9. Particles

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1 A realistic Example

In this chapter, we will see how Particles move according to Quantum Mechanics!
The Hamiltonian, is of high significance in this procedure!
It is what the time evolution of a system depends on!
As we have seen, this comes from the fact that it plays a vital role in the Time Independent Schrödinger Equation!

$$i\hbar\frac{\partial |\Psi\rangle}{\partial t} = H|\Psi\rangle \tag{1}$$

We will talk about non-relativistic particles and the Original Schrödinger Equation.

In classical Mechanics, the Hamiltonian, or Energy of a System is given by the sum of Kinetic and Potential Energy. We will now take a look at the Quantum version of the Hamiltonian!

Suppose that the Hamiltonian Operator is a constant and is a multiple of P, the momentum operator. say H=cP, where c is that multiple!
In Quantum Mechanics, such a Hamiltonian is reasonable for a particle
Lets try to plug the wavefunction in our equations, but since we are talking about time-dependence, the wavefunction is also a function of time t, $\psi(x,t)$
We said that H = cP and that

$$i\hbar\frac{\partial\left|\Psi\right\rangle}{\partial t} = H\left|\Psi\right\rangle \tag{2}$$

, so we can combine everything and get:

$$i\hbar\frac{\partial\left|\psi(x,t)\right\rangle}{\partial t} = -i\hbar c\frac{\partial\psi(x,t)}{\partial x} \tag{3}$$

and now if we cancel out the terms:

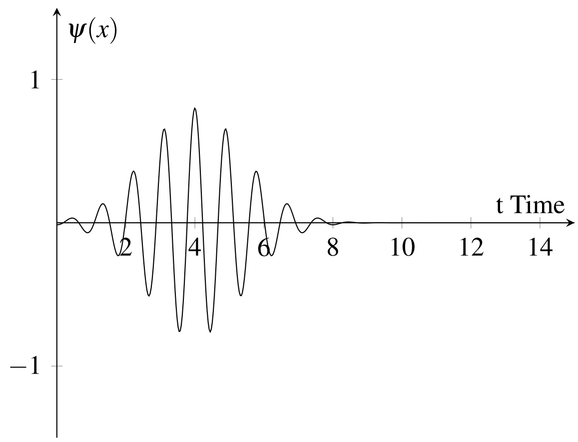
$$\frac{\partial\left|\psi(x,t)\right\rangle}{\partial t} = -c\frac{\partial\psi(x,t)}{\partial x} \tag{4}$$

Which is a very simple equation:
Any function of (x-ct), will solve the equation!
You could do the calculations and see what this is true, but I think this is very obvious and trivial!
Instead, we will see how $\psi(x-ct)$ behaves:
If we start at t=0, which means that: $\psi(x-ct) = \psi(x)$, and that is how we will denote it!(This wavefunction at time t=0)
We don't want any random function of (x-ct), since we know that the total probability musty be 1, meaning:

$$\int_{-\infty}^{\infty}\psi^*(x)\psi(x)\,dx = 1 \tag{5}$$

In other words, we want $\psi(x)$ to collapse to 0 at infinity, so the integral doesn't blow up!!

The wavefunction $\psi(x)$, in a diagram with time, form what we call a **Wave Packet**!
For example:



