The Mathematics of Quantum Mechanics: An Introduction

A wave function:

\[
\text{f}(x) \ := \ \frac{x}{\left(1 + x^4\right)} \quad \text{i} := 0 \ldots 100 \quad z_i := -5 + \frac{i}{10}
\]

The basis of modern Quantum Mechanics (QM) is that particles exhibit wave properties. So, let us define a simple function \( f(x) \) that looks like a wave in a finite region of space. Our "particle" is confined to this region (-5,5) by some means.

Probability density and normalization:

\[ N := \int_{-5}^{5} f(x) \cdot \overline{f}(x) \, dx \quad N = 0.555 \]

\[ g(x) := \frac{1}{\sqrt{N}} \cdot \overline{f}(x) \]

\[ I := \int_{-5}^{5} g(x) \cdot g(x) \, dx \quad I = 1 \]

The function \( f(x) \) when squared and integrated between the two limits gives us 0.555. For certain reasons, we want to work with functions that give 1 when squared and integrated between limits. So, we multiply it by an appropriate constant, as you can see. This process of finding a constant \( N \) that can be used to make the square-integral equal to 1 is called "normalization." We say that we have normalized \( f(x) \). From now on, we will work with the normalized \( f(x) \), which we designate as \( g(x) \).

Plot and see what the square of the normalized function looks like:

The square of the normalized wave in QM is related to the probability distribution of the "particle" we are interested in. The dashed line shows that the "particle" has almost no probability of being found near the ends or at the center of the interval, but has two spots on either side of the center where its probability density is a maximum.

Normalizing the wave ensures that the total probability of the wave in the interval (-5,5) is 1, i.e., we are 100% certain of finding the particle somewhere in this space.

Average value of \( x \) for the wave:

\[ x_{av} := \int_{-5}^{5} x \cdot g(x) \, dx \quad x_{av} = 0 \]

The average of a property of a distribution is obtained by multiplying the property with the distribution and integrating over the limit. Let us look at average position. It is reasonable that the average "position" of the wave is the middle of the interval.
In QM, we say that the position "operator" and the momentum "operator" are complementary variables. We are limited by the standard deviations or uncertainties from knowing the value of both these variables for a particle simultaneously and exactly. The entire foundation of classical mechanics is in specifying all dynamical variables exactly and simultaneously. This is the fundamental difference between QM and classical mechanics.

Operators:

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Operators act on the wave, not its square:

Note that \( \frac{d^2}{dx^2}g(x)^2 \) both acted on \( g(x) \), not \( g(x)^2 \). Changing the order of where we place the differential operator drastically changes the result almost all the time:

\[
-\int_{-5}^{5} \frac{d^2}{dx^2}g(x)^2 \, dx = 2.753 \cdot 10^{-4}
\]

The "operator" \( x \) is simply a multiplication by \( x \). Therefore, its placement in the integral is not critical but we still put it between the two \( g(x) \)'s for consistency.

The mathematics of QM is basically one in which we allow various linear operators (we will define "linear" later) to operate on the wave function (not its square). Each operator corresponds to a physical property or "observable" of the system. In order to get a numerical value for the property corresponding to a particular operator, we will let the operator act on the wave function—actually, its "complex conjugate" (to be defined later)—and integrate over the relevant interval of space. This is what we did to get the average values for \( x, \ x^2, \ D_x, \) and \( D^2x \) above.

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**Exercises:**

1. Let \( f(x) = \sin \left( \frac{n \pi}{a} x \right) \) where \( n \) is an integer = 1,2,3, ... Find the normalization constant \( N \) in the interval \((0,a)\), given that

\[
\int_{0}^{a} \sin \left( \frac{n \pi}{a} x \right) \sin \left( \frac{n \pi}{a} x \right) \, dx = \frac{1}{2} \left( -\cos(n \pi) + n \pi \right)
\]

Remember that \( \sin(n \pi) = 0 \) for all integers \( n \), and \( \cos(n \pi) = 1 \) if \( n \) is even, \( -1 \) if \( n \) is odd.

2. Define the normalized wave function \( g(x) \) in terms of the normalization constant and \( f(x) \).

3. What is the average value of \( x \) for this system? The integral you need is:

\[
\int_{0}^{a} \sin \left( \frac{n \pi}{a} x \right) \cos \left( \frac{n \pi}{a} x \right) \, dx = \frac{1}{4a} \left( -2 \sin(n \pi) \cos(n \pi) + n^2 \pi^2 - \cos(n \pi)^2 \right) + \frac{1}{4 \pi^2} \left( n \pi \right)^2
\]

4. What is the average value of \( x^2 \)? The integral you need is:

\[
\int_{0}^{a} \sin \left( \frac{n \pi}{a} x \right) \cos \left( \frac{n \pi}{a} x \right) \, dx = \frac{1}{12} \left( -6 \pi^2 \sin(n \pi) \cos(n \pi) + 2 \pi^3 \pi - 6 \pi^2 \cos(n \pi) + 3 \cos(n \pi) \sin(n \pi) + 3 \pi \right) \]
5. What is the average value of $D_x$? This one is easy and you should know how to do it. (Hint: what is $d(\sin kx)$?)

6. What is the average value of $D^2x$? Don't forget the negative sign in the definition of $D^2x$. You should be able to use the integral in Exercise 1 to do this. (Why?)

7. What is the uncertainty in $x$?

8. What is the uncertainty in $D_x$?

9. What is the product of $\sigma_x$ and $\sigma_{Dx}$?

10. Consider the function $f(x) = e^{-ax^2}$ or $\exp(-ax^2)$. What is the result of the operator $D^2x$ acting on this function? i.e., what is $\frac{d^2}{dx^2}f(x)$?

11. If some function $h(x)f(x)$ is added to $-\frac{d^2}{dx^2}f(x)$, we may be able to define a differential equation of the form:

$$-\frac{d^2}{dx^2}f(x) + h(x)\Phi(x) = k\Phi(x)$$

where $k$ is a constant. What is $h(x)$? The result of Ex. 10 should tell you what it needs to be. The equation you get is very closely related to the Schrödinger equation, which is the basis of QM. [If you get this far and get confused, please e-mail me and I will send you an example that might make matters clearer.]

Operators and their "eigen"functions:

Let us define an operator as $H = \left( \frac{d^2}{dx^2} + h(x) \right)$. Then, Ex. 11 is to show that, for the $f(x)$ we have selected in Ex. 10, the following relationship is satisfied: $Hf(x) = k\cdot f(x)$. Such pairings of operators and functions have a special significance in QM. In this case, we will say that the $f(x)$ we used in Ex. 10 and 11 is an eigenfunction of operator $H$. The constant $k$ is called the eigenvalue.

Note that only certain pairs of operators and functions satisfy this relationship. For example, the operator $D_x$ acting on the $f(x)$ above will not give you a constant × the same function. However, $D_x$ acting on a different function, say $\exp(-ax)$, will give us the type of relationship we are looking for.

$$\frac{d}{dx}e^{-ax} = -ae^{-ax}$$

So, here $-a$ is the eigenvalue, and we have showed that the function $\exp(-ax)$ is an eigenfunction of the operator $D_x$.

I agree that this is all rather mysterious at this point. Hopefully we will make sense of it all soon. The good news is that you have just completed the most complicated mathematics you will need for this course!