PHYSICS 137A NOTES

Typeset notes for Physics 137A: Quantum Mechanics I
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University of California, Berkeley

Fall 2022

Contents

Introduction

This course is titled **Quantum Mechanics I**. Eric and Andrew both took this course in Fall 2022.

0.1 Basic Syllabus Info

Here, there is some basic information regarding the syllabus for this course as it was taught in Fall 2022.

Professor and GSI Info

A little bit about the professor and the GSIs:

- **Professor**: Irfan Siddiqi (irfan_siddiqi@berkeley.edu)
- **GSI 1**: Avirukt Mittal (avirukt@berkeley.edu)
- **GSI 2**: Serah Moldovsky (serah_moldovsky@berkeley.edu)

Office hours were different for each professor and GSI and were available by appointment as well.

0.1.1 Lecture and Discussion Info

Now, a bit about the lectures and discussions.

- **Lectures**: M/W/F, 09:00 - 10:00, Physics Building 4
- **Discussions**: M, 18:00 - 19:00, Evans 60 **or** T, 17:00 - 18:00, GSPP

Lectures and discussions both start on Berkeley time (10 minutes after posted start time), and lectures end one minute before the hour.

0.1.2 Course Materials

For this course, there are two required textbooks: Griffiths Intro to Quantum Mechanics and Shankhar Principles of Quantum Mechanics. It is recommended, though, that you consult other resources to get a better and more thorough grasp on the material.

0.1.3 Grading Breakdown

Here is everything factored into the grade:

- **Homework**: One assignment per week, due Friday at 17:00. Lowest dropped. Total 30%
- **Midterm**: Split over two days, 10/17 and 10/19, in class. Total 30%.
- **Final**: Will cover everything. On 12/16 from 19:00 - 22:00. Total 40%

There is no curve in this class, so just do the best that you can! To succeed in this course, it's important to come to lectures, do the homework, and read the materials in advance. With all of this, success is guaranteed!

PART I

PRE-MIDTERM

Lecture 1 (8/24)

The first lecture of Physics 137A was held on **Wednesday, August 24**. It covered the basics of the course syllabus and an introduction of blackbody radiation.

1.1 ‖ Why Quantum Mechanics?

Quantum mechanics was developed as a way to better describe physical observations. By the eighteenth century, we effectively mastered principles of Newtonian mecahnics, but we could not describe what was happening when objects glow when heated. So before we begin studying quantum mechanics, let's take a look at how we got here.

1.2 ‖ Blackbody Radiation

Blackbody radiation refers to the phenomenon that when a solid object, such as a cube of matter, is heated to a temperature T, it begins to glow.

- **1742:** It was observed that different objects (made from different materials) at the same temperature glow the same colour.

- **1800s:** The methods of spectroscopy get better, and we are now able to analyze light to a much higher degree of precision.

- **1854:** Kirchoff develops the modern theory of blackbody radiation. He imagined that there is a function $R(\lambda, T)$ which represents the emissive power per unit area of a blackbody. He also developed a the modern model of a blackbody − an object that allows light and bounces many times, and it generates a temperature T due to the bouncing. Here's an example of $R(\lambda, T)$ vs. λ:
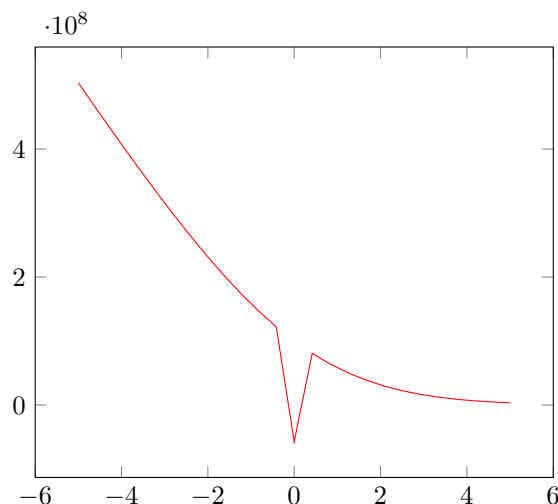
There are a few characteristics of this curve that make intuitive sense. At $\lambda = 0$, there is no wave, so the blackbody radiation intensity should be 0. At large wavelengths, the light carries very low energy, and thus the radiation intensity is also very low.