Wave Packet

In our case, every feature of the function, moves to their right with uniform velocity, namely c! In other words, the wave packet above, maintains its shape as time increases!
We used the letter c to denote the constant/speed to define the Hamiltonian, but that was no random choice. c is the letter we use to denote the speed of light, $3 \cdot 10^8$. This doesn't however mean that the particle is a photon! It actually is a very similar description to that of a neutrino moving at the speed of light!
But there is a problem with this! The neutrino cannot travel to the left here! It only goes to the right, since, according to our equations, it can have negative energy!
But that is simply the result of a negative momentum! That doesn't make sense right? A particle moving with towards one direction has positive and towards the other it has negative?
Here is where the antiparticles enter the scene. Take a wild guess and try to find who used them to solve this problem! If you guessed Paul Dirac then you are right!
For our purpose, we will allow the energy to be negative!
Based on our equations, the particle can only exist in a state where it travels with uniform velocity, meaning it cannot change its velocity!
Given these statements, the Classical equations of motion, Hamilton's equations are:
$\frac{\partial H}{\partial p} = \dot{x}$ and $\frac{\partial H}{\partial x} = -\dot{p}$
Or $\frac{\partial H}{\partial p} = c$ and $\frac{\partial H}{\partial x} = 0$
The momentum is conserved as we noted earlier!
In this example, Quantum Mechanics tells us that both probability distributions and expectation values travel with velocity c, or that the expectation value of position, can be described by the Classical Equation of Motion!

2 Free Particles

In the world as we know it, only mass-less bodies can travel at the speed of light! That is, based on Relativity the boundary of the Universe! All known particles, except gravitons and photons move with velocities lesser than c. We call **nonrelativistic** the particles that travel at speeds a lot lot lower than c, or velocities that for us humans can make sense!

Nonrelativistic Particles follow the laws of motion that Newton discovered and formulated.
In such particles, meaning free nonrelativistic, the usual Hamiltonian, is equal to :

$$\frac{P^2}{2m} \tag{6}$$

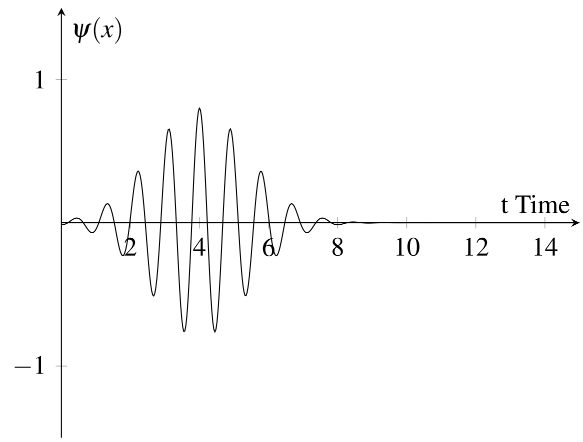
With the term free particle, we mean that no forces act upon it, therefore, we can ignore the potential energy!(Only when talking about free particles)
We only care about the Kinetic Energy, or T, which in Quantum Mechanics is equal to

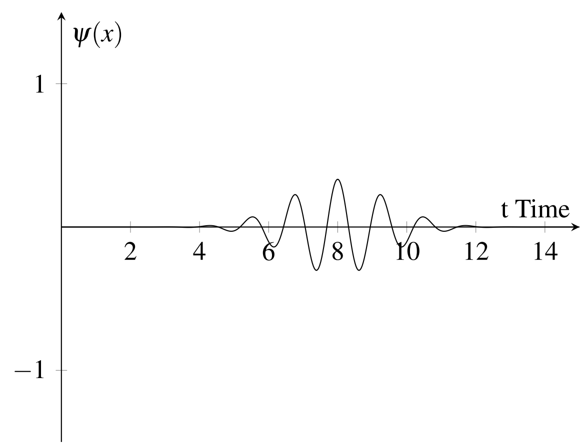
$$\frac{P^2}{2m} \tag{7}$$

This time, since the momentum is squared, the sign of the particle's Energy, doesn't depend on the direction the particle is moving.
Let's now try to solve the Schrödinger Equation with this Hamiltonian!
We have said that $P = -i\hbar\partial_x$! That means that the $P^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$
And now if combine this with our Hamiltonian, we get:
$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Now we can rewrite the Schrödinger Equations :

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} \tag{8}$$

This time, unlike the previous example ($\psi(x-ct)$, waves of different wavelength move differently with different velocities. This results in the wave packet to flatten out!





