California Institute of Technology
Physics 2a Recitation
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Daunting Uncertainty
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"Not only does God play dice but... he sometimes throws them where they cannot be seen." — Stephen Hawking

Contents

1 Introduction to quantum mechanics

These Notes provide a short introduction to quantum mechanics, first examining the two-state system (through light polarization) and then calculating the energies of a quantum particle in an infinite well.

1.1 The puzzle of polarizations

In an electromagnetic wave traveling in the $\vec{k} \parallel \hat{z}$ direction, the electric field may point in any direction perpendicular to $\hat{z}$, i.e.,

$$\vec{E} \propto \hat{s} = \cos\phi\,\hat{x} + \sin\phi\,\hat{y} = \begin{pmatrix}\cos\phi \\ \sin\phi\end{pmatrix} \tag{1}$$

where the angle ϕ defines the **polarization**. We see that all polarizations (for the given propagation direction) can be written as a combination of the $\hat{x}$ and $\hat{y}$ polarizations:

$$\hat{x} = \begin{pmatrix}1 \\ 0\end{pmatrix} \tag{2a}$$

$$\hat{y} = \begin{pmatrix}0 \\ 1\end{pmatrix} \tag{2b}$$

These polarization states are shown in Figure 1.

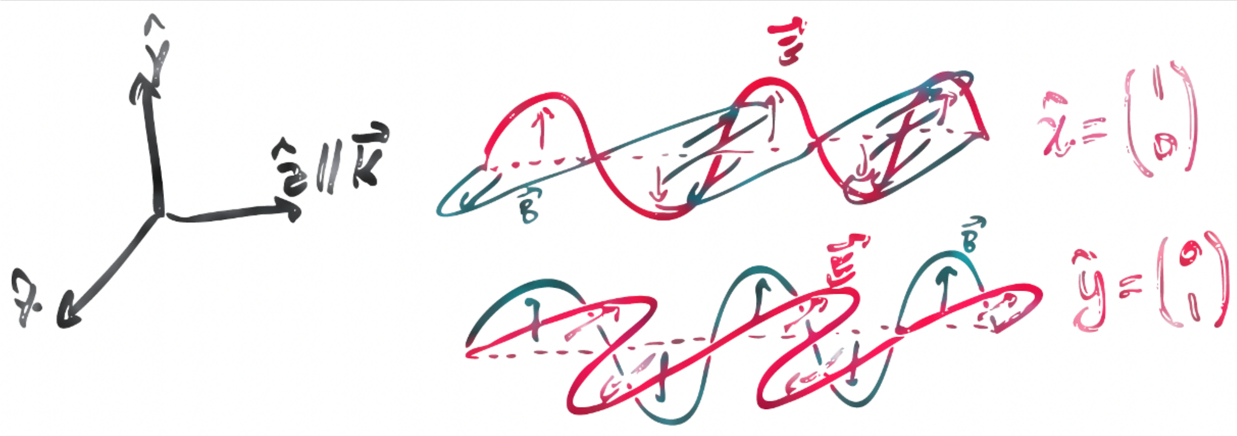

Figure 1: Polarization states of light.

A **polarizer** is a kind of filter which picks out a given kind of polarization. For example, an $\hat{x}$ polarizer will "filter out" the component of incoming light which is polarized in the $\hat{y}$ direction. To see how a polarizer works, we first consider a field which is polarized in the $(\hat{x} + \hat{y})/\sqrt{2}$ (a polarization 45° between $\hat{x}$ and $\hat{y}$):

$$\vec{E} = E_0 \frac{\hat{x} + \hat{y}}{\sqrt{2}} \tag{3}$$

where we are not writing the time dependence.

