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# Part 4. Quantum Mechanics

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## Alice's adventures in a quantum wonderland

Alice drinks a bottle of “drink me” and becomes as small as an atom. She finds the world totally unfamiliar, compared to the familiar classical world when she was of normal size.

- 1 When she knows where she is, she doesn't know how fast she is walking; When she knows how fast she is walking, she doesn't know where she is.
- 2 Walking in the brightness helps her to know better where she is.
- 3 Walking in the brightness, Alice finds the apparently continuous beams of light hits her as bullets: one shot after another in a discrete way. And she feels hurt more by the “bullet” of blue light than the “bullet” of red light.
- 4 She no longer has to enter a room through a door. She has a small chance to cross the wall and enter the room directly (although more likely she gets bounced back).
- 5 With fine-tuned speed, she can greatly enlarge the wall-crossing chance by using the front and back wall of the room together.
- 6 If she still prefers to walk through doors, she can walk through two doors at the same time. She is then likely to appear in the room somewhere, but never somewhere else.
- 7 She met an electron and made friend with him. However, soon, Alice was unable to find this electron friend out from other electrons no matter how hard she tries.

I don't know how to talk about a person as small as an atom consistently, but let us imagine that she is now just an atom, but somehow she can still record and tell her experiences.

In this part, let us find out what happens in the microscopic world, where the laws of nature is quantum mechanics. Let me tell that the learning experience of quantum mechanics will be very different from special relativity. Knowing it in advance helps for your learning.

## Quantum mechanics and special relativity are of different “feeling”

- Special relativity is based on 2~3 simple postulates – everyone knowing general physics knows what they mean physically. The logical sequence of these postulates may be counter intuitive. But after thinking, you can know what these consequences mean physically and that provides you a unique way to model them explicitly in your mind.
- Quantum mechanics is based on about 5 fundamental postulates. Each postulate looks mathematical. You may scroll to the summary of this part to get a quick feeling, not to be scared by their appearances. They tell you how to compute things. But they do not give you a physical idea in your mind (known as interpretations of quantum mechanics) to think about what's really happening.

Due to the differences, in this part we will not start from throwing the postulates to your face. Instead, we will spend a longer time to explain why we are forced to impose these “exotic” postulates. Afterwards we will happily test what we can do with these postulates as usual.

The exact number of postulates of quantum mechanics depends how you formulate it. You will see 4, 5, 6 in different books.

The interpretations of quantum mechanics is still an open question. There are a few possible interpretations in the market now. But we don't know which is correct (and we don't know even if it's possible to figure out the correct one).

# 1 The Nature of Light

## 1.1 Is Light Particle or Wave?

The nature of light was studied and debated for thousands of years. In the classical era (until 1900s), the key debate about light can be summarized as: Is light particle or wave? To be clear, let us summarize what particles and waves are. I encourage you to tap a basin of water or throw stones into a lake, to watch the nature of classical waves if you haven't done so before.

### Nature of classical particles

- 1 Can be counted and labeled as 1, 2, 3, ...
- 2 Have definite locations (or mass centers).
- 3 Have energy & momentum with  $E = p^2/(2m) + V$ .
- 4 When two particles meet, they collide.

### Nature of classical waves

- 1 Is oscillation with continuously variable amplitude.
- 2 Extended objects without definite locations.
- 3 Have frequencies  $\nu$  and wavelength  $\lambda$ .
- 4 When two waves meet, they overlap on top of each other.

Now that you know very well what classical particles and waves mean, let us explore the nature of light.

### Is light particle or wave? The debate in the history

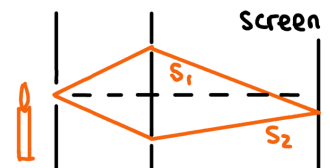
- ▶ As early as 400BC, Democritus asserted that all things are made of atoms (tinny particles) including light.
- ▶ In the early 17th century, optics was developing very fast led by microscopes, telescopes and so on. In 1630s, Descartes considered light as wave. In 1660, Grimaldi discovered diffraction of light, which behaves like water wave.
- ▶ Newton discovered the dispersion of light (1666). He considered light as particles and dispersion is interpreted as mixing and separation of different particles (1672).
- ▶ Hooke and company strongly criticized Newton's particle theory of light and supported the wave theory.
- ▶ In 1704, Newton published "Opticks" (Hooke died in 1703). Due to his impact at that time, the particle theory of light dominated.
- ▶ In 1801, Young made a double-slit experiment. After that and further developements (for example the Poisson spot) the wave theory become dominate again.
- ▶ In 1861, Maxwell published his equations of E&M. Electric field, magenetic field and light is then unified in one theory, where light appeared in the form of wave solutions.

Maxwell's equations concludes the debate about the *classical* nature of light – light is wave, and its mathematical equations are found from the first principle. However, the nature of light starts to look surprisingly different again once we step into the modern era.

The whole thing started at an "ultraviolet catastrophe". The observed radiation from black body does not agree with Boltzmann's theory of statistical physics for short wavelength light. In 1900, Planck suggested that light is emitted and absorbed in a quantized way to solve the problem. This is the first indication of the quantum world historically. Here we will not follow a historical order, but instead show you two more intuitive experiments made slightly later, where classical physics fails.

### The double-slit experiment

The double-slit experiment is an important turning point in the history for the wave theory of light. Let us review it here. As in the figure below, two beams of light travel through two slits and meets on the screen. The experiment needs to be explained by the wave theory of light.



On the screen, the pattern looks



The position of the bright and dark bands on the screen can be computed by comparing distances  $s_1$  and  $s_2$  on the figure.

▶ If  $s_1 - s_2 = 0, \lambda, 2\lambda, \dots$ , then light from both trajectories oscillate towards the same direction (constructive interference), and they leave bright bands on the screen.

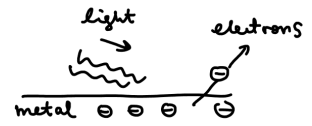
▶ If  $s_1 - s_2 = \lambda/2, 3\lambda/2, \dots$ , then light from both trajectories oscillate towards different directions (destructive interference), and they leave dark bands on the screen.

For the double-slit experiment to work, the light wave must at the same time go through two slits. If we block one slit, the originally dark spots will become bright again.

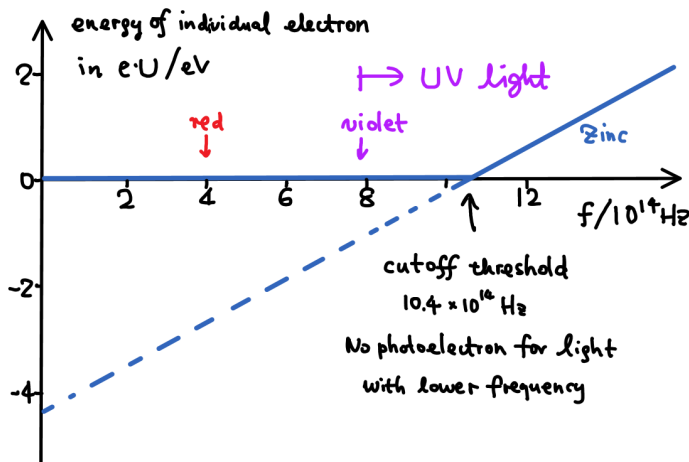
## 1.2 The Photoelectric Effect

### The photoelectric effect

Consider the experiment in the margin figure. A beam of light shines on metal. Apart of reflection light, what else do we expect to see?



- In 1887, Hertz noted that electrons can be knocked out by light. Such electrons are called photoelectrons. He also noted that the effect needs ultraviolet (UV) light.
- In 1902, Leonard studied the effect in more details. The energy of individual photoelectron increases with the frequency of light, but independent of the intensity of light. For each type of material, there is a cutoff frequency  $\nu_0$ , below which there is no photoelectron emission at all. The situation is plotted in the below figure.



### Summary of photoelectric effect

Dependent on	$I$	$\nu$
# of PE	Y	N
Energy of PE	N	Y
threshold	N	Y

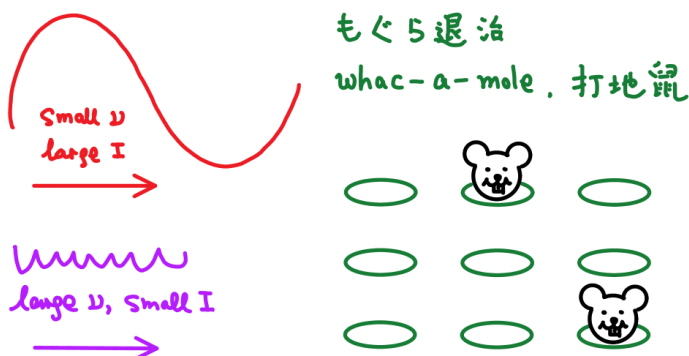
Here PE = photoelectron,  $I$  and  $\nu$  are the intensity and frequency of the incident light, respectively.

Why UV light with high enough frequency can knock out electrons? While light with lower frequency cannot knock out electrons no matter how strong is the beam of light. This surprising effect cannot be explained in classical E&M, and gives us a clue about quantum mechanics.

Honestly, when I learned this I did not feel surprised though the textbook told me to feel so. Trust me, it's indeed surprising. If you are not convinced, let's instead think about the following game.

### The surprising whac-a-mole

Whac-a-mole is a game to knock mice back to their holes. As physicists, instead of thinking how to knock them back, let's model why they come out. Assume they come out because they are scared by earthquake.



Imagine two types of earthquakes:

- ▶ Red earthquake has low frequency but very very large shaking amplitude.
- ▶ Violet earthquake has high frequency but very very small shaking amplitude.

Which earthquake is more likely to scare mice out?

In reality, the red earthquake is of course more scary. But if we correspond this game to the photoelectric effect experiment, what the experiment tells is that

- ▶ The violet earthquake can scare some mice out despite of the small amplitude it has (indeed if it is stronger it can scare more mice out).
- ▶ No matter how strong the red earthquake is, it does not scare *any* of the mice out.

### The photoelectric effect cannot be explained by classical E&M

Now have you started to feel that the photoelectric effect is surprising? Classical E&M cannot explain photoelectric effect. In classical E&M, electrons are shook by light, just as the mice shook by earthquake. When the intensity (i.e. shake amplitude) of the light is large enough, some electrons are shook so hard that they fly out of the metal. However, now whether electron leaves the metal depends on frequency instead of intensity. This poses a serious problem for the classical theory of light.

### Intensity still matters

When photoelectrons can come out, the number of photoelectrons indeed depend on the intensity of light. The stronger light, the more photoelectrons. But the key puzzle is why the threshold of whether photoelectrons come out does not depend on intensity.