3 Time Independence

Before moving to solving the time-dependent Schrödinger Equation, we first need to solve the time-independent!

$$H\left|E_j\right\rangle = E_j\left|E_j\right\rangle \tag{9}$$

or by expanding the Hamiltonian:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x) \tag{10}$$

Since it is time-independent, we have removed the time dependence of the wavefunction too, meaning it is only a function of x!

We have seen earlier, the solution to this is an exponential, namely $\psi(x) = e^{\frac{ipx}{\hbar}}$, and its eigenvalue is $E = \frac{p^2}{2m}$, which makes sense, since E is the energy eigenvalue!
We saw in chapter 4, that in order to turn the time-independent result into a time-dependent, we simply multiply it by: $e^{\frac{-iEt}{\hbar}}$, which if we execute gives us:
$\psi(x,t) = e^{\frac{i(px-\frac{p^2t}{2m})}{\hbar}}$, and using that in combination with the Fourier transform integrals, we can find $\tilde{\psi}(p)$.

$$\psi(x,t) = \int \tilde{\psi}(p)(e^{\frac{i(px-\frac{p^2t}{2m})}{\hbar}})\,dp \tag{11}$$

Like this, you can find $\tilde{\psi}(p)$ by starting with any position wavefunction at t=0, then using the Fourier Transforms, and lastly letting it evolve!
Again, the wave packet will change its shape as time progresses since the waves travel at different velocities.
However, the whole wave packet, will travel at velocity $\langle \frac{p}{m} \rangle$, just like a classical particle would.
Using everything we have said in this chapter, we can calculate the time dependent, momentum representation wavefunction!

$$\tilde{\psi}(p,t) = \tilde{\psi}(p)e^{\frac{i(px-\frac{p^2t}{2m})}{\hbar}} \tag{12}$$

That translates to the fact that only the phase changes with time, while the magnitude stays the same. That means that P(p) doesn't change as time progresses!
This is obvious, since the momentum is conserved, however this **only applies for Free Particles**.

4 Velocity

So far, we haven't talked about the relation between momentum and the momentum operator!
From Classical Mechanics, we get that $v = \frac{p}{m}$ and $v = \dot{x}$.
The Quantum Mechanics Version of that, is:

$$v = \frac{d\,\langle\Psi|X|\Psi\rangle}{dt} \tag{13}$$

Using everything we have said about the terms of this equation, we can rewrite :

$$v = \frac{d}{dt}\int \psi^*(x,t)x\psi(x,t)\,dx \tag{14}$$

We know that $\langle\Psi|X|\Psi\rangle$ changes with time, since, well, it depends on time.
Now I suggest you take a look at chapter 4 before moving on!

If you recall, we have said that

$$\frac{d}{dt}\langle L\rangle = \frac{i}{\hbar}\langle [H,L]\rangle \tag{15}$$

or in English, the expectation value of L is given by the $\frac{i}{\hbar}$ multiple of the expectation value of the commutator of the Hamiltonian with that observable!
We can apply this to velocity and get:

$$v = \frac{i}{\hbar}\langle [H,X]\rangle \tag{16}$$

and using the definition of the Hamiltonian,

$$v = \frac{i}{\hbar}\langle [\frac{P^2}{2m},X]\rangle \tag{17}$$

but since the term $\frac{1}{2m}$ is simply a constant, we can take it out, and we see that:

$$v = \frac{i}{2m\hbar}\langle [P^2,X]\rangle \tag{18}$$

All we now need to do is compute $[P^2,X]$
If we carry on the calculation, we get that $[P^2,X] = P[P,X] + [P,X]P$.
(Try to mathematically come to the same result as an exercise)
We had found the commutation relation between P and X earlier, namely $-i\hbar$, so we can combine everything and get that:

$$v = \frac{i}{2m\hbar}\cdot -2\hbar i\langle P\rangle \tag{19}$$

or

$$v = \frac{\langle P\rangle}{m} \tag{20}$$

or that

$$\langle P\rangle = mv \tag{21}$$

The Average of Momentum equals to the mass times velocity!

