8. Waves and Particles

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1 Continuous Function

1.1 Wave Function Review

From now on, we will be using wavefunctions a lot more and we will see why they are called wavefunctions, and also see about their physical meaning.
We have already used wavefunctions and their notation, namely $\psi(\lambda)$.
I wrote it as a function of λ, because the wavefunction depends on the observable we initially choose to work with, and up until now we have denoted almost all observable with L.
Now what is really important, is that in the same state, a different observable produces a different wave function. That is another key difference between state-vector and wavefunction.
Generally, if we indeed work with an observable L, we say that $\psi(\lambda)$ is the wave function in the L-basis, or mathematically:
$\psi(\lambda) = \langle\lambda|\Psi\rangle$

There are two main ways of thinking of $\psi(\lambda)$.
First of all, you can simply think of it as the set of components of the state vector in a particular basis. This is what we have thought of the wavefunction for 7 chapters now and it is not wrong, however there is also a different way of seeing the wavefunction: We can also think of it as a complex-valued function of λ, where $P(\lambda) = \psi^*(\lambda)\psi(\lambda)$

1.2 Functions as Vectors

Since the beginning of these chapters, we have only studied systems, that have finite dimensions. We haven't generalized anything to more dimensions than we are given. For example a spin, has finite, and very very limited number of possible state, namely two, +1 and -1.
But Particles can have infinite possible values! Any moving particle, can be found at any real value of the axis it is moving along, for example along the x-axis, it can be found at any x!
x is a continuous infinite variable.
Based on the title of this section I think you already know were we are going!
When we have continuous observables in a system, it follows that the wavefunction must also be continuous!
Now here comes the interesting part! If you think of vectors as a simple arrow pointing in a specific point in the space, then we cannot substitute a vector with a function. However, if we look at vectors from a wider point of view, as mathematical objects satisfying certain axioms, a function can form a vector space. And to be honest we have worked in such vector spaces from the beginning! A Hilbert space is such a vector space!
For example, a set of complex functions $\psi(x)$, of a single real variable x, where $\forall x, \psi(x) \in C$, and $x \in R$ satisfy the mathematical axioms to define a vector space.
More specifically, here are all the axioms:
1) The sum of any two functions is also a function
2) Addition of functions is associative and commutative
3)There exists a zero function, such that when added to any other function, the result is that other function
4) $\forall\psi(x)$**,** $\exists -\psi(x) \ | \ \psi(x) + (-\psi(x)) = 0$ *(The symbol |, means such that)*
5) The product of a function with any complex number gives a function, and the multiplication is linear.
6) The distributive property holds

Since we now continuous, we can't simply sum over them with a classical discrete sum $\sum$

That means that the following changes need to be made:
1) Integrals take the place of sums

2) Probability Densities replace Probabilities

3) The Kronecker delta is replace by the Dirac delta function

1.2.1 Integrals take the place of Sums

We will replace the sum $\sum_i$, with an integral $\int dx$.
We could do a rigorous math proof, but that is not the goal of this subsection, (but you could try it as an exercise!).

This is probably the best time to warn you that from now on, we will get into way more math and use a lot of calculus and multivariate calculus. I would highly suggest you to have a knowledge about these topics before moving on, otherwise you won't gain even half of the knowledge there is to absorb in these last few chapters, which I believe are the most interesting!
Lets now consider a bra $\langle\psi|$ and a ket $|\phi\rangle$, and define their inner product:

$$\langle\Psi|\Phi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\phi(x)dx \tag{1}$$

Which should come to you as no surprise!

1.2.2 Probability Densities Replace

Since x is continuous, the probability it has to be in any exact value is virtually 0.
So instead of asking what is the probability that the particle is at the exact position x, we will ask, **What is the probability that the particle lies between two x values, say between x=a and x=b.**
We now defined the Probability Density as:

$$P(a,b) = \int_a^b P(x)dx = \int_a^b \psi^*(x)\psi(x)dx \tag{2}$$

It is pretty obvious, that total probability must be 1, we should have a normalized vector:

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1 \tag{3}$$

1.2.3 The Kronecker is replaced by the Dirac Delta Function

The delta function, is nothing but a more generalized Kronecker delta.
In an integral, we can't use the Kronecker Delta because it is based on discrete variables. Here comes again the genius of Paul Dirac!
We use the function $\delta(x-x')$ that is defined as:

$$\int_{-\infty}^{\infty} \delta(x-x')F(x')dx' = F(x) \tag{4}$$

The delta function is 0 when $x \neq x'$, and when x=x', it is just ∞ enough so that the area under $\delta(x)$ is 1. Overall, it is a function that is nonzero over an infinitesimal interval ε, but on that interval it has the value $\frac{1}{\varepsilon}$, thus making the area equal to 1.