As this curve represents emissive power per unit area, the area (the integral) under the curve is finite, and describes the total emissive power. Stefan's law then states that the total radiation is proportional to T^4. Mathematically speaking, this means that

$$R(T) = \int_0^\infty R(T, \lambda) d\lambda = \sigma T^4$$

Wein's law describes a relationship between the maximum wavelength of a blackbody curve to its temperature. Specifically, he found that $\lambda_{max} T = 2.898 \times 10^{-3}$, or in other words $\lambda_1 T_1 = \lambda_2 T_2$.

Then, Rayleigh and James calculated, numerically, that at high wavelengths this curve is approximated by

$$R(T) = \frac{8\pi k_B T}{\lambda^4} \tag{1.1}$$

Notice that we have λ^4 in the denominator of this equation, meaning that our function should, in theory asymptote very quickly at low λ values, However, this is not what we see in experiments! This discrepancy between the classical theory and observed is most commonly referred to as the **ultraviolet catastrophe.**

1.3 ‖ Derivation from First Principles

Let's now go back to first principles and try to build up a black body and see how it behaves. For simplicity, consider a cube of side length L [INSERT TIKZ HERE]. Now, recall standing waves on a line: [INSERT TIKZ HERE] To figure out the eigennodes for such a setup, all we do is solve the wave equation we learned in E&M:

$$\nabla^2 \psi(\vec{r}, t) = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \psi(\vec{r}, t)$$

The quantum version of this equation will look similar, so it's good to remind ourselves of it. This is a second-order differential equation, which means that we need to specify the boundary conditions. In this case, our boundary condition is that ψ must vanish at the cavity walls:

$$\psi(x = 0, y, z, t) = \psi(x = L, y, z, t) = 0$$

From this, we get our standard solution of a sine wave:

$$\psi(\vec{r}, t) = A(t) \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

Here, $k_i = \frac{n_i \pi}{L}$. In other words, our equation is of the form $A(t)B(x, y, z)$. Essentially, we've separated the time parts and the space parts into different pieces, which is exactly what we would expect in the standing wave case. Mixing them together gives us traveling waves. If we now consider an electron in our box, we get an oscillating EM field, which will be important when we continue this next lecture.

Lecture 2 (8/26)

The second lecture of Physics 137A was held on **Friday, August 26**. It picked up where the previous lecture left off on the black body model and explained why quantum mechanics is needed.

2.1 ‖ Last Time: Modeling the Black Body

Quickly recapping what happened last time: we modeled a black body in a cube of side length L and are trying to understand where the Rayleigh-Jeans law comes from, as well as understanding how to reconcile it with the Ultraviolet Catastrophe.

2.2 ‖ Energy Density

Last lecture, we threw in electrons into the black body and saw that those electrons would bounce off the wall, creating an oscillating electric field. This means there must be some energy $\vec{E}$ contained in our box from this. Now, we want to calculate energy density. How do we do this? The Poynting vector. In order to compute the energy density, we will need the number of modes and the energy per mode of this oscillation:

> **Insight:** Energy Density = # of N (modes) × Energy per mode

Let's think about modes in a cube. We know that we must satisfy the wave equation:

$$\nabla^2 \psi(\vec{r}, t) = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \psi(\vec{r}, t)$$

We also know that we hacve a solution of the following form (given our boundary conditions that ψ must vanish at the edges):

$$\psi(\vec{r}, t) = A(t)\sin(k_x x)\sin(k_y y)\sin(k_z z) = A(t)B(x, y, z), \text{ where } k_i \frac{n_i \pi}{L}$$

We have an equation and a solution to that equation: let's plug it in!