5 Quantization

1) Start with a Classical System. Turn the sets of momenta and positions to p_i and x_i to generalize them. The system has a Hamiltonian, which is a function of p_i and x_i.
2) Replace the Phase-Space with a Linear Vector Space. The State-Space is now represented by a wavefunction.
3) Replace the positions and Momenta p_i and x_i with the Operators, P_i and X_i, where $X_i\psi(x) = x_i\psi(x)$ and $P_i\psi(x) = -i\hbar\partial_{x_i}\psi(x)$
4) The Hamiltonian is now an operator given by $\frac{P^2}{2m}$.

The Hamiltonian can then be used in either Schrödinger Time Dependent or Time Independent Equation, where the one tells us how the wavefunction evolves over time, and the other tells us how to find the eigen vectors and values of the Hamiltonian.
Quantization is the transformation from Classical Equations of Motion to Quantum Equations.

Quantum Mechanics describes how the world actually works, and Classical Mechanics, how the averages of quantities behave, whenever the wavefunction maintains its shape!

6 Forces

The world would be very boring if all particles were free! Thankfully, forces exist!
As we have seen in Classical Mechanics, the force on any given particle is the sum of forces that all other particles exert on it!
There also exists a Potential Energy Function, denoted by $V(x)$, that are the forces that the environment exerts on a given particle! It is a function of position, since it isn't the same for a ll location. For example, the potential energy is different here on Earth of a particle, and different on the Moon, for the exact same particle.
We have seen in Classical Mechanics, that $F(x) = -\partial_x V(x)$ or

$$\frac{md^2x}{dt^2} = -\frac{\partial V(x)}{\partial x} \tag{22}$$

That is in Classical Mechanics. In Quantum Mechanics, our approach is different!
V(x) becomes an Operator V that gets added to the Hamiltonian!
When V acts on the wavefunction, it multiplies it by V(x).

$$V\psi(x) = V(x)\psi(x) \tag{23}$$

Just like in Classical Mechanics, once forces are included, $\frac{dp}{dt} \neq 0$! Instead,

$$\partial_t p = F \tag{24}$$

or,

$$\partial_t p = -\partial_x V(x) \tag{25}$$

That said, in Quantum Mechanics, as I just said, we simply modify the Hamiltonian, as

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{26}$$

Which means, that our Schrödinger Equation, becomes:

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{27}$$

or

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) \tag{28}$$

The new term obviously affects how ψ evolves over time.
Also, having added this new term, there is a new commutator of X and H, namely [X,V], but both operators simply multiply by x and V(x) respectively, so i think it is obvious that they commute!
What does that mean and why is it so important?
It means that the connection between velocity and momentum is unaffected by Forces in Quantum Mechanics, and as stated by Newton, $\dot{p} = F$, is also true for Quantum Mechanics!

Lets now try to calculate $\partial_t \langle P \rangle$
The way to do this is to take the commutator of the the Hamiltonian with P, as we did before with X.

$$\frac{d\langle P \rangle}{dt} = \frac{i}{2m\hbar}\langle [P^2, P] \rangle + \frac{i}{\hbar}\langle [V,P] \rangle \tag{29}$$

The first term is 0, since an operator commutes with any function of itself, and because it is the definition of the conservation of momentum!
The second term is equal to:

$$[V,P] = i\hbar\partial_x V(x) \tag{30}$$

, which is something we will prove soon.
That results in

$$\frac{d\langle P \rangle}{dt} = -\langle \frac{dV}{dx} \rangle \tag{31}$$

Now to prove equation 30, we will let the commutator act on a wavefunction

$$[V,P]\psi(x) = -V(x)i\hbar\partial_x\psi(x) - -i\hbar\partial_x V(x)\psi(x) \tag{32}$$