1.1.1 Passing through $\hat{x}$ and $\hat{y}$ polarizers

When this electromagnetic wave passes through an $\hat{x}$ polarizer, the electric field $\vec{E}'$ of the wave that comes out is simply the $\hat{x}$ component of $\vec{E}$:

$$\vec{E}' = (\hat{x} \cdot \vec{E})\hat{x} = \frac{E_0}{\sqrt{2}}\hat{x} \tag{4}$$

Note that the **intensity** of light is proportional to the square of the amplitude of the field,

$$I \propto |\vec{E}|^2 \tag{5}$$

Therefore, we see that the initial intensity $I \propto E_0^2$ and the final intensity $I' \propto E_0^2/2$, i.e., the polarizer drops the intensity of the light by half. However, now let us consider passing $\vec{E}'$ (the output of the $\hat{x}$ polarizer) through *another* polarizer, this time in the $\hat{y}$ direction.

Since $\vec{E}'$ is only in the $\hat{x}$ direction, that means that the $\hat{y}$ polarizer completely blocks the incoming wave, so that the output field and intensity are

$$\vec{E}'' = 0 \tag{6a}$$

$$I'' \propto 0 \tag{6b}$$

This makes sense—one polarizer blocks the $\hat{x}$ component of the light, and the other blocks the $\hat{y}$ component of the light. There is nothing left (Figure 2).

Figure 2: Light which first passes through an $\hat{x}$ polarizer and then a $\hat{y}$ polarizer.

1.1.2 Passing through $\hat{x}$, $(\hat{x} + \hat{y})/\sqrt{2}$, and $\hat{y}$ polarizers

Now, instead of considering a series of just a $\hat{x}$ polarizer and a $\hat{y}$ polarizer (which we know should block all of the light), we now consider sticking a $(\hat{x} + \hat{y})/\sqrt{2}$ polarizer in between.

Since the $\hat{x}$ polarizer is the first polarizer just like in the previous case, the electric field that comes out of it is the same, i.e.,

$$\vec{E}' = \frac{E_0}{\sqrt{2}}\hat{x} \tag{7}$$

We now consider the second polarizer, which is oriented in $\hat{n} = (\hat{x} + \hat{y})/\sqrt{2}$. Then the output field $\hat{E}''$ of the second polarizer is

$$\vec{E}'' = (\hat{n} \cdot \vec{E}')\hat{n} = \frac{1}{2} E_0 \frac{\hat{x} + \hat{y}}{\sqrt{2}} \tag{8}$$

The final $\hat{y}$ polarizer then grabs out the $\hat{y}$ component of $\vec{E}''$:

$$\vec{E}''' = \frac{1}{2\sqrt{2}} E_0 \tag{9a}$$

$$I''' \propto \frac{1}{8} E_0 \tag{9b}$$

This is very peculiar: the final field (and thus intensity) is *not* zero! Adding a polarizer in between a series of $\hat{x}$ and $\hat{y}$ polarizers (which we know should by themselves filter out all light) somehow allows *more* light through. In other words, sticking a "polarization filter" between two filters which can filter out everything can somehow allow *more* stuff through (Figure 3)!

Figure 3: The same situation as in Figure 2, but with a $\hat{n} = (\hat{x} + \hat{y})/\sqrt{2}$ polarizer inserted in between.

In the case of electromagnetic waves, this may not be an issue. There is no inherent reason why waves should behave like particles, with "polarization" being a property that can just be filtered out.

1.1.3 Photons are particles

However, we know that light is actually made of particles, called **photons**, whose individual properties can be measured. In this case, the probability of a photon with a polarization passing through a polarizer is proportional to the intensity of light.

However, if an individual photon can have a polarization, it seems very bizarre that adding an additional filter can actually increase the amount of probability of a photon passing through.

There are a few interesting observations here:

- It is already strange that, to match classical electromagnetic waves, the question of whether or not a photon passes through a filter is probabilistic.

- It is very strange that adding a filter which selects based on polarization could ever *increase* the probability that a photon can pass through. It rather suggests that the polarizer's act of measuring the photon's polarization *itself* modifies the polarization.