2.2.1 | Solving for the Dispersion Relation

Plugging in, we get:

$$-(n_x^2 + n_y^2 + n_z^2)\frac{\pi^2}{L^3} A(t)B(x, y, z) = \frac{1}{c^2} B(x, y, z)\frac{\partial^2}{\partial t^2} A(t) = -\omega^2 t$$

Notice that this differential equation is in the same form as an oscillator, and we know that a solution to this such an equation is in the form $A(t) = A_0 \cos(\omega t) + \varphi$, which gives us

$$\omega^2 = \frac{c^2\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2)$$

Remember that $n_i \in \mathbb{Z}$, so this means that ω also takes on discrete values. Therefore, note that for large values of ω we see that there are many different ways to write n_i, which is also known as the dispersion relation.

Now, let's circle back to the first question that we asked: how many nodes are in the box? Well, let's break it down.

2.2.2 | Many Nodes

Our lowest-order node occurs at $n = 1$, and the only way to achieve this is to have one of $n_x, n_y,$ or n_z be equal to 1. Then, as we increase n, we have more and more possible combinations of $n_x, n_y,$ and n_z values.

2.2.3 | Density of States

For simplicity, let $g(\omega)$ denote the number of nodes per unit frequency ω. In other words,

$$g(\omega) = \frac{dN(\omega)}{d\omega}$$

This m,eans, therefore, that the number of nodes from 0 to ω frequency (denoted $N(\omega)$ is

$$N(\omega) = \int_0^\omega g(\omega)d\omega$$

If we recall our previous equation and rearrange the terms:

$$n_x^2 + n_y^2 + n_z^2 \le \frac{\omega^2 L^2}{c^2\pi^2}$$

we see that this is simply modeling the equation of a sphere centered at the origin with radius $\frac{\omega L}{c\pi}$! And so, to calculate $N(\omega)$, we need only to calculate the volume of this sphere. It's important to remember, however, that this sphere will cross into quadrants of negative n_is, so we need to only compute the volume of the sphere where all n_is are positive: namely, one eighth of the sphere:

$$N(\omega) = \frac{1}{8}\left(\frac{4}{3}\pi\frac{\omega^3 L^3}{c^3\pi^3}\right)$$

As we can see, the volume of the cube L^3 has popped up here. Let's denote it V for simplicity moving forward. Now, let's convert our angular frequency to regular frequency, using the conversion $\omega = 2\pi f$:

$$N(f) = \frac{8\pi^3 f^3 V}{6c^3\pi^2}$$

$$\therefore g(f) = \frac{dN(f)}{df} = \frac{4\pi f^2 V}{c^2}$$

However, we need to account for the polarization of our waves,so we actually need to multiply everything by 2 (for each of the possible wave polarizations), giving us:

$$\boxed{g(f) = \frac{8\pi f^2}{c^3}V}$$

This is correct both classically and for the quantum scale.

2.3 ‖ Quantum Mechanics is Needed

The previous equation we derived is true both for the classical model and the quantum model, since all we really invoked was some basic geometry. However, we are now about to see exactly where these two worlds bifurcate and our classical models fall apart.

2.3.1 | Classical Calculation

In our classical model, each mode is excited with $k_B T$ energy (from Thermodynamics). Do, the energy density between frequencies f and $f + df$ is

$$\boxed{g(f)df k_B T}$$

Now, let's plug this into our equation:

$$g(f) = \frac{8\pi}{c^3} f V k_B T df$$

For simplicity, let's introduce an energy density per volume (call it ρ):

$$\rho(f, t) = \frac{8\pi}{c^3} f^2 k_B T$$

Now, let's convert to wavelengths, using the conversions $f = \frac{c}{\lambda}$ and $df = -\frac{c}{\lambda^2} d\lambda$. This negative sign is important to remember, because it will flip the limits of our integral. Plugging in, we get:

$$\rho(\lambda) = \frac{8\pi}{c^3} \frac{c^2}{\lambda^2} \frac{c}{\lambda^2} k_B t = \boxed{\frac{8\pi k_B T}{\lambda^4}}$$

And so, we've attained our Rayleigh-Jeans law as desired! But, there's one important problem that we will need to fix with quantum mechanics:

> **Insight:** Some modes at some energies are not excited. In other words, this means that <u>not all states are allowed</u>, and <u>not all energies are allowed</u>.