An approximation of the delta function is: $\frac{n}{\sqrt{\pi}}e^{-(\pi x)^2}$ as a function n.

1.3 Linear Operators

In Quantum Mechanics, we also need Operators.
A linear operator in a space of functions, when acting on the sum of two functions, it returns the sum of the separate results, and when acting on a multiple of a function, it returns the same multiple of the original result.

We will now define two operators that we will use a lot in this and the next chapters.
First of all we will define **X**, as a simple operator, that when acting on a function it returns the x multiple of that function: *(Where x is real)*

$$X\psi(x) = x\psi(x) \tag{5}$$

We also define the Operator ∇, which is defined as the differentiation operator:

$$\nabla\psi(x) = \frac{\partial\psi(x)}{\partial x} \tag{6}$$

Note that the partial derivative notation I used is just be more general, because as we will see, the wavefunction is also a function of time!

Let's now check if these operators are Hermitian, although it is pretty obvious!
Let's start with X!
Since $X\psi(x) = x\psi(x)$, we can write:

$$\langle\Psi|X|\Phi\rangle = \int \psi^*(x)x\phi(x)dx \tag{7}$$

and

$$\langle\Phi|X|\Psi\rangle = \int \phi^*(x)x\psi(x)dx \tag{8}$$

Since x is real, we can clearly see that the two integrals are complex conjugates of each other, hence **X** is Hermitian.

Let's Now do the same for ∇:
The two sandwiches are:

$$\langle\Psi|\nabla|\Phi\rangle = \int \psi^*(x) \;\; \partial_x\phi(x)dx \tag{9}$$

and

$$\langle\Phi|\nabla|\Psi\rangle = \int \phi^*(x) \;\; \partial_x\psi(x)dx \tag{10}$$

Don't confused with notation! the ∇ operator can also be written as D and is called the del operator or nabla, and the ∂_x notation is simply the derivative of the function that follows with respect to x. There a ton of different notations for differentiation, like Euler's, Lagrange's, Leibniz's which we are using. What we are getting with the del operator is actually the gradient of each wavefunction each time. However, since we are in one dimension, namely x, we could instead of using partial notation, simply use $\frac{d}{dx}$. Later we will use x as the generalized coordinates!
That said, we could rewrite the above as :

$$\langle\Psi|\nabla|\Phi\rangle = \int \psi^*(x) \;\; \frac{d\phi(x)}{dx}dx \tag{11}$$

and

$$\langle\Phi|\nabla|\Psi\rangle = \int \phi^*(x) \;\; \frac{d\psi(x)}{dx}dx \tag{12}$$

To determine whether the del operator is Hermitian, all we need to do is compute the integrals and compare the results.
Using Integration by parts, we get that:

$$\langle\Psi|\nabla|\Phi\rangle = \int \psi^*(x) \;\; \frac{d\phi(x)}{dx}dx \tag{13}$$

$$\langle\Phi|\nabla|\Psi\rangle = -\int \psi^(x) \;\; \frac{d\phi^*(x)}{dx}dx \tag{14}$$

We know clearly see that the Del operator is not Hermitian. It is actually **Anti-Hermitian**!
Overall we see that
$X^\dagger = X$
$\nabla^\dagger = -\nabla$
All we need to do in order to turn it into a Hermitian, is to multiply it by -i. (And $\hbar$ for

the balance of units later on)
So now we have a Hermitian Operator, $-i\hbar\nabla$ which when acting on a function $\psi(x)$, is defined as:

$$-i\hbar\nabla\psi(x) = -i\hbar\frac{\partial\psi(x)}{\partial x} \tag{15}$$

2 The State of a Particle

In Quantum Mechanics, as opposed to Classical Mechanics, when we say we know everything about a system, we don't mean that we know the momenta and the positions of all particles!
Actually, that would be impossible! As we will soon see and prove, **you cannot know both momentum and position of a particle simultaneously!** We can know x or p.