### Einstein's explanation of the photoelectric effect

Inspired by Planck's 1900 explanation of black body radiation, Einstein proposed in 1905 that in the photoelectric effect, light can be considered as a collection of tiny particles (now known as *photons*). Each photon has energy

$$E = h\nu = h\frac{c}{\lambda} = \hbar\omega, \quad (1)$$

where  $h = 6.6 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$  is the Planck constant, and  $\hbar = h/(2\pi) = 1.1 \times 10^{-34} \text{ m}^2 \text{ kg s}^{-1}$  is the reduced Planck constant.

This explains the photoelectric effect (and Alice's experience [3](#) in her wonderland). Because an electron is likely to be hit by one photon instead of multiple photons together (if a person is hit by car, it is almost impossible that the person is hit by two cars at the same time). Thus whether the electron is knocked out of the metal is determined by the energy of the photon  $E$ , and thus its frequency  $\nu$ , instead of the intensity of light.

Classical light can be considered a "coherent state" of many photons. In a rough sense, coherent means that the **E** and **B** fields of the photons add coherently (instead of cancel each other in a disordered way).

### The everyday photoelectric effect

We actually don't have to do experiments to find out the photoelectric effect. We know that strong sunlight hurts our skin. To reduce the hurt, we can use sunscreen (sun cream). For example, after applying SPF 30 sunscreen and stay under the sun for 30 minutes, in principle, your skin damage equals to staying 1 minute under the sun.

How SPF 30 sunscreen works? To prevent damage to your skin (prevent sunlight reaching your skin), it should do either of the below for you:

### Quantities describing waves

- ▶ Wavelength  $\lambda$ : length of a period of oscillation.
- ▶ Wavenumber  $k \equiv 2\pi/\lambda$ : number of radians the wave oscillates per unit distance.
- ▶ Period  $T \equiv \lambda/v$ : time duration of a period of oscillation. Here  $v$  is the phase velocity of wave. For light,  $v = c$ .
- ▶ Frequency  $\nu \equiv 1/T$ : number of oscillations per unit time.
- ▶ Angular frequency  $\omega \equiv 2\pi\nu$ : number of radians the wave oscillates per unit time.

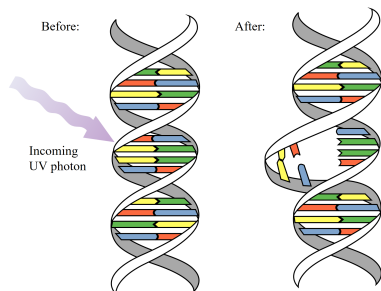
### Photon, quanta and quantization

- ▶ The "tiny" particle as building block of light is called photon.
- ▶ In general, the "tiny" particle (or quasi-particles where there is no actual particle) as building block of some form of energy (including matter itself, or the rotation, oscillation of matter, etc) is called quanta. In this sense, photon is the quanta of light. We will see that there are many other types of quantas that makes up our world.
- ▶ The feature that the quantas can be counted one by one (instead of being continuous) is that the quantas are "quantized".

- ▶ Reflection: reflect 29/30 of the light away. But, why you don't look like a mirror after applying sunscreen?
- ▶ Absorption: absorb 29/30 of the light before it reaches your skin. But, why don't you look black after applying sunscreen?

This is because sunscreen does not reflect or absorb all frequencies of light. It is much more effective on UV light. Indeed you look different after applying sunscreen if you take a photo in the UV light frequency band.

Why the UV light hurts your skin more than the visible light (which dominates energy of sunlight)? The reason is the same as the photoelectric effect (but what get knocked is not electrons but chemical bonds).



Also, in the winter, when you get close to a heater, you feel as warm as being under the sun. However, you don't have to apply sunscreen around a heater. This is because the heater radiation is dominated by the IR light.

And also you do not have to apply sunscreen when using your phone or microwave ovens, either.

### Does the photon wavelength change? The Compton effect

In the photoelectric effect, we have discussed how the electrons behave when light shines on them. What about the photons themselves? Let the incoming photon wavelength be  $\lambda$  and the outgoing photon wavelength be  $\lambda'$ . Are they equal?

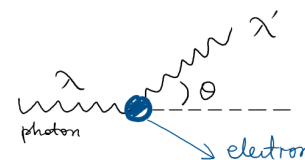
In classical E&M,  $\lambda = \lambda'$ . The incoming light (which has oscillatory electric field) shakes the electrons, and then the shaken (i.e. accelerated) electrons runs away, at the same time emits outgoing light of the same frequency.

When the electrons got hit by light, they get additional kinetic energy. Where does the additional kinetic energy come from? In classical E&M, the kinetic energy come from the reduction of the intensity of light, i.e. the outgoing light has small intensity.

However, the above energy argument must be wrong in a quantum theory. A photon cannot further reduce its intensity. Then, where would the kinetic energy of the electron come from? A photon has nothing to lose but its wavelength (recall  $E = hc/\lambda$ ). Thus we must have  $\lambda' > \lambda$ . As a good exercise, assuming that the electrons are free without any binding energy, then energy-momentum conservation together with quantization  $E = hc/\lambda$  gives

$$\lambda' - \lambda = \frac{h}{m_e c} (1 - \cos \theta) . \quad (2)$$

Up to the angular factor  $1 - \cos \theta$ , the shift of wavelength is  $\lambda_c \equiv h/(m_e c) \simeq 2.4 \times 10^{-12} \text{m}$ , known as the Compton wavelength. And the effect is observed by Compton (1923) and known as the Compton effect. Since the Compton wavelength corresponds to X-ray wavelength of light, the effect is hard to observe for observable light, and clearly visible when the wavelength of light is as short as X-ray.



### The dimension of $\hbar$

It is interesting to note the dimension of  $\hbar$ : it connects mass, speed and length. This relates to the question: why there is a fixed size of atom, such that the electron does not fall into the nuclei. From dimension analysis, the electron mass is a fundamental quantity of nature. Through speed of light  $c$  (enter from Coulomb's law) and  $\hbar$  (and a dimensionless strength of interaction  $\alpha$ ), the electron mass scale  $m_e$  got converted to the atomic length scale  $\hbar/(m_e c \alpha)$ , known as the Bohr radius. Thus, from dimensional analysis, before putting in any dynamics, we already expect that we need such a fundamental constant. We will see it explicitly in the part of atoms.

### Wait! Haven't you said that the particle theory of light is dead?

In the last subsection 1.1, I have already told you that the Newtonian particle theory of light is dead. Now, why Einstein dare to use particles to explain light again?

The photon that Einstein proposed is not a "classical particle" as we usually imagine. It has the feature of particles in that its energy is quantized and it appears to interact with the electron in the same way as two point particles collide.

Haven't I said that the particle theory of light contradict is killed by the double-slit experiment? Now let's see how the photons behave in the double-slit experiment.

### Planck scale and quantum gravity

In addition to the Bohr radius, we can also make another scale out of  $\hbar$  once gravity is concerned. The scale is the Planck energy  $E_p = \sqrt{\hbar c^5/G} \sim 10^9 \text{J} \sim 500 \text{kWh}$ , approximately the kinetic energy of an operating train. This scale puts together quantum and gravity, and is the scale of quantum gravity.

Consider two electrons, each has kinetic energy comparable to a running train, collide head-to-head. The collision is energetic enough to produce a microscopic black hole. Such collisions need to be studied with quantum gravity. We still don't have a full understanding of quantum gravity, though there is a decent candidate known as string theory.

## 1.3 The Single Photon Double-Slit Experiment

### The single photon double-slit experiment

In section 1.1, we have reviewed the double-slit experiment. Imagine that we reduce the intensity of light. Eventually, in the extremely-low intensity limit, each time we are doing double-slit experiment with only one photon. What is the outcome of such a single photon double-slit experiment? Suppose that we put a sensitive film on the screen which can record every photon. What's the status of the film as time goes on?

The experiment was carried out in 1909 by Taylor. The result looks like the figures to the right. Two features are clearly spotted in the result:

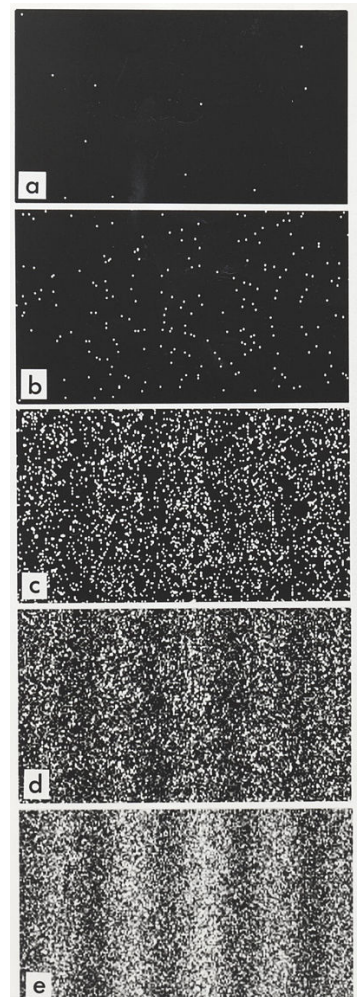
- 1 At the early stage of the experiment (panels (a) and (b) of the figure), clearly, the photon postulate is supported: Indeed we see a few "particles" on the screen. Each photon leaves one point on the screen.
- 2 As the experiment goes on (from panels (c) to (e)), more and more photons pass the slits. Interference patterns emerges. Indeed there are bright bands where the photons are more likely to reach and dark bands where the photons cannot reach.

How to interpret this result?

Considering that the intensity of incoming light is low enough, one photon already reaches the screen and leaves an unchangeable record before the other photon starts off. Thus the photons can be considered as independent.

Each photon behave independently but ends up at different points on the screen for the same experimental setup. Thus there must be some randomness in the photon behavior.

So the position of a photon on the screen should satisfy a probability distribution (as a smoothed version of panel (e)). The probability is large at bright bands and vanishes at dark bands, forming interference patterns.





You may ask where the randomness come from. We will come back to this point when discussing quantum measurement. The short answer at the moment is that there is no unique fundamental answer to the origin of randomness. But we have a well-defined way to compute the probability distribution. In this section, let us focus on another question, along the line of particle-wave debate of light.

### Is a photon particle or wave?

If you think the photon is a particle in the classical sense. Then recall how the interference patterns are formed:

- ▶ The photon must have gone through both slits. But how can a particle go through both slits at a time? Note that the photon is not supposed to further split into even smaller particles. Otherwise that contradicts the photoelectric effect, and contradicts the fact here that each photon leaves one point on the screen.
- ▶ The dark band of the interference pattern indicate destructive interference (cancellation between two branches). When particles meet, they collide. How can they stay at the same position and cancel each other?

So you probably change your mind and consider photon as a wave in the classical sense. Then

- ▶ Why photons arrive at the screen one by one, and one photon is the smallest building block of energy? Can't we continuously reduce the energy of wave by continuously reduce the amplitude of oscillation?
- ▶ Why each photon leaves one point on the screen, instead of a weak but complete interference pattern?