This comes from Max Planck. Because not all energies or states are allowed, there needs to be some minimum energy. This is where quantum mechanics comes in.

2.3.2 | Quantum Calculation

It's now time to fix the issue of not all energies being allowed with quantum mechanics. Planck tells us that we need a minimum energy. More notably, he also tells us that this energy is quantized, and so the energy per node is then $E_n = nhf$. Som our average energy is

$$\bar{E} = \sum_{n=0}^{\infty} nhf \frac{e^{-\frac{nhf}{k_B T}}}{\sum_{n=0}^{\infty} e^{-\frac{nhf}{k_B T}}}$$

We need that fraction to normalize the probability. Also, some may recall the exponent as our Boltzmann

factor. For simplicity, let $x = e^{-\frac{hf}{k_B T}}$. Now, we plug into all of our equations:

$$\bar{E} = hf \sum_{n=0}^{\infty} n \frac{x^n}{\sum_{n=0}^{\infty} x^n} = hf \frac{x}{1-x} = \frac{hfe^{-\frac{hf}{k_B T}}}{1 - e^{-\frac{hf}{k_B T}}} = \boxed{hf \frac{1}{e^{\frac{hf}{k_B T}} - 1}}$$

$$\therefore \rho(f, t) = \frac{g(f)}{V} \bar{E} = \frac{8\pi hf^3}{c^3} \frac{1}{e^{\frac{hf}{k_B T}} - 1}$$

$$\therefore \boxed{\rho(\lambda) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}}$$

Many will recognize that last equation as the <u>Plack Radiation Formula</u>. Now, this is correct. How does this solve the ultraviolet catastrophe we discovered in the first lecture? Well, in the limit, this equation will reduce to the correct formula, especially taking into account the quantization of energies.

2.4 The Bohr Atom

Now that we've reconciled this, let's take a look at the atom. More specifically, the Bohr model of the atom.

As Planck solved the ultraviolet catastrophe, he introduced the idea that energy is quantized, and thus only some energies are allowed. Another big issue in modern physics at the time was that the classical framework for the structure of an atom was completely unstable.

2.4.1 The Electron Dies

An electron orbiting the nucleus of an atom that is positively charged is bound to collapse into the nucleus, and if this were true, then the lifetime of the universe would be incredibly short. This needed to be fixed.

2.4.2 Matter is a Wave

Thus, Bohr theorized that, just like the quantum calculation for the allowed energies, atoms must have quantized angular momenta. That is,

$$L = m_e v_e r$$

where L is a quantized value. The only way this configuration is stable is if the electrons are *standing waves*, and as a result, **all particles are waves**. So instead of the electron orbiting the nucleus as if it were a circle, it looks like a wave instead. This is the problem de Broglie solved when he derived the relation that $\lambda = \frac{h}{p}$. This important fact, combined with the derivation we saw previously, is exactly why we need quantum mechanics.

2.5 How Do we Gain Intuition?

All of the calculations and approximations that we did involve a bunch of guesses for values and equations that do not at all appear intuitive in the classical sense. So, where do these guesses come from, and how can we make our own when the time comes? Quantum mechanics is designed to equip us with the tools necessary to understand such approximations, and as we delve deeper, we will gain a different type of intuition for the scale of the very small. In the next lecture, we will formally begin our quantum mechanical study.

Lecture 3 (8/29)

The third lecture of Physics 137A was held on **Monday, August 29**. It discussed the wave description of matter and made a brief introduction to operators.