2.1 Position and its Eigenstuff

If the position of a particle is an observable, then we set its operator to be **X**. The X we saw previously.
The eigenvalue of X are the possible values of position that can be observed and the eigenvectors represent the states of definite position!
What are the eigenvalues, and in which states, we know the definite position?
We will denote the eigenvalues with x_0, meaning that:
$X|\Psi\rangle = x_{-}|\Psi\rangle$
or
$x\psi(x) = x_0\psi(x)$
We can rewrite this as

$$(x - x_0)\psi(x) = 0 \tag{16}$$

That means that if $x \neq x_0$, then $\psi(0) = 0$, so for any given eigenvalue x_0, the wavefunction **can** be nonzero only at one point! Namely $x = x_0$.
Here comes the delta function to save the day make sense out of the statement above!
$\delta(x - x_0)$
Every real number x_0 is an eigenvalue of X, and the corresponding eigenvectors are function, called eigenfunctions, namely $\delta(x - x_0)$, that are infinitely concentrated at $x = x_0$.
We can translate this mathematically, and write: $\psi(x) = \delta(x - x_0)$, which also makes a lot of sense, sense the wavefunction that represents a particle that is know to be at x_0, is 0 $\forall x$, except x_0, where it obviously is 1.

2.2 Momentum and its eigenstuff

Position was easy to understand because it was very intuitive. Momentum, unfortunately isn't!
For a second forget the classical definition of $p = mv$!
Let's start off with the Abstract Mathematical way of defining it!

The Momentum Operator is denoted as P and is defined, as expected:

$$P = -i\hbar\nabla \tag{17}$$

or, a less fancy notation:

$$P = -i\hbar D \tag{18}$$

(D is the exact same as ∇, but less intimidating!)
We also know from the Linear Operators Section that

$P\psi(x) = -i\hbar\frac{d\psi(x)}{dx}$

In Quantum Mechanics, we often use units, so that $\hbar$ is simplified to 1(magnitude of 1). It is tempting, but we will not do that here!

Now, for the eigenstuff, we have seen the definition many times, so we all know what follows:

$$P\,|\Psi\rangle = p\,|\Psi\rangle \tag{19}$$

or

$$P\psi(x) = p\psi(x) \tag{20}$$

Where p is an eigenvalue of P.
Using that $P\psi(x) = -i\hbar\frac{d\psi(x)}{dx}$
we can rewrite eq. 20 as

$$-i\hbar\frac{d\psi(x)}{dx} = p\psi(x) \tag{21}$$

or, using basic algebra:

$$\frac{d\psi(x)}{dx} = \frac{ip}{\hbar}\psi(x) \tag{22}$$

The solution for such an equation is an exponential, namely:

$$\psi_p(x) = Ae^{\frac{ipx}{\hbar}} \tag{23}$$

I used the subscript p to show that it is an eigenvector of P with the specific eigenvalue p. It is a function x thought!

The term A is a constant that is not determined by the eigenvector equation, but we

require the wavefunction to be normalized to unit probability!
An example is the eigenvector of the x component of the spin, say the state right!

$$|r\rangle = \frac{1}{\sqrt{2}}|u\rangle + \frac{1}{\sqrt{2}}|d\rangle \tag{24}$$

The factor $\frac{1}{\sqrt{2}}$ is there to make sure that the total probability is equal to 1.
To things short, we get that the result is that A = $\frac{1}{\sqrt{2\pi}}$, so that:

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}} \tag{25}$$

We can now take3 the inner products of x and p and see that:

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{ipx}{\hbar}} \tag{26}$$

and

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{-ipx}{\hbar}} \tag{27}$$

The equation 25 is a momentum eigenstate!
So far, we have been using ψ to represent position, but also momentum eigenvectors!
$\psi(x)$ is a generalized symbol for no matter which function we are talking about.

We can now see why these functions are called wavefunctions!
The eigenfunctions of the momentum operator are sine and cosine waves!
The wavelength of $e^{\frac{ipx}{\hbar}}$ is given by $\lambda = \frac{2p\hbar}{p}$, since when we add it to the variable x, nothing changes!
Momentum is related to wavelength!