## 1.4 A Wave-Particle Duality, and from Light to All Matter

### A wave-particle duality

Is a photon particle or wave? This may be a wrong question to ask.

We have listed the properties of particles and waves in section 1.1. But who told us that microscopic matter must be classified into one of them following our classical experience?

It turns out that microscopic matter has some natures of classical particles, and some natures of classical waves together. The full properties of classical particles or waves emerges exclusively in the classical limit when macroscopic matter is considered.

### Not only for photons, but for all matter quanta

Now that light (considered waves before the quantum evolution) share some natures of particles, would matter like electrons, atoms, etc (considered particles before the quantum evolution) share some nature of waves as well?

In 1924, de Broglie proposed that particle-like matter should also have wave-like properties. The de Broglie wavelength of a particle is proposed to be

$$\lambda = h/p . \quad (3)$$

Though sounds crazy at that time, the de Broglie matter wave is verified in experiments. For example, the interference patterns in the single photon double-slit experiment above is also observed using electrons, atoms, and so on.

### The which-way experiment

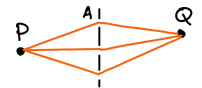
You may want to further see which slit on earth the photon goes through. To do so, you put a detector on one of the slit. If the photon goes through this slit, the detector reports it. However, once a detector is placed, the interference pattern vanishes.

There are many more confusing results, including compromise which-way experiment (1987), delayed choice (1999), weak measurement (2012), and so on. But here we have already enough surprises to explore at the moment and will not discuss these experiments here.

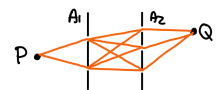
### From double-slit to path integral

(Optional) One can generalize the single-photon double-slit experiment by adding

- ▶ more slits on a board  $A$



- ▶ more boards  $A_1, A_2, \dots, A_n$



The interference pattern at  $Q$  is the phase interference among all these paths. This should still apply if we have an infinite number of boards and each board has an infinite number of slits on it.

What does a board with an infinite number of slits mean? It can be considered as free space with no board at all! The probability amplitude of photon traveling in free space between  $P$  and  $Q$  can be computed by summing over the interferences of all paths. This approach is known as the path integral formulation of quantum mechanics, as mentioned in the part of action principle.

## Non-relativistic quantum mechanics

Although quantum mechanics is initiated from photons, photons move at speed of light and thus is relativistic by its nature. The quantum theory consistent with special relativity (quantum field theory) was established much later than the non-relativistic quantum mechanics. This relativistic theory is beyond the scope of the current course.

Thus, now let us switch our attention from photons to massive microscopic particles, such as electrons, atoms, etc. They are non-relativistic at low energies. And our focus is how Newtonian mechanics get generalized into non-relativistic quantum mechanics. We will call non-relativistic quantum mechanics just quantum mechanics for short.

## More success of matter wave

In fact, crystal diffraction experiments are relatively easier ways to prove matter waves. The diffraction pattern of electrons are observed as early as 1927. Also the matter wave postulate immediately inspired Schrödinger to ask the question: what is the wave equation of matter wave? He then derived the Schrödinger equation in 1925 and published it in 1926.

## The wave and particle properties of a quanta

- ▶ Quantized (particle-like). Quantas are discrete and can be counted.
- ▶ Superposition (wave-like). Like waves, quanta obeys linear equations of motion. One can thus add one solution and another to make a third solution.
- ▶ Energy and angular frequency (connection of wave and particle). The particle-like energy and the wave-like angular frequency is related by the Planck formula

$$E = \hbar\omega . \quad (4)$$

- ▶ Momentum and wavenumber (connection of wave and particle). The particle-like momentum and the wave-like wavenumber is related by the de Broglie formula (3)

$$p = \hbar k . \quad (5)$$

We will expand some of these properties in great detail in the next section, and study a few other wave-like and particle-like properties in later sections.

## (Optional) A field of particles

The wave nature of particles provides us new insight about whether fundamental particles are the most “fundamental” objects. Think about water wave propagating on water surface. These water waves are not fundamental. They are excitations of the more fundamental water surface. Similarly, particles can be considered as excitations of more fundamental fields. For example, photons are excitations of E&M field (which you have learned), and electrons are excitations of electron field (which you probably have not learned so far). The quantum theory of studying these more fundamental fields is known as “quantum field theory”, which consistently put special relativity into the framework of a quantum theory.

## 2 The Quantum Wave Function

As we discussed, all matter has wave properties. How to describe wave? We are familiar with plane waves with angular frequency  $\omega$  and wave number  $k$ , it looks like  $\exp(ikx - i\omega t)$ . It is a function of space and time, and a special example of wave function.

## The quantum wave function

We assert that a quantum state  $|\psi\rangle$  is described by a wave function. For a quanta (quantum particle) moving in one spatial dimension, the wave function can be written as  $\psi(x, t)$ . In general,  $\psi$  can take complex values. This wave function completely describes the quantum nature of the particle.

Why bother to introduce a wave function? What's its physical meaning? In the below subsections we will answer these questions. But before to proceed, let me remind you that at a given time, a whole function  $\psi(x, t_0)$  contains much more information than the position and momentum of a particle (which are two real numbers). Thus a quantum state contains much more information than a classical state. We will see this again and again later.

## What is the symbol $|\psi\rangle$ ?

Don't be scared by the strange appearance of  $|\psi\rangle$ . For the moment being, it means nothing more than a state (the status of the quantum particle). In the part of quantum information, you will see why this notation is convenient.



## 2.1 The Wave Function as a Probability Amplitude

### The wave function is a probability amplitude

From the single quanta double-slit experiment, we learned that we have to introduce probability into the theory of quantum mechanics in a fundamental way. The wave function is a probability amplitude, such that  $|\psi(x, t)|^2$  is the probability density:

The probability to find the particle between  $x$  and  $x + dx$  is  $|\psi(x, t)|^2 dx$ .

This is known as the Born's rule and is the physical meaning of the wave function.

This explanation is first discovered by Born (1926).

For a complex number,  $|\psi|^2 \equiv \psi^* \psi$ , where star denotes complex conjugate.

### Features of the wave function in probability theory

As a probability amplitude, we can immediately read off a few features of  $\psi(x, t)$ :

► The wave function is normalized as

$$\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = 1, \quad (6)$$

because it describes a particle, and the probability to find the particle once in the whole space is one.

► If we prepare many copies of the same state, and measure the position  $x$  of the particle for each copy, the average value (called the *expectation value*) of the position is

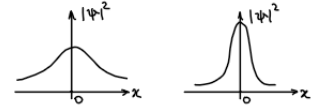
$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x, t)|^2 dx. \quad (7)$$

► More generally, the expectation value for a function of position  $f(x)$  is

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x) |\psi(x, t)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x, t) f(x) \psi(x, t) dx. \quad (8)$$

### Why we want $\langle f(x) \rangle$ ?

Because  $\langle x \rangle$  does not provide us enough information about the distribution. We want to know more. For example, the two below distributions:



They have the same  $\langle x \rangle$ . But in the left panel the value of  $x$  is less certain because the distribution is broader, while in the right panel we have a better idea where to find the particle. This information is encoded in  $\langle x^2 \rangle$ .

### Remaining questions

We now already know a lot about the quantum state. However, you may have the following questions:

- 1 So far only  $|\psi(x, t)|^2$  appears in the description. So why we use  $\psi(x, t)$  as the fundamental object?
- 2 How to relate  $\psi(x, t)$  to the single quanta double-slit experiment?
- 3 We have shown how to extract position information from  $\psi(x, t)$ . However, we need to extract the momentum information as well to know the state better. Can we and how do we do it?
- 4 We have only discussed the  $x$  dependence of  $\psi(x, t)$ , what about the  $t$  dependence?

We will address 1 and 2 in section 2.2, 3 in section 2.3, and 4 in section 5.1.

## 2.2 Consequence of Superposition and Linearity

### The world is linear

Superposition is the key feature of wave. Mathematically, superposition means linearity: if wave functions  $\psi_1$  and  $\psi_2$  are solutions of the wave equation, then  $c_1\psi_1 + c_2\psi_2$  is also a solution, where  $c_1$  and  $c_2$  are arbitrary complex-valued constants.

The water waves and E&M waves are approximately linear when the amplitude is small. However, quantum mechanics asserts that the wave function is *exactly* linear.

### Double-slit and the interference in probability

Suppose  $\psi_1(x)$  and  $\psi_2(x)$  are the solutions going through slit 1 and slit 2, respectively. Then from linearity,  $\psi(x) = \psi_1(x) + \psi_2(x)$  is also a solution. From the symmetry of the double-slit setup, this should be the actual solution that we look for.

At the dark bands, though  $\psi_1 \neq 0$ ,  $\psi_2 \neq 0$ , they cancel such that  $\psi_1 + \psi_2 = 0$ .

Thus, if we block a slit (say slit 2), the dark band is no longer dark since the probability density to have particle at the (originally) dark band is  $|\psi_1|^2 \neq 0$ . However, if we allow both slits, the probability density becomes  $|\psi|^2 = |\psi_1 + \psi_2|^2 = 0$ .

Linearly adding up probability amplitude  $\psi$  is how quantum mechanics. This is totally different from adding up probabilities in our classical life.

The probabilities are non-negative, and has no interference when adding them up. For example, if we buy a lottery and then buy another. The probability to win simply adds up. The probability of buying one lottery will not cancel the probability of buying the other.

However, adding probability amplitude is different. Because

$$|\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + \psi_1^*\psi_2 + \psi_2^*\psi_1 . \quad (9)$$

The first two terms correspond to adding up probabilities. But there are two additional interference terms  $\psi_1^*\psi_2 + \psi_2^*\psi_1$ . They are not positive definite and can cancel the whole thing.

### Why probability amplitude?

Now we know why we introduce probability amplitude in quantum mechanics: Because we treat probability as waves. Waves are linear in amplitude, but not in energy or intensity. This is a general feature of waves. For example, the intensity of light and the energy of water waves are both proportional to amplitude squared.

Here we have written  $\psi(x, t) \sim \psi(x)$  for a time-independent problem. We will later see that it is indeed consistent. Also, we are not careful about complex phases at this moment.

### Global and relative phases

Here, the relative phase (a phase is  $e^{i\alpha}$  for real  $\alpha$ ) between  $\psi_1$  and  $\psi_2$  has physical effects. Because the phase controls constructive interference, destructive interference or something in between.

However, a global phase of the whole wave function  $\psi$  (if we do not do further superpositions or enlarge the system) is unobservable (and thus unphysical). Because a global phase does not affect the probability density  $|\psi|^2$ .