Which is equal to :

$$[V,P]\psi(x) = -i\hbar V(x)\partial_x\psi(x) + -i\hbar V(x)\partial_x V(x)\psi(x) \tag{33}$$

Using the Chain rule, we get that:

$$[V,P]\psi(x) = -i\hbar V(x)\partial_x\psi(x) + i\hbar(\partial_x V(x)\cdot\psi(x) + \partial_x\psi(x)\cdot V(x)) \tag{34}$$

Now if we expand everything:

$$[V,P]\psi(x) = -i\hbar V(x)\partial_x\psi(x) + i\hbar\partial_x V(x)\cdot\psi(x) + i\hbar V(x)\partial_x\psi(x) \tag{35}$$

Lastly Cancelling the terms we prove that :

$$[V,P] = -i\hbar\partial_x V(x) \tag{36}$$

7 The Limitation of Classical Equations

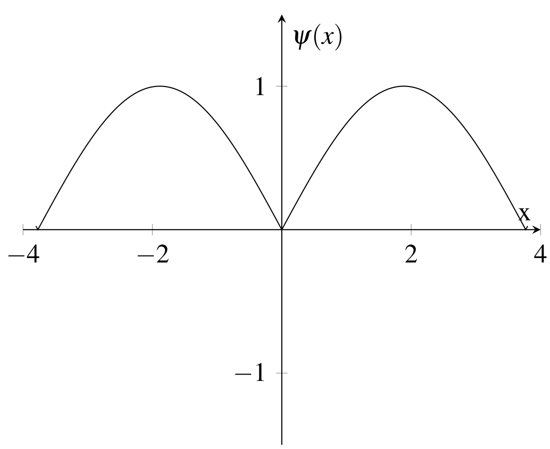
You probably think that $\langle x \rangle$ follows the trajectory of a classical particle, and that we have proved it! However, this is not true, and we have proven something different!
The reason this is not true, is because

$$\langle f(x) \rangle \neq f(\langle x \rangle) \tag{37}$$

which means that

$$\frac{d\langle P \rangle}{dt} \neq -\frac{dV(\langle x \rangle)}{d\langle x \rangle} \tag{38}$$

The Classical Equations, are approximation, only whenever, we can replace $\langle \frac{dV}{dx} \rangle$ with $\frac{dV(\langle x \rangle)}{d\langle x \rangle}$! That happens, only when V(x) varies slowly compared to the size of the wave packet.
If V varies rapidly, a narrow spike-like wave packet will get broken down into a scattered wave.
This also happens to a badly scattered wave



This is an approximation to the Binodal Function Centered, where although $\langle x \rangle = 0$, $\Delta x > 0$.

Consider the wave packet above!
$f(\langle x \rangle)$ is a function of the center of the wave packet, while $\langle f(x) \rangle$ represents, $-\frac{d\langle P \rangle}{dt}$.
If we suppose that $f = x^2$, that means that $\langle x \rangle$ is equal to 0, but, $\langle x^2 \rangle > 0$.
Knowing that, we can deduce that

$$\frac{d\langle P \rangle}{dt} = -\frac{dV(\langle x \rangle)}{d\langle x \rangle} \tag{39}$$

, only when $\langle f(x) \rangle = f(\langle x \rangle)$!
That means, that the Quantum Equations look like the Classical, only when the wave

packet is **localised** and **coherent**.
Usually, if a particle's mass is pretty large, then the wave function tends to be well concentrated! However, if V(x) has no sharp spikes, as we said earlier it varies very slowly compared to the size of the wave packet, we can make the transition from $\langle f(x)\rangle$ to $f(\langle x\rangle)$. When it doesn't it breaks up and even a nice cocentrated wave function will be spread out!