3 Fourier Transforms

There is no way way to know both momentum and position simultaneously, as we have said 10 times already!
We can though, know each individually!
We now need to define another wavefunction, for the momentum representation, which we will denote by $\tilde{\psi}(p)$, and it is defined as

$$\tilde{\psi}(p) = \langle P|\Psi\rangle \tag{28}$$

So that $P(p) = \tilde{\psi}^*(p)\tilde{\psi}(p)$
Having now two wavefunctions, we can express the state in two different basis.
(But both represent the state-vector!)

We have said in the beginning, that:

$$I = \sum_i |i\rangle \langle i| \tag{29}$$

As expected, because momentum and position are continuous variables, and they define basis, $|x\rangle$ and $|p\rangle$ respectively, we can write;

$$I = \int dx\, |x\rangle \langle x| \tag{30}$$

and

$$I = \int dp\, |p\rangle \langle p| \tag{31}$$

Now lets try to something that is useful and will help us a lot.
Suppose we know the the wavefunction of a state-vector Ψ and we want to find out $\tilde{\psi}(p)$!
We know that $\tilde{\psi}(p) = \langle p|\Psi\rangle$,a dn we can use it, by sandwiching equation 30 between $\langle p|$ and $|\Psi\rangle$. That will simply give us:

$$\tilde{\psi}(p) = \langle p| \int dx\, |x\rangle \langle x||\Psi\rangle \tag{32}$$

or, by using the rules of integration,:

$$\tilde{\psi}(p) = \int dx\, \langle p|x\rangle \langle x|\Psi\rangle \tag{33}$$

Now $\langle x|\Psi|$ is the definition of $\psi(x)$ and that $\langle p|x\rangle$ is equation 27, or simply

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{-ipx}{\hbar}} \tag{34}$$

We can now add everything together, to get that:

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int dx\; e^{\frac{-ipx}{\hbar}}\, \psi(x) \tag{35}$$

Similarly, for the opposite situation, meaning we know the $\tilde{\psi}(p)$, we can find $\psi(x)$ by:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int dp\; e^{\frac{ipx}{\hbar}}\, \tilde{\psi}(p) \tag{36}$$

These are **Fourier Transforms of each other!**

4 Commutators

From earlier Chapters, we had seen that:

$$[L,M] = i\hbar\{L,M\} \tag{37}$$

That means that we could enrich our knowledge if we compute **[X,P]**
From eqs. 5 and 17, we can compute the product of X and P and then the product of P and X and subtract them!

But in order for this to make sense, we need to have a function $\psi(x)$ to act on it so we see the difference!
First of all $XP\psi(x)$ is:

$$XP\psi(x) = -i\hbar x\frac{d\psi(x)}{dx} \tag{38}$$

and the product $PX\psi(x)$:

$$PX\psi(x) = -i\hbar\frac{dx\psi(x)}{dx} \tag{39}$$

By using differentiation rules, we can rewrite equation 39 as:

$$PX\psi(x) = -i\hbar x\frac{d\psi(x)}{dx} - i\hbar\psi(x) \tag{40}$$

Now subtracting the two, we get that:

$$[X,P]\psi(x) = i\hbar\psi(x) \tag{41}$$

That means that when the Position Momentum Commutator acts on any function, it multiplies it by $i\hbar$
We can rewrite this as:

$$[X,P] = i\hbar \tag{42}$$

This is key to proving the Heisenberg Uncertainty Principle, but what is also interesting, is that $X,P = 1$ from equation 37

5 Heisenberg's Uncertainty Principle

We have seen in Chapter 5 that

$$\Delta A\Delta B \geq \frac{1}{2}|\langle\Psi|[A,B]|\Psi\rangle| \tag{43}$$

If we now substitute X and P, we get

$$\Delta X \Delta P \geq \frac{1}{2} | \langle \Psi | [X, p] | \Psi \rangle | \tag{44}$$

and then replacing [X,P] with the previously found $i\hbar$, and using some of algebra, we get:

$$\Delta X \Delta P \geq \frac{1}{2} | i\hbar \langle \Psi | \Psi \rangle | \tag{45}$$

But since $\langle \Psi | \Psi \rangle = 1$ and we only care about the real values, hence the $|.....|$, we finally see that:

$$\Delta X \Delta P \geq \frac{1}{2} \hbar \tag{46}$$

or

$$\Delta X \Delta P \geq \frac{\hbar}{2} \tag{47}$$

There is no experiment that can beat this limitation!