I hope this relates the single-quanta double-slit experiment to the wave function of a quanta, and explains Alice's observation [6] at the beginning of this part.

### Plane waves as building blocks of wave functions in free space

In math, linearity allows us to expand the wave function with a complete set of basis. Physically, the importance of basis is that we can first understand these simple states, and then consider a general state as a weighted average of these simple states.

The basis are the solutions of the wave equation and of course depend on detailed problems: for a particle moving in potential  $V(x)$ , the solutions (and thus basis) depend on the form of  $V(x)$ . For most of this part (unless explicitly stated), we will be interested in the case of a constant  $V$  (or gluing a few stages of motion where each stage has constant  $V$ ). For constant  $V$ , happily the basis of the wave function are the familiar plane waves

$$\psi_p(x, t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i(px - Et)/\hbar} . \quad (10)$$

Here we have used  $p = \hbar k$  and  $E = \hbar\omega$  to replace wave vector and angular frequency

with momentum and energy of the quanta. Positive and negative  $p$  indicates that the wave is moving to the right and left, respectively. Again, be reminded that by wave or oscillation here, there is nothing changing positions periodically as for water wave or E&M wave. But rather what really oscillates is the *probability amplitude*.

Thanks to linearity, a general state of quanta can be written as a superposition of the plane waves

$$\psi(x, t) = \int_{-\infty}^{\infty} dp \, c(p) \psi_p(x, t), \quad (11)$$

where  $c(p)$  are complex valued functions of  $p$ . Here  $\psi(x, t)$  can be thought of as a weighted average of plane waves  $\psi_p(x, t)$  with weight  $c(p)$ . And  $c(p)$  can be thought of as how much of  $\psi_p(x, t)$  is contained in a state  $\psi(x, t)$ .

Superposition opens up the possibility to consider more exotic objects, such as the Schrödinger's cat (section 7) and quantum entanglement (the next Part).

## 2.3 Extracting momentum information from the wave function

In Newtonian mechanics, to describe a state, we would like not only to know the position of the particles but also how they move (momentum). Now that a wave function describes the state of a quanta, we also would like to know how to extract the information of momentum from the wave function.

### States with certain and uncertain momentum

What is the momentum of a wave function  $\psi(x, t)$ ? We have a few observations:

- ▶ For plane wave  $\psi_p$ , we know that its momentum is  $p$ .
- ▶ For general  $\psi$ , we do not expect a definite answer because of superposition. For example, the state can be  $\psi = \psi_{p_1} + \psi_{p_2}$  ( $p_1 \neq p_2$ ). What's the momentum of  $\psi$ ? The state does not have a definite momentum, but rather we have probabilities to find the state with momentum  $p_1$  and  $p_2$ .

### Computing expectation value involving momentum

We have shown how to compute an expectation value  $\langle f(x) \rangle$  for a function of position of the particle. For the momentum of the particle, we hope to find a similar formula

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) \hat{p} \psi(x, t) dx. \quad (12)$$

Is it possible? Here we have put a hat to momentum  $p$ . Why? We hope  $\hat{p}$  to tell information about momentum. However, we cannot simply take  $\hat{p} = p$ . Because the RHS does not have  $p$  elsewhere in the equation. Thus putting a number  $p$  in the integral does not make sense. So how to extract momentum information from the wave function?

For example, if we take a plane wave  $\psi = \psi_{p_1}$ , we should expect  $\hat{p}\psi_{p_1} = p_1\psi_{p_1}$ . If we take  $\psi = \psi_{p_2}$ , we should expect  $\hat{p}\psi_{p_2} = p_2\psi_{p_2}$ . Is this possible for the same  $\hat{p}$ ?

This suggests that we take  $\hat{p}$  as a differential operator (known as the momentum operator), instead of a number:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \equiv -i\hbar \partial_x, \quad (13)$$

### Plane waves are not normalized

We required the  $\psi$  being normalized:  $\int |\psi(x, t)|^2 dx = 1$ . Unfortunately a plane wave cannot be normalized since this integral diverges for  $\psi_k(x, t)$ . Physically it is because finding the plane wave at anywhere in space is a constant:  $|\psi_k(x, t)|^2 = \text{const}$ . Thus the normalization factor (whose square is probability density) is zero. An analogue is that, if you guess an integer from 1 to 10, you can win by chance 1/10. But if you guess a number uniformly distributed from  $-\infty$  to  $\infty$ , your chance to win is zero.

If you really worry about this normalization, you may choose to do one of the follows:

- ▶ Start from finite volume of space, and take the volume of space infinity after all calculations.
- ▶ Consider a wave packet – a collection of plane waves, which locally looks like plane waves but can be normalized properly. Physically, we can never make an exact plane wave

But they make things unnecessarily complicated. We thus leave the plane waves unnormalized. The factor  $1/\sqrt{2\pi\hbar}$  is not a normalization factor but just for future convenience.

### Reconsidering normalizations

You may be puzzled here: If I take  $\psi = \psi_{p_1}$  and  $\hat{p} = p_1$ , then isn't  $\int \psi_{p_1}^* p_1 \psi_{p_1} dx = \infty$ ?

You are right! This is because  $\psi_{p_1}$  cannot be normalized.

To fix this, we may reconsider the expectation value and define:  $\langle \hat{p} \rangle_r = \langle \hat{p} \rangle / \langle 1 \rangle$ , where  $\langle 1 \rangle \equiv \int \psi_{p_1}^* \psi_{p_1} dx$ .

At first sight, this seems stupid: I am trying to make sense of  $\infty/\infty$ . However, in physics, this indeed makes sense: Plane waves in infinite space does not exist in its exact form in nature. This is the origin of the divergence. We thus can first *regularize* the infinity by considering wave packets close enough to plane waves, or plane waves in a finite box. In such physical problems, the infinities are canceled and we get the desired result  $\langle \hat{p} \rangle_r = p_1$  for

$$\psi = \psi_{p_1}.$$

where the  $\partial_x$  in the very RHS is just a short hand notation of  $\partial/\partial x$ . We assert that (13) applies not only for free space, but also for non-constant  $V$ .

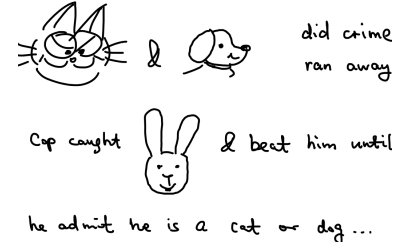
More generally, the expectation value  $\langle f(x, \hat{p}) \rangle$  can be extracted from the wave function as

$$\langle f(x, \hat{p}) \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) f(x, \hat{p}) \psi(x, t) dx . \quad (14)$$

### 3 Observables and Measurements

When talking about expectation values in the previous section, we implicitly mean measurements: measuring many identical quantum states and take the average. In this section, let us address the question of measurements more carefully. Especially, if we only have one system and do a measurement once, how do we address the probability of measurement outcomes?

We have talked about a key difficulty: When measuring momentum, what happens if the state does not have definite momentum? In this section we will address the theory of measurements in quantum mechanics: observables, states and measurement outcome.



#### Observables are represented by operators

To talk about measurements, we should start with what we can measure – observables. For example, position and momentum are observables. In the example of momentum operator  $\hat{p} = -i\hbar\partial_x$ , we learned that a number may not be enough to represent an observable. For position,  $x$  as a number can also be considered as a special operator  $\hat{x} = x$ . In general:

An observable is represented by an operator  $\hat{O}$  in quantum mechanics.

Moreover, for the observable outcome being real numbers instead of complex numbers, we require that the observables are Hermitian operators:  $\hat{O}^\dagger \equiv (\hat{O}^*)^T = \hat{O}$ .

#### Classical measurements are simple

In classical theories, theorists never worried about measurements:

- ▶ A classical state always have definite values of observables.
- ▶ A classical measurement can be made in an infinitely gentle way which do not disturb the system.

Quantum systems do not have above features. Thus, measurement is a key part of the quantum mechanics theory.

#### States with definite values of observables

Among the quantum states, some states have definite value  $\lambda$  of  $\hat{O}$ :

$$\hat{O}\psi_\lambda(x) = \lambda\psi_\lambda(x) . \quad (15)$$

In other words, the operator acting on the wave function is equal to the number  $\lambda$  acting on the state. For these states, when we measure  $\hat{O}$  on the state, we get definite outcome  $\lambda$ . Mathematically, we call the state  $\psi_\lambda(x)$  an eigenstate (or sometimes eigenfunction in math) of  $\hat{O}$  with eigenvalue  $\lambda$ .

Examples:

- ▶ Momentum eigenstates: The plane waves are momentum eigenstates with definite momentum. Indeed, we already know that plane wave  $\psi_p$  defined in (10), and

$$\hat{p}\psi_p(x) = p\psi_p(x) . \quad (16)$$

When we measure the momentum of this state, we definitely get  $p$ .

- ▶ Position eigenstates: What kind of states have definite position? Recall the probability amplitude nature of the wave function, the state with definite position  $q$  should only take value at one particular position  $q$ , and vanish everywhere else. This function is

In this section we will talk about the time around the measurement  $t_m$  and suppress the time variable of the wave function for short:  $\psi(x, t_m) \rightarrow \psi(x)$ .

known as a Dirac  $\delta$ -function defined as

$$\psi_q(x) = \delta(x - q) \equiv \begin{cases} 0, & \text{if } x \neq q \\ \infty \text{ with } \int_{-\infty}^{\infty} \delta(x - q) = 1, & \text{if } x = q \end{cases} \quad (17)$$

We can test that  $\psi_q(x)$  is indeed an eigenstate of  $\hat{x} = x$ :

$$\hat{x}\psi_q(x) = q\psi_q(x) . \quad (18)$$

This is because if  $x \neq q$ ,  $\psi_q(x) = 0$ . We thus have  $x\psi_q(x) = q\psi_q(x)$ . When we measure the position of this state, we definitely get  $q$ .

Unfortunately,  $\psi_q$  cannot be properly normalized either. Again, if you'd like to properly normalize  $\psi_q$ , you can either study particle in a finite box, or a physical narrow peak instead of the  $\delta$ -function.

For the eigenstates, the outcome of measurement is simple: we get the corresponding eigenvalue once measured. However, what about superpositions, such as two plane waves  $\psi_{p_1} + \psi_{p_2}$ , or two Dirac  $\delta$ -functions  $\psi_{q_1} + \psi_{q_2}$ ?

### Measurement outcome for a general state

For superpositions when measuring  $\hat{O}$ , we decompose the general state in eigenstates.

► For observables taking discrete results: The decomposition is

$$\psi(x) = \sum_i c_i \psi_{\lambda_i}(x) , \quad (19)$$

where  $\psi_{\lambda_i}$  is the eigenstate of  $\hat{O}$  with eigenvalue  $\lambda_i$ . The probability for the measurement outcome being  $\lambda_i$  is  $|c_i|^2$ . After the measurement, the wave function “collapse” to  $\psi_{\lambda_i}$ .

