Intermat: Complex Numbers In Quantum Mechanics

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1 Introduction

"*If you think you understand quantum mechanics, you don't understand quantum mechanics.*" - Richard Feynman

Over the past approximately 100 years, physics has undergone something of a revolution. Our own Niels Bohr was one of the first to propose revolutionary and controversial theories, including the quantization of energy on an atomic scale. This (broadly speaking) contradicted classical physics, and many were highly skeptical of the new ideas put forward by Niels Bohr, Max Planck, Albert Einstein, Arthur Compton, and others. However, it would turn out that an entirely new world and a completely new field of research emerged: quantum mechanics.

Quantum mechanics is (very briefly explained) the study of physical phenomena at the atomic scale of size and energy. It is at once incredibly fascinating, incredibly difficult, and incredibly strange, as the quote above also suggests. One of the most fundamental (and strangest) aspects is that nothing can be calculated with absolute precision. Probabilities can be calculated for a particle's location, but one can never be certain. Nor can one simultaneously determine both a particle's speed and position—this is Heisenberg's uncertainty principle. Well, the goal of this section is not to explain quantum physics either. That would be doomed to fail from the start (and, of course, the blame lies entirely with the author). The goal is to show that complex numbers naturally also play a role in this complex (!) world.

A classic example from quantum physics is the case of a particle in an infinite potential well. Here, one must imagine a particle essentially confined to a region on the x-axis between the lines $x=0$ and $x=a$, as illustrated to the right. Note that we haven't drawn the particle itself, since we cannot precisely determine its position anyway. The idea, however, is that the particle can move in one dimension along the x-axis between 0 and a, with the lines representing infinitely high barriers. For a (quantum) physicist, it is immensely interesting to determine such a particle's possible energies, the probability of various positions, and so on. The approach to tackling this is by solving the following (rather formidable) differential equation, known as the (time-dependent) Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi \tag{1}$$

There are many new symbols and letters in this equation, but we won't expend energy on understanding everything. The key point to note is that the imaginary unit appears in the differential equation!

Solving this equation is certainly no easy task, so we won't attempt it here. However, it's essential to mention that a solution to the equation is a function $\Psi(x, t)$ of two variables: position x and time t. This solution is called the particle's wavefunction. The wavefunction contains information about the particle, which can be utilized with the appropriate mathematics.

Surprisingly (or perhaps not), it turns out that the particle can only have certain discrete energies (a conclusion derived from the differential equation). This phenomenon is called energy quantization. In this case, the energy levels are given by:

$$E_n = \frac{\hbar^2 \cdot n^2 \cdot \pi^2}{2 \cdot m \cdot a^2} \tag{2}$$

With some advanced mathematical gymnastics, it can be shown that for the n'th energy level, Ψ takes the form:

$$\Psi_n(x, t) = A \cdot e^{-\frac{i\cdot\hbar\cdot n^2\cdot\pi^2\cdot t}{2\cdot m\cdot a^2}} \cdot \sin\left(\frac{\pi \cdot n \cdot x}{a}\right) \quad \text{for } x \in [0, a] \tag{3}$$

Here, it is implied that: $\Psi_n(x, t) = 0$ when $x \notin [0, a]$ This function, which includes the complex exponential function as a factor (as is the case for many wavefunctions), will now be used to predict where on the x-axis we can expect to find the particle.

At first glance, it might seem that the particle is just as likely to be located near *0* as near a, or even in the middle for that matter. So, if we imagine many identical systems set up like this, the symmetry suggests it would be reasonable to expect the average position of the particle to be $\frac{a}{2}$. In other words, the particle is, on average, located in the middle.

Let's attempt to calculate this and see if our assumption holds true. It is indeed fundamental that $|\psi(x, t)|^2$ is a probability density function that describes the particle's position in the n'th energy state. In other words, we have the condition that:

$$\int_{-\infty}^{\infty} |\psi_n(x, t)|^2 \, dx = 1 \tag{4}$$

This means that the factor A must be chosen such that the above integral equals 1. The constant A is referred to as the normalization constant. Since $|\psi(x, t)|^2$ is a probability density function, it follows that the integral:

$$\int_{x_1}^{x_2} |\psi_n(x, t)|^2 \, dx \tag{5}$$

This expression gives the probability of finding the particle within the interval $[x_1, x_2]$. From this, it also follows that the probability of finding the particle at a specific position x_0 is zero. This is one of the fundamental differences between classical mechanics and quantum mechanics. In classical mechanics, the position of a particle can be pinpointed exactly, but in quantum mechanics, the position is described by a probability distribution, and the probability of finding the particle at any exact point is zero.