A very similar experiment can be done with electrons, and is called the **Stern–Gerlach experiment**. Roughly the same experimental results can be achieved with them. However, unlike light polarization, the spin of an electron can point in all three directions of space, x, y, and z. Electron spins are an example of a **two-state system**.

1.2 Postulates of quantum mechanics in the two-state system

In this Section, we describe the **postulates** (i.e., fundamental *rules*) of quantum mechanics, and give examples in the context of the two-state system.

1.2.1 Quantum states

The state of a particle is described by a **vector** (an object following certain rules regarding addition, scalar multiplication, etc.), with complex numbers allowed. It should be **normalized**, i.e., its length should be 1.

In the two-state system, an example of a state is:

$$\vec{\psi} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{10}$$

We note that its length is, indeed, 1:

$$\vec{\psi} \cdot \vec{\psi} = 1 \tag{11}$$

1.2.2 Observables

Anything which can be observed is a **Hermitian** operator, called an **observable**.

In the case of the two-state system, Hermitian operators can be represented as matrices. Hermiticity in this case means that transposing a matrix and complex conjugating all of its entries leads to the same original matrix.

In the two-state system, one example of a Hermitian matrix is the $\hat{S}_x$ operator, which measures the spin of the particle in the $\hat{x}$ direction (we have ignored some unimportant prefactors):

$$\hat{S}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{12}$$

We see that the matrix is Hermitian. Note that a "hat" is often placed on an operator to notate that it is an operator (instead of, e.g., a regular number). This does not indicate that it is a unit vector.

1.2.3 Possible measurements

For a given observable (represented by an operator $\hat{A}$), the only possible measurement outcomes are its **eigenvalues**, i.e., if a is a possible outcome of a measurement of $\hat{A}$, that means that

$$\hat{A}\vec{\phi} = a\vec{\phi} \tag{13}$$

for some state $\vec{\phi}$—this is just the usual eigenvalue equation. Moreover, measurement of $\hat{A}$ on the state $\vec{\phi}$ (which is its eigenvector) will *only* return its corresponding eigenvalue, in this case a.

For example, for the $\hat{S}_x$ operator, we can calculate the characteristic equation:

$$\det\left(\hat{S}_x - \lambda\hat{I}\right) = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1 = (\lambda+1)(\lambda-1) = 1 \tag{14}$$

We see that the only possible measurement outcomes of $\hat{S}_x$ are $\lambda = +1$ and $\lambda = -1$. Note that zero is *not* an option in the two-state system.

We can then calculate the eigenstates of $\hat{S}_x$. For $\lambda = +1$, this is

$$\vec{\psi}_{x+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{15}$$

For $\lambda = -1$, this is

$$\vec{\psi}_{x-} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{16}$$

1.2.4 Measurement probabilities

For a general state, the probability of measuring each outcome of $\hat{A}$ is given by the square of the coefficient in front of its decomposition in terms of the eigenvectors of $\hat{A}$.

This sounds a little abstract, but an example should help. The state in Equation 10 can be rewritten as

$$\vec{\psi} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\vec{\psi}_{x+} + \frac{1}{\sqrt{2}}\vec{\psi}_{x-} \tag{17}$$

We see that $\vec{\psi}$ (which should be *normalized*) can be written as a combination of $\vec{\psi}_{x+}$ and $\vec{\psi}_{x-}$. For Hermitian operators, this is *always* possible.

The coefficient in this decomposition in front of $\vec{\psi}_{x+}$ is $1/\sqrt{2}$. Therefore, the probability of measuring the corresponding eigenvalue ($\lambda = +1$) is $(1/\sqrt{2})^2 = 1/2$. The same is true of $\vec{\psi}_{x-}$, so the probability of measuring $\lambda = -1$ is also $1/2$. Reassuringly, these sum to one.

1.2.5 Measurement collapse

Once a measurement is made, the state **collapses** and is **projected** to the eigenspace of states with the measured eigenvalue.