► For observables taking continuous results: The decomposition is

$$\psi(x) = \int c(\lambda) \psi_{\lambda} d\lambda , \quad (20)$$

where  $\psi_{\lambda}$  is the eigenstate of  $\hat{O}$  with eigenvalue  $\lambda$ . The probability density for the measurement outcome being  $\lambda$  is  $|c(\lambda)|^2$ . After the measurement, the wave function “collapse” to  $\psi_{\lambda}$ .

Examples:

► Momentum measurement: Equation (11) realizes equation (20). After the measurement, the probability density to find  $p$  is  $|c(p)|^2$ .

► Position measurement: A state  $\psi(x)$  can always be written as

$$\psi(x) = \int_{-\infty}^{\infty} \psi(q) \delta(x - q) dq . \quad (21)$$

After the measurement, the probability density to find  $q$  is  $|\psi(q)|^2$ . This reproduces the Born's rule, i.e. the probability amplitude interpretation of a quantum wave function.

### “Collapse” of wave function?

What does “collapse” of a wave function after a measurement mean? We mean the wave function becomes the corresponding eigenstate as indicated by the meaning of the word collapse. However, currently there is no unique understanding about dynamically why and how the collapse happen. This question is related to the interpretation of quantum mechanics. We will address it briefly in the epilogue section.

At the beginning of this part, when Alice is walking in the brightness, her position keeps being measured. Thus she knows better where she is. This explains [2].

### Wave Function Collapse Algorithm

Interestingly, the collapse of the quantum wave function has inspired the classical programming world. The [Wave Function Collapse Algorithm](#) is developed to dynamically generate infinitely sized 2D or 3D maps. The algorithm is inspired by the quantum superposition and collapse of the wave function.

## 4 The Uncertainty Principle

We have lots of uncertainties in our classical life due to lack of information. For example, before your exam score is released, your teacher tells you only the mean and standard derivation (uncertainty) of score distribution. What can you tell from this information? If the standard derivation is small, you are more certain about your score, but less certain about your ranking (as a small mistake may bring you from top to below mean). If the standard

derivation is large, you have less idea about your score but can estimate better your ranking based on usual performance.

In the quantum world, even if we have complete knowledge of the state, we still have uncertainties. For example, what happens if you measure the position of a plane wave?

In this section, let us make this question better defined and more general.

### Uncertainty is quantified by standard derivations

Talking about precision (or uncertainty), the corresponding quantity in statistics is the standard derivation. Given a state:

► Uncertainty of the state's position  $\sigma_x$  is  $\sigma_x \equiv \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ .

► Uncertainty of the state's momentum  $\sigma_p$  is  $\sigma_p \equiv \sqrt{\langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle} = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2}$ .

### The uncertainty principle

In math, a **Kennard inequality** tells that for  $\hat{p} = -i\hbar\partial_x$ :

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}. \quad (22)$$

This is the uncertainty principle, first discovered by Heisenberg in 1927.

We are trying to pack all the difficulties into math. As a result, though (22) is a logical consequence, we do not have an intuitive understanding about what happens. Instead of proving (22), let us see some examples.

### Understanding the uncertainty principle from waves

Let's see a few examples of wave functions:

► Plane waves:  $\psi_p = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$ ,  $\sigma_p = 0$  and  $\sigma_x = \infty$ .

► Gaussian wave packet:

$$\psi(x) = \frac{1}{\sqrt{\sigma_x} \sqrt{2\pi}} e^{-\frac{x^2}{4\sigma_x^2}}. \quad (23)$$

It's simple to check that  $\sigma_x$  is indeed the standard derivation for  $x$ . To calculate  $\sigma_p$ , noting that  $\langle \hat{p} \rangle = 0$  and  $\langle \hat{p}^2 \rangle = \hbar^2/(4\sigma_x^2)$ . Thus  $\sigma_p = \hbar/(2\sigma_x)$ . The Gaussian wave packet exactly saturates the uncertainty principle.

As the wave packet does not have definite momentum, different momentum eigenstates in the superposition do not move equally fast. That indicates that the wave packet will spread over time. We will see that it's indeed the case in section 5.1.

And going through the math proof does not make me feel it being more intuitive. That's why I choose to hide the math here and leave it for a proper quantum mechanics course. You will find it more intuitive once you realize that  $\psi(x)$  and  $c(p)$  are Fourier transform to each other. For Fourier transformation in general, the original function and the image admits an uncertainty principle. But this is beyond the scope of this course.

### Understanding the uncertainty principle from particles

Can we first measure  $x$  and then measure  $\hat{p}$  for the same state, and thus get both position and momentum information precisely?

The quick answer is no, because after a quantum measurement, the state collapses to the eigenstate. But this argument still seems mysterious. Let us consider a scenario in which we can see what actually happens.

### Wave vs particle viewpoints

There is a subtle difference between understanding the uncertainty principle from waves and particles: From waves, we are talking about the intrinsic fuzziness of quantum states. This is more precise in the sense of a principle of uncertainty. From particles, we see that fundamentally when measuring a microstate's position we have to change its

momentum. These two aspects are nevertheless consistent with each other.



Any measurement must act some interaction on the system and thus must change the system.

For example, you see an apple because light is reflected by the apple and is detected by your eyes. The light pushes the apple at the same time.

Classically, the reaction on the system can be made as small as one wants. However, quantum mechanically it is not possible.

To measure the position precisely, one needs to use a wave packet of light with shorter wavelength. We at best have  $\sigma_x \sim \lambda$ .

From de Broglie's relation,  $p_\lambda \geq \hbar/\lambda$  and thus shorter wavelength implies larger  $p_\lambda$ . The reflection of light transfers momentum of order  $p_\lambda$  to the measured object. Thus the object has a momentum uncertainty of order  $\sigma_p \sim p_\lambda$ . As a result, we at least need  $\sigma_x \sigma_p \sim \hbar$ .



### Optional: The quantum non-cloning theorem

You may think of another way to invalidate the uncertainty principle: What about clone the state into two copies, and measure position and momentum respectively?

Unfortunately, your brilliant idea has been elaborately blocked by the theory of quantum mechanics, by the quantum non-cloning theorem – no machine can clone an unknown state without destroying the original copy.

To prove that, we need to extend our language a little: including states of a cloning machine and multiple outcome states. Also, it is convenient to use the abstract notation  $|\text{object}\rangle$  to denote the quantum state of the object. If a quantum cloning machine  $|M\rangle$  exists, it does the follows: for any given quanta state  $|\psi\rangle$ , the machine transforms the state as

$$|M\rangle|\psi\rangle \rightarrow |M_\psi\rangle|\psi\rangle|\psi\rangle, \quad (24)$$

where  $|M_\psi\rangle$  is the state of the machine after the transformation. Now, consider two states  $|1\rangle$  and  $|2\rangle$ . We expect

$$|M\rangle|1\rangle \rightarrow |M_1\rangle|1\rangle|1\rangle, \quad |M\rangle|2\rangle \rightarrow |M_2\rangle|2\rangle|2\rangle. \quad (25)$$

Now what about the state  $\alpha|1\rangle + \beta|2\rangle$ ?

- 1 From how a cloning machine should work, we should get  $|M_*\rangle(\alpha|1\rangle + \beta|2\rangle)^2$ .
- 2 From linearity of quantum mechanics, we should get  $\alpha|M_1\rangle|1\rangle|1\rangle + \beta|M_2\rangle|2\rangle|2\rangle$ .

Although we don't know the final state of the machine  $|M_1\rangle$ ,  $|M_2\rangle$  and  $|M_*\rangle$ , the above 1 and 2 cannot be consistent. Because 1 contains  $\alpha\beta|1\rangle|2\rangle$  which is not part of 2. We thus conclude that a quantum cloning machine is impossible. Linearity is the key to prove the non-cloning theorem.

### What is possible about cloning

It's important to note the conditions of the non-cloning theorem.

It is possible to produce many copies of a known state. However, the ability of producing a known state does not help you to measure the position and momentum of an unknown state.

It is possible to clone a state and at the same time destroy the original copy. Obviously this does not help you to invalidate the uncertainty principle either.

A joke says when Heisenberg knows where he is, he doesn't know how fast he is walking. So does Alice for item 1 at the beginning of this part.

## 5 The Schrödinger Equation

We have talked about the interpretation of quantum states and measurements. They belong to the properties of the state at a given time.

But more importantly, physics is about given an initial condition, how to predict the state after some time. In other words, it is important to know the equation of motion which governs the time evolution of the system. In quantum mechanics, this governing equation is the Schrödinger equation.

## 5.1 The Schrödinger Equation

### Extracting energy from a wave function: the Schrödinger equation

We discussed in section 2.3 that the operator  $-i\hbar\partial_x$  can extract momentum from a plane wave  $\psi_p(x, t) \propto \exp[i(px - Et)/\hbar]$ , and consequently any superposition of plane waves, and thus a general wave function.

How to extract the information of energy from a wave function? We can do it in two ways:

- 1 Using the relation  $E = \frac{p^2}{2m} + V(x)$  and replacing  $p \rightarrow \hat{p}$ .
- 2 Noting that applying  $i\hbar\partial_t$  on plane waves directly extract their energies.

These two ways must be consistent. We thus get an equation

$$i\hbar\partial_t\psi(x, t) = \hat{H}\psi(x, t), \quad \hat{H} \equiv -\frac{\hbar^2\partial_x^2}{2m} + V(x) \quad (26)$$

This is the Schrödinger equation, and  $\hat{H}$  is called the Hamiltonian (the operator corresponding to energy). The LHS connects the state of a given time to a later time by the appearance of  $\partial_t$ .

In this part, we have been talking about one-dimensional problems. For future reference, the Schrödinger equation with three spatial dimensions takes the form

$$i\hbar\partial_t\psi(\mathbf{x}, t) = \hat{H}\psi(\mathbf{x}, t), \quad \hat{H} \equiv -\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{x}) \quad (27)$$

### We are not deriving it

Here by arguments and extrapolations, we show that the Schrödinger equation is a natural thing to expect. But we are not deriving the Schrödinger equation. Rather, the Schrödinger equation is a fundamental postulate of quantum mechanics.

The Schrödinger equation appears to be derived here because we have treated: The plane waves are the quantum state in free space with  $V = \text{const}$  (even for constant  $V$ , we only argued that the plane waves are the natural thing to expect). But now, we are extrapolating to include non-constant  $V$ .

### The spreading wave packet

We have argued that wave packets spread because its uncertain momentum. How to see this in calculations?