2 Tasks

2.1 Task 1: Show that $A = \sqrt{\frac{2}{a}}$for the first energy state thus, for $n = 1$

First, let's define the integral:

$$\int_0^a |\psi_1(x,t)|^2 \, dx = 1 \tag{6}$$

let's expand the squared absolute value. We know that $e^{-\frac{i \cdot \hbar \cdot n^2 \cdot \pi^2 \cdot t}{2 \cdot m \cdot a^2}}$ got a complex number, thus we can expand the squared part the the conjugate of $e^{-\frac{i \cdot \hbar \cdot n^2 \cdot \pi^2 \cdot t}{2 \cdot m \cdot a^2}}$

$$\int_0^a A \cdot e^{-\frac{i \cdot \hbar \cdot 1^2 \cdot \pi^2 \cdot t}{2 \cdot m \cdot a^2}} \cdot \sin\left(\frac{\pi \cdot 1 \cdot x}{a}\right) \cdot A \cdot e^{\frac{i \cdot \hbar \cdot 1^2 \cdot \pi^2 \cdot t}{2 \cdot m \cdot a^2}} \cdot \sin\left(\frac{\pi \cdot 1 \cdot x}{a}\right) \, dx = 1 \tag{7}$$

Now let's reduce and combine the values. As we know $e^{-\frac{i \cdot \hbar \cdot n^2 \cdot \pi^2 \cdot t}{2 \cdot m \cdot a^2}}$ and the conjugate of it cancels eachother out.

$$\int_0^a A^2 \cdot \sin^2\left(\frac{\pi \cdot x}{a}\right) \, dx = 1 \tag{8}$$

In this integral A^2 is a constant, so let's bring it out of the integral.

$$A^2 \cdot \int_0^a \sin^2\left(\frac{\pi \cdot x}{a}\right) \, dx = 1 \tag{9}$$

We have now isolated the squared sine, so now we can use u-sub to make it easier to calculate.

$$u = \frac{\pi \cdot x}{a} \to \frac{du}{dx} = \frac{\pi}{a} \to \frac{a}{\pi} \cdot du = dx \tag{10}$$

And let's calculate the new intervals by putting a in x's place. We dont need to put 0 in as we now it just equals 0.

$$u = \frac{\pi \cdot a}{a} = \pi \tag{11}$$

$$A^2 \cdot \int_0^\pi \sin^2(u)\ \frac{a}{\pi} du = 1 \tag{12}$$

let's take the other constant out of the integral.

$$A^2 \cdot \frac{a}{\pi} \int_0^\pi \sin^2(u)\ du = 1 \tag{13}$$

Now that we have isolated sine we can use a trick to rewrite it.

$$\sin^2(x) = \frac{1 - \cos(2x)}{2} \tag{14}$$

$$A^2 \cdot \frac{a}{\pi} \int_0^\pi \frac{1 - \cos(2u)}{2}\ du = 1 \tag{15}$$

Now we can split up the fraction in two and split up the integral in two.

$$A^2 \cdot \frac{a}{\pi} \int_0^\pi \frac{1}{2} - \frac{\cos(2u)}{2}\ du = 1 \tag{16}$$

$$A^2 \cdot \frac{a}{\pi} \int_0^\pi \frac{1}{2}\, du - \int_0^\pi \frac{\cos(2u)}{2}\ du = 1 \tag{17}$$

now we can evaluate the integrals.

$$\int_0^\pi \frac{1}{2}\, du = [\frac{u}{2}]_0^{pi} = \frac{\pi}{2} - (\frac{0}{2}) = \frac{\pi}{2} \tag{18}$$

$$\int_0^\pi \frac{\cos(2u)}{2} = [\frac{-\sin(2u)}{4}]_0^\pi = \frac{-\sin(2 \cdot \pi)}{4} - (\frac{-\sin(2 \cdot 0)}{4}) = 0 \tag{19}$$

Now we are left with the first integral and the constants.

$$A^2 \cdot \frac{a}{\pi} \cdot \frac{\pi}{2} = 1 \tag{20}$$

Let's combine the fractions and reduce.

$$A^2 \cdot \frac{a \cdot \pi}{2 \cdot \pi} = 1 \tag{21}$$

π cancels eachother out.

$$A^2 \cdot \frac{a}{2} = 1 \tag{22}$$

now let's divede a over 2 on both side of the equation.

$$A^2 = \frac{1}{\frac{a}{2}} = \frac{2}{a} \tag{23}$$

now we can take the square root of both sides

$$\sqrt{A^2} = \sqrt{\frac{2}{a}} \tag{24}$$

$$\boxed{A = \sqrt{\frac{2}{a}}} \tag{25}$$

We have now solved the first task.