8 Action in Quantum Mechanics

Classical Mechanics, has a very powerful principle, the **Principle of Least Action**, and it is very helpful when trying to solve the equations of motion!
Now the question arises:
Is there a Quantum Mechanics Version of this principle?
Fortunately, Richard Feynman was also bothered by this question! And what would any logical person do? Yup, just like we would have done it, he invented the Path Integrals, to satisfy the requirements and finally provide the world, with a Quantum Principle of Least Action.

In Classical Mechanics, Action is given by the time integral of the Lagrangian across two points in time:

$$A = \int_{t1}^{t2} L(x,\dot{x})\, dt \tag{40}$$

Where the Lagrangian L is given by the Kinetic - potential Energy, or simply

$$L = \frac{m\dot{x}^2}{2} - V(x) \tag{41}$$

In Quantum Mechanics, having the history of the particle offers us nothing, due to uncertainty. So, instead, given it starts at (x_1,t_1), the right question to ask is:
What is the probability it will show in (x_2,t_2), if an observation is made.
or, an even better question:

Given a particle starts at $(x_1,t_1), whatistheamplitudeitwillshowupin (x_2,t_2)$**?**

We can say that, since the probability is the square of absolute value of the complex amplitude!
We define that amplitude as

$$C(x_1,t_1;x_2,t_2) \tag{42}$$

or simply

$$C_{1,2} \tag{43}$$

This means state of the particle is $|\Psi(t_1)\rangle = |x_1\rangle$.
Over the time interval $t_2 - t_1$, the state evolves to $|\Psi(t_2)\rangle = e^{\frac{-iH(t_2-t_1)}{\hbar}} |x_1\rangle$.
Therefore, the amplitude to detect the particle at $|x_2\rangle$ is

$$C_{1,2} = \langle x_2 | e^{\frac{-iH(t_2-t_1)}{\hbar}} | x_1 \rangle \tag{44}$$

Let $t = t_2 - t_1$.
We can now break the interval into two smaller intervals of size $\frac{t}{2}$.

$$e^{-\frac{iHt}{\hbar}} = e^{\frac{-iHt}{2\hbar}} e^{\frac{-iHt}{2\hbar}} \tag{45}$$

We can insert the Identity Operator in the form $I = \int dx \, |x\rangle \langle x|$ in our equation to write our final integral:

$$C_{1,2} = \int dx \, \langle x_2 | e^{\frac{-iHt}{2\hbar}} | x \rangle \langle x | e^{\frac{-iHt}{2\hbar}} | x_1 \rangle \tag{46}$$

In English, that means that the amplitude or square root of the probability to get from x_1 to x_2 over the time interval we denote as t, $(t_2 - t_1)$, is an integral over all the possible points between the start and the end points!
For every infinitesimal time interval ε, we simply include to our equation a factor: $e^{\frac{-i\varepsilon H}{\hbar}}$.
Between each of these factors we insert the integral form of the Identity Operator, $I = \int dx \, |x\rangle \langle x|$. That means that $C_{1,2}$, becomes a multiple integral over all the locations in between.
The Integrad, or the function whose integral we take, is the sum of all the expressions:

$$\langle x_i | e^{\frac{-i\varepsilon H}{\hbar}} | x_{i+1} \rangle \tag{47}$$

Now if you remember,in chapter 4, we had defined Unitarity Operator exactly as the term sandwiched, namely : $U(\varepsilon) = e^{\frac{-i\varepsilon H}{\hbar}}$!
Using this, we can rewrite the whole product, as

$$\langle x_2 | U^N | x_1 \rangle \tag{48}$$

or

$$\langle x_2 | UUUU ... | x_1 \rangle \tag{49}$$

Where N, is the amount of infinitesimal epsilon intervals that constitute to time interval t!
What Feynman Discovered and changed a lot of things, is that we can express all of these terms with a simpler terms: $e^{\frac{iA}{\hbar}}$, where A is the Action for each individual path, hence the term path integral, which mathematically is defined as:

$$C_{1,2} = \int_{paths} e^{\frac{iA}{\hbar}} \tag{50}$$