Let us focus on the simplest case:  $V = 0$ . One can verify that the following wave function satisfies the Schrödinger equation:

$$\psi(x, t) = \sqrt{\frac{\sigma}{\sqrt{2\pi}(\sigma^2 + i\beta t)}} e^{i(kx - \omega t)} e^{-\frac{(x - v_g t)^2}{4(\sigma^2 + i\beta t)}} \quad (28)$$

where  $v_g \equiv \hbar k/m$ ,  $\beta \equiv \hbar/(2m)$  and  $\omega \equiv \hbar k^2/(2m)$ . Here  $\sigma$  is a free parameter, indicating the spatial spread of the wave function at  $t = 0$ .

This solution is known as the Gaussian wave packet because the probability density is

$$|\psi(x, t)|^2 = \frac{\sigma}{\sqrt{(2\pi)(\sigma^4 + \beta^2 t^2)}} e^{-\frac{\sigma^2(x - v_g t)^2}{2(\sigma^4 + \beta^2 t^2)}}. \quad (29)$$

This is indeed a Gaussian wave packet at any time. The spatial spread of the wave

### Why spreading?

Why the wave packet is spreading? Intuitively, a wave packet contains waves with different momentum. These waves travel at different speeds. Thus, after a while, the superposition disperse and the wave packet spreads.

function is

$$\sigma_x(t) = \sqrt{\sigma^2 + \frac{\beta^2 t^2}{\sigma^2}} . \quad (30)$$

### The stationary state Schrödinger equation

Solutions of the Schrödinger equation with definite energy  $E$  is of particular interest. This is because:

- Physically, energy is conserved. If we start with a state with definite energy and keep it isolated, it will continue to have definite energy.
- Mathematically, with definite energy, the Schrödinger equation is greatly simplified. In general, the Schrödinger equation (26) is a partial differential equation. For a state with definite energy, we can solve the time part trivially and reduce it to an ordinary differential equation in the  $x$  direction only.

For a state with definite  $E$ , the Schrödinger equation breaks into two parts:

- The time part is  $i\hbar\partial_t\psi(x,t) = E\psi(x,t)$ . This can be solved as  $\psi(x,t) = e^{-iEt/\hbar}\psi(x)$ . Thus the time dependence in the wave function is a simple phase.

- The Hamiltonian part is

$$\left[ -\frac{\hbar^2\partial_x^2}{2m} + V(x) \right] \psi(x) = E\psi(x) . \quad (31)$$

This equation is known as the stationary state Schrödinger equation.

The stationary state Schrödinger equation (31) is a powerful tool to explore the quantum wonderland. In the reminder of the section, we will make use of the stationary state Schrödinger equation to consider various types of potentials and how the wave function  $\psi(x)$  behaves in these cases.

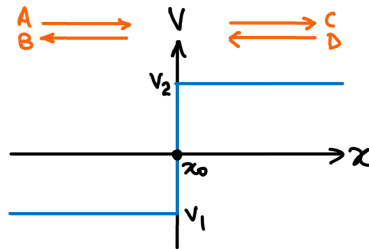
## 5.2 A Step in the Potential

Here and in subsequent subsections, we focus on square potentials where the potential is a constant at most places, except having a sudden change at the connection points. For such potentials, plane waves still work at almost everywhere, except that at connection points continuous conditions have to be imposed. This avoids the math difficulty of solving the Schrödinger equation as a differential equation.

### The step potential

Consider the potential in the stationary state Schrödinger equation (31):

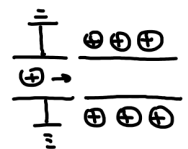
$$V = \begin{cases} V_1, & \text{if } x < x_0 \\ V_2, & \text{if } x > x_0 \end{cases} \quad (32)$$



Labels  $A, B, C, D$  in the figure will be used in the box below.

### Realization of a step

For example, a charged quanta travelling from zero electric potential to non-zero electric potential realizes a step potential if the transition is sharp.



### Wave function away from the step

For the step potential, when  $x \neq x_0$ ,  $V$  is a constant. The stationary state Schrödinger equation reduces to

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) = (E - V)\psi. \quad (33)$$

It has very simple solutions. It is the same plane wave solutions which have motivated us to “derive” the Schrödinger equation:

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x}, & \text{if } x < x_0 \\ Ce^{ik_2x} + De^{-ik_2x}, & \text{if } x > x_0 \end{cases} \quad (34)$$

where  $A, C$  denote waves moving to the right,  $B, D$  denote waves moving to the left, and

$$k_1 \equiv \frac{1}{\hbar}\sqrt{2m(E - V_1)}, \quad k_2 \equiv \frac{1}{\hbar}\sqrt{2m(E - V_2)}. \quad (35)$$

### The connection conditions

What happens to the point  $x_0$ ? There must be two relations between  $A, B, C$  and  $D$ . This is because, mathematically, Eq. (34) is a second order differential equation and thus should have only two integration constants. Physically, if we set  $D = 0$ , then it becomes a problem of an incoming wave  $A$  scatter at the potential and thus  $B$  and  $C$  should be fixed. Thus there are two relations between  $A, B, C$  and  $D$ .

The relations are

- $\psi(x)$  is continuous. Otherwise,  $\partial_x\psi(x_0) \rightarrow \infty \Rightarrow$  infinite momentum  $\Rightarrow$  unphysical.
- $\psi'(x)$  is continuous. Otherwise,  $\partial_x^2\psi(x_0) \rightarrow \infty \Rightarrow$  infinite energy  $\Rightarrow$  unphysical.

Applying these two relations to connect the two branch of solutions in Eq. (34):

$$\begin{aligned} Ae^{ik_1x_0} &= \frac{k_1 + k_2}{2k_1}Ce^{ik_2x_0} + \frac{k_1 - k_2}{2k_1}De^{-ik_2x_0}, \\ Be^{-ik_1x_0} &= \frac{k_1 - k_2}{2k_1}Ce^{ik_2x_0} + \frac{k_1 + k_2}{2k_1}De^{-ik_2x_0}, \end{aligned} \quad (36)$$

### Scattering into classically allowed region with $E > V_1$ and $E > V_2$

As we mentioned, when setting  $D = 0$ , the problem is reduced to a scattering problem.  $A$  is the incoming wave coming from  $x \rightarrow -\infty$ ,  $B$  is the reflection wave and  $C$  is the outgoing transmission wave.

Here we first consider the case when the energy of the state is large enough, such that if the state was a classical particle, then it is able to reach  $x > x_c$  regime.

From Eq. (36) we get

$$\begin{aligned} C &= \frac{2k_1}{k_1 + k_2}e^{i(k_1 - k_2)x_0}A, \\ B &= \frac{k_1 - k_2}{2k_1}e^{i(k_1 + k_2)x_0}C = \frac{k_1 - k_2}{k_1 + k_2}e^{2ik_1x_0}A. \end{aligned} \quad (37)$$

In general, there are transmission and scattering waves. This is different from the particle mechanics that the particle always goes through (because it has enough energy).

### Scattering into classically forbidden region with $V_1 < E < V_2$

Now we consider the case  $E < V_2$ . In this case, classically the particle is unable to reach the  $x > x_c$  regime.

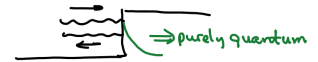
In this case,  $k_2$  becomes imaginary. When  $x > x_0$ ,

$$\psi(x) = Ce^{-|k_2|x} . \quad (38)$$

We are forced to have  $D = 0$  because the  $D$  term blows up at  $x \rightarrow \infty$ . The formal solution of  $C$  is the same as Eq. (37).

How the particle can enter the classical forbidden regime even if the  $V_2 > E$ ? This is because formally the effective “kinetic energy”  $\hbar^2 k_2^2 / (2m) < 0$  when  $k_2$  is imaginary.

An exponentially small part of wave function can enter the classical forbidden regime. This is completely different from classical particles and has profound implications. We shall uncover some of them later, namely tunneling, a consistent picture of identical particles.



However, in the wave perspective, it is not that hard to understand – E&M wave into a conductor has similar exponentially decaying properties (instead of vanish immediately).

## 5.3 The Potential Barrier: Reflection and Tunneling

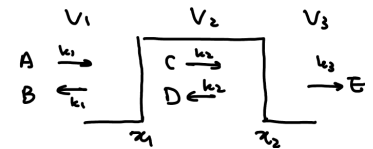
Now we modify the step potential further: Let’s join two steps to make a potential barrier.

### Scattering on a potential barrier

Consider the potential barrier illustrated in the figure. The detailed calculation will be left as an exercise. And here we shall use the experience we got from the step potential to study qualitative features here.

The way of solving this problem is similar to the last subsection: In principle we just have to solve an array of 4 equations at  $x_1$  and  $x_2$ , to determine 4 relations between 5 coefficients.

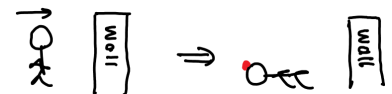
Practically, it is convenient to start from the outgoing wave  $E$ . Given  $E$ , we get  $C$  and  $D$ . And given  $C$  and  $D$ , we get  $A$  and  $B$ . In other words, given non-vanishing  $A$ , we always have non-vanishing  $E$ , even in the case that  $E < V_2$ .



### The quantum tunneling effect

In the case  $E < V_2$ , classically the particle can never go from  $A$  to  $E$  because there is a barrier to block it.

However, in quantum mechanics, no matter how high the barrier is (in the real world the barrier is always finite), there is an exponentially small part which goes into the barrier and escapes out to  $E$ . This is a key feature of quantum mechanics.

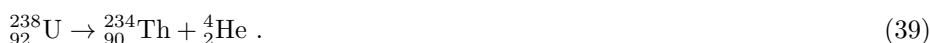


This is why at the beginning of this part, the quantum Alice observe that she can sometimes walk into a wall to enter a room in item 4.

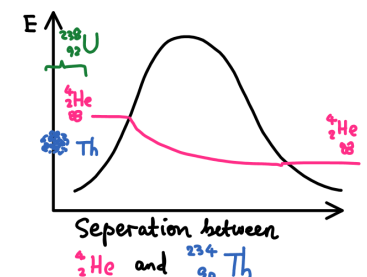
### Example of tunneling: $\alpha$ -decay

Heavy elements may be unstable. They may emit an  $\alpha$  particle, i.e. the Helium nuclei  ${}^4_2\text{He}$  and the remaining part becomes another element. This process is known as the  $\alpha$ -decay.

For example, the following process can happen:



Here the  ${}^{234}_{90}\text{Th}$  part of the nuclei provides a binding potential for the  ${}^4_2\text{He}$  part of the nuclei. They are together to form the  ${}^{238}_{92}\text{U}$ . But the  ${}^4_2\text{He}$  has a small chance to escape,



and this is the  $\alpha$ -decay of  ${}^{238}_{92}\text{U}$ .