This probably also sounds a little abstract, but what it means is that, if you measured S_x for our state $\vec{\psi}$ (in Equation 10) and measured +1, then the state would *become* $\vec{\psi}_+$.

In other words, measuring will actually *change* the state by removing all of the components of the state which are incompatible with the measured value.

1.2.6 Time evolution of a state

A state $\vec{\psi}$ will follow the **time-dependent Schrödinger equation**, which gives how the state evolves with time. This is

$$i\hbar \frac{\partial \vec{\psi}}{\partial t} = \hat{H}\vec{\psi} \tag{18}$$

where $\hat{H}$ is an operator (or observable) called the **Hamiltonian**, which is basically the energy. Here, i is the imaginary unit and $\hbar$ is a constant called **Planck's constant**.

Let us consider a Hamiltonian of the following form:

$$\hat{H} = E_0 \hat{S}_x = \begin{pmatrix} 0 & E_0 \\ E_0 & 0 \end{pmatrix} \tag{19}$$

We see that $\vec{\psi}_{x+}$ would obey

$$i\hbar \frac{\partial \vec{\psi}_{x+}}{\partial t} = \hat{H}\vec{\psi}_{x+} = E_0 \vec{\psi}_{x+} \tag{20}$$

which is solved by an exponential time dependence:

$$\vec{\psi}_{x+}(t) = \vec{\psi}_{x+} e^{-iE_0 t/\hbar} \tag{21}$$

Similarly, for $\vec{\psi}_{x-}$,

$$i\hbar \frac{\partial \vec{\psi}_{x-}}{\partial t} = \hat{H}\vec{\psi}_{x-} = -E_0 \vec{\psi}_{x-} \tag{22}$$

so that

$$\vec{\psi}_{x-}(t) = \vec{\psi}_{x-} e^{-iE_0 t/\hbar} \tag{23}$$

Therefore, the state in Equation 10 evolves as follows:

$$\vec{\psi}(t) = \frac{1}{\sqrt{2}}\vec{\psi}_{x+}(t) + \frac{1}{\sqrt{2}}\vec{\psi}_{x-}(t) = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-iE_0 t/\hbar} + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{iE_0 t/\hbar} = \begin{pmatrix} \cos(E_0 t/\hbar) \\ -i\sin(E_0 t/\hbar) \end{pmatrix} \tag{24}$$

To see the impact of this, we can consider a separate operator S_z (which measures the $\hat{z}$ component of the spin):

$$S_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{25}$$

We see that S_z has the eigenvectors $\psi_{z+} = (1, 0)$ and $\psi_{z-} = (0, 1)$, with respective eigenvalues +1 and −1.

We can decompose $\psi(t)$ into these eigenvectors:

$$\vec{\psi}(t) = \cos(E_0 t/\hbar)\begin{pmatrix}1\\0\end{pmatrix} - i\sin(E_0 t/\hbar)\begin{pmatrix}0\\1\end{pmatrix} = \cos(E_0 t/\hbar)\psi_{z+} - i\sin(E_0 t/\hbar)\psi_{z-} \tag{26}$$

The measurement probabilities for S_z are given by the squares of the coefficients in the decomposition in Equation 26. The probabilities P_{z+} and P_{z-} actually evolve in time as

$$P_{z+} = |\cos(E_0 t/\hbar)|^2 = \cos^2(E_0 t/\hbar) P_{z-} = |-i\sin(E_0 t/\hbar)|^2 = \sin^2(E_0 t/\hbar) \tag{27a}$$

or

$$P_{z+} = \frac{1+\cos(2E_0 t/\hbar)}{2} \tag{28a}$$

$$P_{z-} = \frac{1-\cos(2E_0 t/\hbar)}{2} \tag{28b}$$

1.3 Postulates of quantum mechanics in the infinite well

We now review the postulates in Section 1.2, but discuss them in terms of a particle in a one-dimensional **infinite well**, i.e., a particle which is forced to lie between $x = 0$ and $x = L$ (Figure 4).