From probability theory, we know that the expected value for the position is found by the integral:

$$\langle x \rangle = \int_{-\infty}^{\infty} x \cdot |\psi_n(x,t)|^2 \, dx \tag{26}$$

2.2 Task 2: We show that for n = 1, the expected value of x is equal to $\frac{a}{2}$

. first show that:

$$\langle x \rangle = \int_0^a x \cdot \frac{2}{a} \cdot \sin\left(\frac{\pi \cdot x}{a}\right)^2 \, dx \tag{27}$$

Given the integral of the expected value for the position, we change the interval to 0 to a.

$$\langle x \rangle = \int_0^a x \cdot |\psi_1(x,t)|^2 \, dx \tag{28}$$

As we know from before $|\psi_n(x,t)|^2$ can be reduced to $A^2 \cdot \sin^2\left(\frac{\pi \cdot x}{a}\right)$, so lets replace it in the integral.

$$\langle x \rangle = \int_0^a x \cdot A^2 \cdot \sin^2\left(\frac{\pi \cdot x}{a}\right) dx \tag{29}$$

We also know the value of A so we can also replace that.

$$\langle x \rangle = \int_0^a x \cdot \sqrt{\frac{2}{a}}^2 \cdot \sin^2\left(\frac{\pi \cdot x}{a}\right) dx = \int_0^a x \cdot \frac{2}{a} \cdot \sin^2\left(\frac{\pi \cdot x}{a}\right) dx \tag{30}$$

We also know from before a way to rewrite $\sin^2(x)$.

$$\langle x \rangle = \int_0^a x \cdot \frac{2}{a} \cdot \sin^2\left(\frac{\pi \cdot x}{a}\right) dx = \int_0^a x \cdot \frac{2}{a} \cdot \frac{1 - \cos(\frac{\pi x}{a} \cdot 2)}{2} \, dx \tag{31}$$

Now lets reduce since the two 2 cancels eachother out.

$$\langle x \rangle = \int_0^a \frac{x}{a} \cdot 1 - \cos(\frac{\pi x}{a} \cdot 2) \; dx \tag{32}$$

now we can split the integral up in two.

$$\langle x \rangle = \int_0^a \frac{x}{a} \; dx - \int_0^a \cos(\frac{\pi x}{a} \cdot 2) \; dx \tag{33}$$

let's solve the first integral.

$$\int_0^a \frac{x}{a}\ dx = \frac{1}{a}\int_0^a x\ dx = \frac{1}{a}\cdot\frac{x^2}{2}|_0^a = \frac{1}{a}\cdot\frac{a^2}{2} - (\frac{1}{a}\cdot\frac{0^2}{2}) = \frac{a^2}{2a} - (0) = \frac{a}{2} \tag{34}$$

now that the first integral is solved let's move on to the second one

$$\int_0^a \cos(\frac{\pi x}{a}\cdot 2)\ dx \tag{35}$$

first we can use u-sub the make it easier.

$$u = \frac{\pi x}{a}\cdot 2 \rightarrow \frac{du}{dx} = \frac{2\pi}{a} \rightarrow \frac{a}{2\pi}du = dx \tag{36}$$

we can also calculate the new interval, and we dont need to calculate the 0 since we know it stays 0.

$$u = \frac{\pi x}{a}\cdot 2 \rightarrow \frac{\pi\cdot a}{a}\cdot 2 = 2\pi \tag{37}$$

$$\int_0^{2\pi} \cos(u)\frac{a}{2\pi}\ du = \sin(u)\cdot\frac{a}{2\pi}|_0^{2\pi} = \sin(2\pi)\cdot\frac{a}{2\pi} - (\sin(0)\cdot\frac{a}{2\pi}) = 0 \tag{38}$$

now we can combine the calculated values.

$$\langle x\rangle = \frac{a}{2} - 0 = \frac{a}{2} \tag{39}$$

now we have calculated what the expected value of x would be when $n = 1$

$$\boxed{\langle x\rangle = \frac{a}{2}} \tag{40}$$