The element  ${}^{238}_{92}\text{U}$  has a half-life of  $10^{17}$  seconds  $\sim 4 \times 10^9$  years (about 1/3 of the age of the universe). Note that the time scale of a typically microscopic process is often a tiny fraction of a second. Such a huge difference in time scales is because of the exponentially small decay rate.

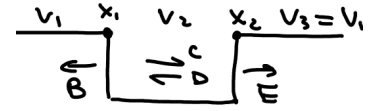
## 5.4 The Potential Well: Scattering and Bound States

What about to connect the two steps differently, to form a potential well?

### The potential well

Consider a potential well as in the side figure. The energy of the quanta classifies the problems into two cases:

- High energy scattering problem: If  $E > V_1$  and  $E > V_3$ , the situation is similar to the discussion in the last subsection.
- Low energy bound state: What if  $E < V_1$  and  $E < V_3$ ? There is no wave coming from  $x \rightarrow -\infty$  or wave going towards  $x \rightarrow \infty$ . As a result, the quantum state is confined inside (or a little bit outside with exponentially decaying amplitude) the potential well.



### Solving the bound state problem

Recall that for the wave function and its derivative to be continuous at  $x_1$  and  $x_2$ , there are 4 conditions. But now there are only 4 variables  $B$ ,  $C$ ,  $D$  and  $E$  and thus there should be at most 3 relations between the 4 variables. What would be the missing condition?

To see that, we apply the continuity conditions for  $\psi(x_1)$ ,  $\psi'(x_1)$  and  $\psi(x_2)$ ,  $\psi'(x_2)$  explicitly. At  $x_1$ ,

$$\frac{k_1 + k_2}{2k_1} C e^{ik_2 x_1} + \frac{k_1 - k_2}{2k_1} D e^{-ik_2 x_1} = 0, \quad (40)$$

$$\frac{C}{D} = \frac{k_2 - k_1}{k_2 + k_1} e^{-2ik_2 x_1}. \quad (41)$$

Similarly (we can do the replacement  $k_2 \rightarrow -k_2$ ,  $k_1 \rightarrow -k_1$ ,  $x_1 \rightarrow x_2$ ,  $C \leftrightarrow D$ ), at  $x_2$

$$\frac{C}{D} = \frac{k_2 + k_1}{k_2 - k_1} e^{-2ik_2 x_2}. \quad (42)$$

They must be consistent and thus

$$e^{2ik_2(x_2 - x_1)} = \left( \frac{k_2 + k_1}{k_2 - k_1} \right)^2 = \left( \frac{1 + i|k_1/k_2|}{1 - i|k_1/k_2|} \right)^2. \quad (43)$$

Recall that  $k_1 = \sqrt{2m(E - V_1)}/\hbar$ ,  $k_2 = \sqrt{2m(E - V_2)}/\hbar$ . Thus the above relation is a requirement on the energy of the state: Only state with such energies can exist. Thus the energy takes a series of discrete values until  $E > V_1$ , after which there is a continuous spectrum.



## Infinite height potential well

Take the limit  $V_1 \rightarrow \infty$ , keeping  $E$  and  $V_2$  fixed. In this case,  $k_1 \rightarrow i\infty$  and as a result, the wave function no longer enters  $x < x_1$  or  $x > x_2$ . In terms of Eq. (43), we now have

$$e^{2ik_2(x_2-x_1)} = 1, \quad \rightarrow \quad k_2(x_2 - x_1) = n\pi. \quad (44)$$

In this case, the left going and right going waves combines into a sine function

$$\psi(x) = 2iC e^{ik_2 x_1} \sin[k_2(x - x_1)] \propto \sin\left[n\pi \left(\frac{x - x_1}{x_2 - x_1}\right)\right]. \quad (45)$$

It is nothing but the standing wave solutions in classical mechanics.

What values can  $n$  take?

Taking negative  $n$  corresponds to flipping the sign of  $k_2$  and just add a negative sign to  $\psi$ .

However, can  $n = 0$ ?

No. Because we start with a particle in the system. If  $n = 0$ ,  $\psi(x) = 0$  and nowhere can we find the particle. Thus we can only have  $|n| = 1, 2, 3, \dots$ . The energies of these states are

$$E_n = \frac{(n\pi\hbar)^2}{2m(x_2 - x_1)^2} + V_2. \quad (46)$$

## The ground state

Let us focus on the  $n = 1$  state. Recall  $n \neq 0$ . Thus the  $n = 1$  state has the lowest energy among all states. This state acts as a “ground” in the energy spectrum and thus known as the ground state.

The ground state is of particular interest in quantum systems. This is because typically a quanta interact with other objects. For example, an electron can emit photons and lower its energy. But once the electron reaches its ground state, the electron can no longer emit photons and thus is stable (assuming the potential does not change).

Naively, we may have expected that the ground state has the same energy as  $V_2$ , since  $V_2$  looks like the “ground” in the potential. However, the ground state energy is in fact higher than  $V_2$ .

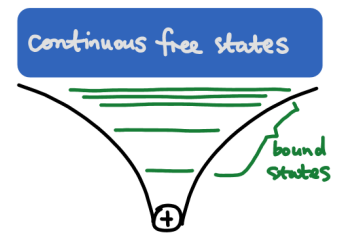
Why? Since we know that the particle is inside the well ( $\sigma_x < x_2 - x_1$ ), uncertainty principle tells that the momentum of the particle cannot be zero. The momentum adds some kinetic energy to the system.

If we make the potential well narrower, i.e. make  $x_2 - x_1$  smaller, then the ground state energy  $E_1$  increases. This is because more uncertainty in momentum is needed.

## Bound states in general

Here we only calculated the case of square potential. And only considered infinite potential well in details. However, the qualitative conclusion is general: If the quantum state does not have enough energy to reach infinity, then the state is a bound state localized in or close to the well. The energy of the state can only take discrete values. There exists a lowest energy state known as the ground state. For example, a nuclei has positive charge and creates a set of bound states that electrons can occupy.

Previously, the effects such as tunneling and bound state, though new in particle mechanics, we can understand using waves in a familiar way. However, the zero-point energy here is an intrinsic combination of particle and wave natures in quantum mechanics – no counter parts with either classical particles or classical waves.

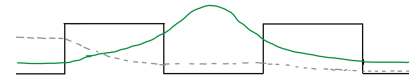


### Optional: Two potential barriers together and resonant tunneling

What about putting two identical potential barriers together? We then have a potential well in between two potential barriers. The potential well can hold bound states in it.

Consider the tunneling problem with such double barrier. Usually, we get double exponential suppression factors. Thus there is doubly small chance to tunnel through double barrier as expected. The situation is illustrated by the gray dashed line in the figure.

However, if we fine-tune the incoming energy to coincide with a bound state energy, then the gray dashed line is not a correct boundary condition for a bound state (for a bound state, both sides should exponentially decay) thus cannot be right. Rather, there is no exponential suppression factor for such tunneling. This situation is known as resonant tunneling.



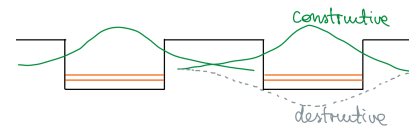
This explains Alice's enhanced tunneling rate (item 5 at the beginning of this part) if we consider the front and back wall as two potential barriers and Alice's incoming energy coincides with a bound state in the room.

### Optional: Two potential wells together and split of ground state

What about putting two identical potential wells together (called "double well")? Each potential well has its own set of bound states. Do the two set of bound states affect each other?

For definiteness, let us call the ground state of the left well  $\psi_L$ , and the ground state of the right well  $\psi_R$ . Both of them have energy  $E$ . Are  $\psi_L$  and  $\psi_R$  the lowest energy state of the system?

Due to linearity of quantum mechanics, we know that the superpositions  $\psi_{\pm} = (\psi_L \pm \psi_R)/\sqrt{2}$  are also solutions of the Schrödinger equation. In fact  $\psi_+$  has slightly lower energy than  $E$  because the wave function takes slightly larger value in the middle barrier (constructive interference), which makes the position of the particle less certain. Similarly,  $\psi_-$  has slightly higher energy due to destructive interference. Thus the original ground state splits into two states, with  $\psi_+$  the true ground state of the theory.



### Optional: Infinite potential wells together and the band theory

What about putting infinitely many identical potential barriers (or wells) together? We get a periodic potential. From the experience of double well, the sign of each local ground state (of an individual well) can make constructive or destructive interferences. There are infinitely many choices. Thus the original ground state splits into an infinite number of states. These states form a continuous band.

The particle energy has to be within the band. And resonant tunneling happens and the quanta can freely travel through potential barriers without suppression.

Here we are talking about the ground state. But for other higher energy states, the same argument applies that the bound state energies are broadened into continuous bands (illustrated by the orange thick lines in the figure).



The infinite potential can be considered as a toy model of a solid. The potential wells are those made by atoms, and the quanta being studied are the electrons. In solid, the energy of the active electrons is determined by statistical physics and the nature of the solid (the "Fermi energy" at low temperature). If the electrons can move in the band, the solid can conduct electric current and thus is a conductor. If the conducting band is fully occupied, the solid is an insulator. The case in between is known as semi-conductor.

#### Quantum mechanics in your phone

You should appreciate quantum mechanics for allowing you to have a cell phone. Indeed, the CPU of your phone is doing classical computing, not quantum computing yet. But the logical gates of a modern classical computer is based on semi-conductors, and thus the band theory of solid state physics. Without quantum mechanics, we cannot understand these theories and there is nothing to guide us for making transistors from semi-conductors.

## 6 Identical Particles

At the beginning of this part, item 7 of Alice's adventure is that she fails to distinguish an electron from another. In the classical world, we can distinguish persons. Why this fails to work in Alice's quantum adventure?

### The classical ways of distinguishing particles all fail

Classically, how we distinguish two persons?

- 1 Intrinsic identifications: Classically, two persons look different. However, for microscopic particles, this fails to work. Because:
  - ▶ Elementary particles: We have only discovered finite types of elementary particles (labeled by mass, spin and charge). Two particles of the same type have the same intrinsic features. For examples, you cannot find any difference between two electrons.
  - ▶ Composite particles (such as atoms): They are bound states. Bound state energies are discrete. For example, if two hydrogen atoms are both in their ground states, or first excited states, we cannot find any difference between the two atoms.
- 2 Extrinsic identification: Classically, two persons are separate. We can follow their trajectories to distinguish them. If Bob is in Beijing, and Charlie is in New York, it's easy to figure out whom is whom even if they look alike.

However, quantum particles can never be in totally different positions. Fundamentally, what separate quantum particles are potential wells. Quantum tunneling tells that the wave function of two particles, say electrons, will always overlap, though the amount may be extremely small. Two electrons are never completely separated.

Those failure of distinguishing quantum particles lead to a fundamental principle of quantum mechanics: the existence of identical particles.