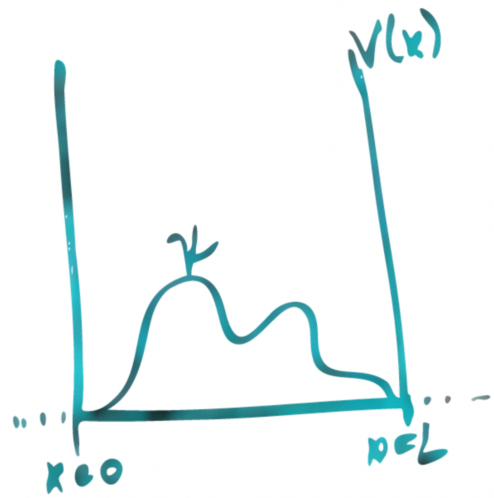

Figure 4: The infinite well quantum system.

There are many similarities (since they are fundamentally the same postulates), but note that a particle in a well is an infinite-state system (and so its behavior can be more complex).

1.3.1 Quantum states

The state of a particle is described by a function (called a **wavefunction**) $\psi(x)$, which should be normalized to 1 in the following sense:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \,\mathrm{d}x = 1 \tag{29}$$

where the integral above is analogous to a "dot product" for functions.

In an infinite well, $\psi(x)$ can only be nonzero within the well, and must vanish at its boundaries.

1.3.2 Observables

Anything which can be observed is a Hermitian operator (also called an observable).

This time, Hermitian operators take the form of linear operators on functions, possibly including derivatives. Some examples include

$$\hat{x}\psi(x) = x\psi(x) \quad \text{(position)} \tag{30a}$$

$$\hat{p}\psi(x) = -i\hbar\frac{\partial\psi(x)}{\partial x} \quad \text{(momentum)} \tag{30b}$$

$$\tag{30c}$$

1.3.3 Possible measurements

For a given observable, the only possible measurement outcomes are its eigenvalues. Eigenfunctions of a given observable will *only* return their eigenvalues upon measurement.

For example, we can consider the energy operator:

$$\hat{H}\psi(x) = \frac{\hat{p}^2}{2m}\psi(x) + V(\hat{x})\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) \tag{31}$$

where $V(x)$ is the potential, which vanishes within the well but is infinity outside of the well (i.e., a particle is confined to be within the well):

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x < 0 \text{ or } x > L \end{cases} \tag{32}$$

For example, in the case of the energy operator $\hat{H}$, we can find the eigenvalues and eigenfunctions:

$$\hat{H}\psi(x) = E\psi(x) \tag{33}$$

where E is the eigenvalue, which we call E to remind ourselves that it is supposed to be an energy.

Within the well, this is the same as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x) \tag{34}$$

We can rewrite this as

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \tag{35}$$

which we recognize to be a harmonic oscillator, which is solved by

$$\psi(x) = A\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) + B\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right) \tag{36}$$

However, we must impose the boundary conditions $\psi(0) = \psi(L) = 0$. The first condition becomes

$$\psi(0) = A = 0 \tag{37}$$

so that

$$\psi(L) = B \sin\left(\sqrt{\frac{2mE}{\hbar^2}} L\right) = 0 \tag{38}$$

If $B \neq 0$, that means that

$$\sqrt{\frac{2mE}{\hbar^2}} L = n\pi \tag{39}$$

where n can be taken to be a positive integer, $n = 1, 2, 3, \ldots$, so that the only allowed energies are

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \tag{40}$$

with normalized eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \tag{41}$$

Note that the spectrum of allowed possible energies is *discrete*, unlike in classical mechanics where it would be able to take any non-negative value.

1.3.4 Measurement probabilities

For a general state, the probability of measuring each outcome of an observable is given by the square of the coefficient in front of it[1].

