Clearly, there is another complementary pair from time dependence if time-dependent is to be considered:

$$\Delta t \Delta \nu \geqslant \frac{1}{4\pi}, \tag{1.17}$$

recall $E = h\nu$

$$\Longrightarrow \Delta E \Delta t \geqslant \frac{\hbar}{2}. \tag{1.18}$$

The above one is understood as lifetime and energy uncertainty (i.e. broadening).

Uncertainty has nothing to do with experimental limitation.

There are the two forms of Heisenberg uncertainty principle. They are fundemental in quantum mechanics and independent of the experimental errors.

The uncertainty arises because for waves, the position and momentum (also energy and time) can not be precisely determined at the same time. This is in contrast to the principles of classical mechanics. In classical, one specifies for a partcile its

$$x : position \tag{1.19}$$

$$v : velocity \tag{1.20}$$

$$V(x) : \text{potential, force acting on the particle} \tag{1.21}$$

then the following motion of the particle is determined. In quantum mechanics, this is impossible.

1.3 The Schrödinger Equation

Schrödinger postulated to treat a particle exclusively as waves(wave mechanics):

$$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}). \tag{1.22}$$

$\vec{r}$ denotes position

This is the time-independent Schrödinger equation and $\psi(\vec{r})$ is wave function, just like what we used for free particles.

Reasoning of the Schrödinger equation:

- The state of a particle is fully described by a wave function: $\psi(x)$.
- $\psi(x)$ satisfies the classical time-independent wave equation

$$\text{1-D: } \frac{d^2}{dx^2}\psi(x) = -(\frac{2\hbar}{\lambda})^2\psi(x). \tag{1.23}$$

$$\text{3-D: } (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi(\vec{r}) = -(\frac{2\hbar}{\lambda})^2\psi(\vec{r}). \tag{1.24}$$

- Total energy must be conserved, recall $\lambda = \frac{h}{\sqrt{2m(E-V)}}$,

$$\therefore (\frac{2\hbar}{\lambda})^2 = \frac{2m(E-V)}{\hbar^2}. \tag{1.25}$$

- Combine Equ.(1.25) and Equ.(1.26), we obtain

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}). \tag{1.26}$$

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ denotes Laplacian.

Note that this is not a derivation, this is just a way of thinking, Schrödinger equation is postulated and tested by experiments. It has no need to “derive” it.