### Classification of quantum particles

To make use of the identical particle postulate, we need a wave function to describe at least two particles. The two-particle wave function  $\Psi(x_1, x_2, t)$  means that the probability to find one particle at  $(x_1, x_1 + dx_1)$  and the other particle at  $(x_2, x_2 + dx_2)$  is  $|\Psi(x_1, x_2, t)|^2 dx_1 dx_2$ .

Since the two particles are identical, we should have  $|\Psi(x_1, x_2, t)|^2 = |\Psi(x_2, x_1, t)|^2$ . Otherwise, we can tell the difference of the two particles by noticing the probability difference that the two particles can be found. Thus,  $\Psi(x_1, x_2, t)$  and  $\Psi(x_2, x_1, t)$  differ at most by

$$\Psi(x_2, x_1, t) = e^{i\alpha} \Psi(x_1, x_2, t), \quad (47)$$

where  $\alpha$  is a real number. Mathematically, this implies (since  $x_1$  and  $x_2$  are just labels that can be swapped)

$$\Psi(x_1, x_2, t) = e^{i\alpha} \Psi(x_2, x_1, t). \quad (48)$$

Thus,  $e^{i\alpha} = \pm 1$ . The multi-particle wave functions are either symmetric or asymmetric under interchange of particles.

There are thus two kinds of multi-particle wave functions which satisfies the identical particle postulate:

- ▶ Symmetric wave functions with  $\Psi(x_1, x_2, t) = \Psi(x_2, x_1, t)$ . The particles described by such wave functions are called bosons. For elementary particles, bosons represents the

Imagine one twin likes more to go to a coffee shop and the other twin likes more to go to a bookstore. You can then distinguish them in a statistical sense, and they are no longer identical.

forces of nature, for example, photons and gravitons.

► Anti-symmetric wave functions with  $\Psi(x_1, x_2, t) = -\Psi(x_2, x_1, t)$ . The particles described by such wave functions are called fermions. For elementary particles, fermions represents the buliding blocks of matter, for example, electrons and quarks.

### Pauli's exclusion principle

For fermions, because of the anti-symmetry of the wave function, the fermions cannot be in the same state. This is because, if two fermions were in the same state, then

$\Psi(x_1, x_2, t) = \Psi(x_2, x_1, t)$ . Considering the definition of fermions,  $\Psi(x_1, x_2, t) = -\Psi(x_2, x_1, t)$ , we get  $\Psi(x_1, x_2, t) = 0$  and thus such systems do not exist.

This is why in a multi-electron atom, electrons do not only occupy the lowest energy states, but also other states if some electrons have already occupied the lowest energy states.

## 7 Epilogue: Summary and What's Next

In the journey of constructing the theory of quantum mechanics, we have met many difficulties. The difficulties are resolved sometimes by applying what we know; and sometimes by introducing new postulates. Now, let us summarize the postulates that we really have to introduce.

### Summary of fundamental postulates of quantum mechanics

- 1 The superposition principle of  $\psi(\mathbf{x}, t)$ : the world is linear.
- 2 Momentum can be represented by an operator  $\hat{\mathbf{p}} = -i\hbar\partial_{\mathbf{x}}$ .
- 3 A measurement is represented by a Hermitian operator  $\hat{O}$ . The operator  $\hat{O}$  defines a complete set of eigenstates  $\hat{O}\psi_{\lambda}(\mathbf{x}) = \lambda\psi_{\lambda}(\mathbf{x})$ . The state to be measured  $\psi(\mathbf{x})$  can be expended by these eigenstates as  $\psi(\mathbf{x}) = \int c(\lambda)\psi_{\lambda} d\lambda$ . The probability density to get value  $\lambda$  from the measurement is  $|c(\lambda)|^2$  and the state collapses to  $\psi_{\lambda}(\mathbf{x})$  after the measurement.
- 4 The wave function obeys the Schrödinger equation

$$i\hbar\partial_t\psi(\mathbf{x}, t) = \hat{H}\psi(\mathbf{x}, t), \quad \hat{H} \equiv -\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{x}) \quad (49)$$

- 5 Particles can be identical in quantum mechanics.

Recall that if the observable take discrete values, the corresponding decomposition is

$$\psi(\mathbf{x}) = \sum_i c_i \psi_{\lambda_i}(\mathbf{x})$$

and the probability to get  $\lambda_i$  is  $|c_i|^2$

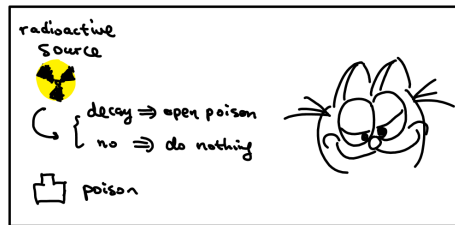
These postulates do not look as simple as those of relativity. This is why it took decades for the sages of the past century to understand the principles of quantum mechanics. Fortunately, once we have understood and accepted these postulates, the quantum world works elegantly and amazingly.

We have discussed how these postulates are natural guesses inspired from experiments, and explored the consequences of these postulates. Having that said, we do not know what “really happens” in quantum mechanics, especially when a measurement is made. Let me mention it further here:

### The Schrödinger's cat: how to understand superposition and measurements?

Traditionally, the Copenhagen (a city where a large part of quantum mechanics is developed) interpretation encourage “shut up and calculate.” However, we may not

like to shut up at a thought experiment known as the Schrödinger's cat:



$$\psi = \psi_{\text{decay}} + \psi_{\text{not}}$$
$$\Rightarrow \text{cat} = \text{alive cat} + \text{dead cat} ?$$

If a quantum process controls whether a bottle of poison opens. And we put the quantum generator, bottle of poison and a cat in a box. Before we open the box and measure the state, what happens to the cat? Is the cat in a superposition of alive and death?

Unfortunately, no firm answer can be given at the moment. The answers differ in different interpretations of quantum mechanics. In some interpretations, one may even so crazy to let both the alive and dead cat live in parallel universes after the measurement, and we are only in one of them!

#### Further reading about the content

- ▶ To learn more, the best way is to read the first a few sections of a proper quantum mechanics book. For example, Griffiths, [Introduction to Quantum Mechanics](#), or Allan Adams, Matthew Evans, and Barton Zwiebach [MIT Open Course on Quantum Mechanics](#) (with videos).
- ▶ [The Principles of Quantum Mechanics](#) by Dirac, though a bit old, is still an excellent introduction.
- ▶ Some other famous books include Shanka, [Principles of Quantum Mechanics](#), Sakuri, [Modern Quantum Mechanics](#).
- ▶ For the developments of quantum mechanics, there is a popular science book in Chinese: Cao, [Does God Play Dice](#).

#### What happens next in a university physics program?

- ▶ Quantum mechanics and advanced quantum mechanics. What I have covered is really a starting point and you need to learn a proper course. You need to learn the algebra of matrices, the quantum harmonic oscillator, angular momentum, approximation methods, and so on.
- ▶ Atom physics, solid state physics and material science. The explanation of matter is all based on quantum mechanics.
- ▶ Quantum field theory. This is how quantum mechanics works with special relativity.

## 8 Exercises

### E1.1 Compton effect

Derive the wavelength shift (2) for the Compton effect.

### E4.1 Time evolution of the eigenstates

What is the form of position eigenstates (quantum states with definite position) and momentum eigenstates for a freely moving particle? At the next moment in time (without measurement or interaction), are they still position and momentum eigenstates?

### E4.2 Uncertainty of the Gaussian wave packet

Compute  $\sigma_x$  and  $\sigma_p$  of the Gaussian wave packet (23). Show that the uncertainty principle is satisfied in a saturated way.

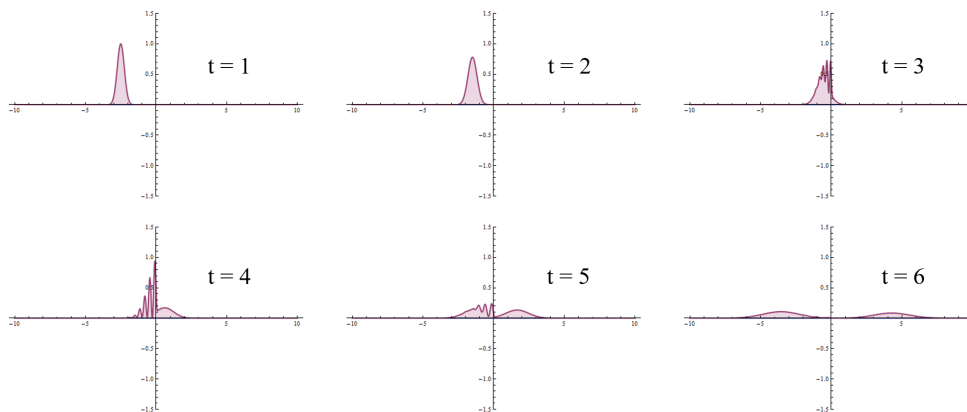
### E4.3 Commutation relations

If  $\psi_q(x)$  is an eigenstate of  $x$  with eigenvalue  $q$ . Can  $\psi_q(x)$  also an eigenstate of  $\hat{p}$ ? Let us answer this question in different ways:

- Physically: show that if  $\psi_q(x)$  is at the same time eigenstate of  $x$  and  $\hat{p}$ , then the uncertainty principle is violated.
- Mathematically: Show that  $\hat{p}(x\psi_q(x)) \neq x(\hat{p}\psi_q(x))$ . Use this observation to prove that  $x$  and  $\hat{p}$  do not share eigenstates.

### E5.1 Time-dependent scattering on a potential barrier

Consider a particle moving towards a barrier-shaped potential, and the incoming energy is lower than the height of the barrier (i.e. the potential energy on the barrier is higher than the total energy of the particle).



- Classically, can the particle pass to the other side of the barrier? Why?
- Quantum mechanically, can the particle pass to the other side of the barrier? Why? Explain it both in terms of continuity of the wave function, and energy conservation.
- Some ripples are observed in the figure below (snapshots of the probability density of the particle). Explain the ripples qualitatively.



## E5.2 Scattering on a potential barrier: math and interpretations

- ▶ Derive the transmission amplitude  $E$  using  $A$  for a potential barrier.
- ▶ Show that the relations between  $A$ ,  $B$  and  $E$  conserves probability.
- ▶ Show that  $E$  is exponentially suppressed if  $E < V_2$ . Find the exponential factor.

## E5.3 Bound states

Consider bound states in a square potential well.

- ▶ Count number of free parameters and number of constraint conditions, to show that energy needs to be quantized for bound states.
- ▶ When measuring the energy of a superposition of bound states with different energies, must the outcome of the measured energy be quantized?
- ▶ Keep the depth of the potential well fixed and increase the width. Shall the number of bound states increase or decrease? Why?

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