To make this more concrete, we can consider a (normalized) wavefunction which is a triangle wave (Figure 5):

$$\psi(x) = \begin{cases} \sqrt{12/L}\,(x/L) & 0 < x < L/2 \\ \sqrt{12/L}\,(1 - x/L) & L/2 < x < L \\ 0 & \text{otherwise} \end{cases} \tag{42}$$

[1]If the spectrum of observables is continuous (as in $\hat{x}$ or $\hat{p}$), this is a bit messier and involves integrals. However, we will ignore such (common) cases in these Notes.

Figure 5: The triangle wave state (Equation 42).

The function $\psi(x)$ can be decomposed into $\psi_n(x)$ (the eigenbasis of $\hat{H}$) via Fourier sine series:

$$\psi(x) = \sum_{n=1}^{\infty} A_n \psi_n(x) \tag{43}$$

where

$$A_n = \begin{cases} 0 & n \,\text{even} \\ \frac{4\sqrt{6}}{n^2\pi^2}(-1)^{(n-1)/2} & n \,\text{odd} \end{cases} \tag{44}$$

Therefore, the probability P_n of measuring an energy E_n is given by $|A_n|^2$:

$$P_n = \begin{cases} 0 & n \,\text{even} \\ \frac{96}{n^4\pi^4} & n \,\text{odd} \end{cases} \tag{45}$$

1.3.5 Measurement collapse

Once a measurement is made, a state collapses and is projected to the eigenspace of states with the measured eigenvalue.

For example, if we measured the energy of our triangle wave state in Equation 42 and measured $E_n = 9\pi^2\hbar^2/2mL^2$ $(n = 3)$, then our state would instantly collapse to

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right) \tag{46}$$

1.3.6 Time evolution of a state

A state $\Psi(x,t)$ (now with the time dependence included) will follow the **time-dependent Schrödinger equation**:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \tag{47}$$

We first note that the eigenstates $\Psi_n(x,t)$ will follow

$$i\hbar \frac{\partial \Psi_n(x,t)}{\partial t} = E_n \Psi_n(x,t) \tag{48}$$

so that

$$\Psi_n(x,t) = \psi_n(x) e^{-iE_n t/\hbar} \tag{49}$$

Then we can use the decomposition in Equation 43 for the triangle-wave state $\psi(x)$ in Equation 42 to write the time-dependent wavefunction:

$$\Psi(x,t) = \sum_{n=1}^{\infty} A_n \Psi_n(x,t) = \sum_{n=1}^{\infty} A_n \psi_n(x) e^{-iE_n t/\hbar} \tag{50}$$

Note that, even though the squared coefficients $|A_n e^{-iE_n t/\hbar}|^2 = |A_n|^2$ will not change over time (i.e., the measurement probabilities for energy might change over time), the different components of the wavefunction will oscillate at different rates and its shape will change (as will the measurement probabilities of other, non-energy operators), see Figure 6.

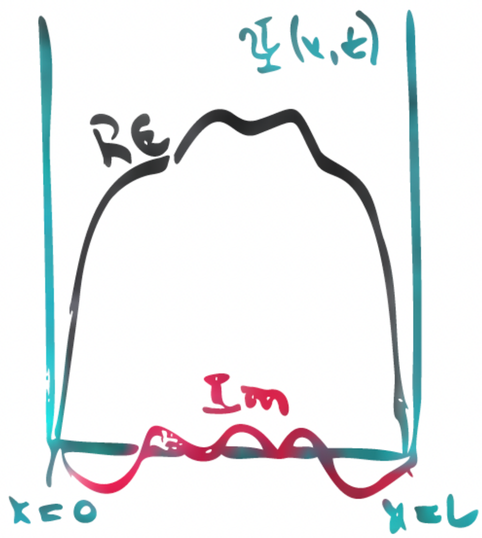

Figure 6: The real and imaginary parts of the triangle wavefunction after some time evolution.