3.1 | Last Time: Everything is a Wave (in Quantum Mechanics)

Last lecture we found that everything is a wave in Quantum Mechanics. This is true, but depending on the unit scales that we're talking about, the true wave descriptions of matter may not show. For instance:

- Electrons: $\lambda_{dB} = e^{-1}$nm, atom size: 1 Å. These sizes are comparable.

- Humans: $\lambda_{dB} = 10^{-36}$nm, size: 1m. These sizes are nowhere near comparable

Since the size of everyday objects are so much larger than that of the deBroglie wavelength, this is why we don't see any quantum effects with the naked eye.

Now back to the quantum realm. Because we've said already that everything is a wave, waves can also interfere with each other. Consider a wave source some distance away from a double slit. If we move the slit apparatus sufficiently far away from the source, the oncoming waves appear to be plane waves instead of circular (or spherical) wave patterns. This is what we mean by plane waves - the fact that the source is infinitely far away from us. To describe this wave, we can measure its electric field, which can be done in the following way:

$$\vec{E} = \vec{E}_0 e^{i(k \cdot r - \omega t + \varphi)}$$

The way we should interpret this expression is as follows: $\vec{E}_0$ is a description of the maximum allowable electric field intensity at any point in time, and $e^{i(k \cdot r - \omega t + \varphi)}$ represents a phase, or in other words, how much of the maximum intensity we are seeing at any point in time. The term $k \cdot r$ represents the spatial component (oscillations per unit space), and ωt represents the temporal component (oscillations in time). The φ represents some overall offset phase, which is determined usually by the system.

> **Insight:** Note that we use a complex exponential here because $|e^{ikx}|^2 = 1$, which is particularly useful when we want it to represent as a percentage of the maximum allowable amplitude.
>
> This convention, we believe, is the fundamental reason why complex numbers exist in quantum mechanics! Any appearance of complex numbers we see later on comes from this convention.

Back to the double slit experiment. Since there are two slits, there are two sources, call them $\vec{E}_1$ and $\vec{E}_2$. Therefore, $E_{tot} = \vec{E}_1 + \vec{E}_2 = \vec{E}_{01} e^{i\delta_1} + \vec{E}_{02} e^{i\delta_2}$. Here, the δ_i represents the spatial and temporal frequencies. Since the intensity scales with $|E|^2 = E \cdot E^\star$ where $E^\star$ represents the complex conjugate, this gives:

$$|E|^2 = E_{01}^2 + E_{02}^2 + \vec{E}_{01}\vec{E}_{02}\left(e^{i(\delta_2 - \delta_1)} + e^{-i(\delta_2 - \delta_1)}\right)$$

$$= E_{01}^2 + E_{02}^2 + 2\vec{E}_{01} \cdot \vec{E}_{02}\cos(\delta_2 - \delta_1)$$

Notice the order of operations here: we summed the two electric field components **before** squaring them. This is important, since had we squared them first, then we would have simply gotten $\vec{E}_{01}^2 + \vec{E}_{02}^2$, which does not exhibit any interference pattern.

3.2 ‖ Wave Description of Matter

So, as we see from the double slit experiment and from our previous discussions on quantum mechanics, particles in the classical sense don't really exist, and everything can be modeled as a wave. So, how do we do this? With the help of a newly-defined **wave function:**

> **Definition 3.1 (Wave Function):** Typically denoted Ψ: a complex function of position and time.

More specifically, Ψ is an amplitude. However, it's not physical (in other words, we can't directly measure it). Despite this, similar to position and momentum in classical mechanics, this wave function contains all of the physical information needed to describe the system.

3.2.1 │ Probability Density

For a while, we had no idea what to do with Ψ and how to make it describe life precisely because it offered no physical significance on its own. However, in 1926, Max Born found that, by taking the square of the modulus of this function, we are able to actually glean something physical from the wave function. This gives us another important concept, notably *probability density*:

> **Definition 3.2 (Probability Density):** $P(\vec{r}, t) = |\Psi(\vec{r}, t)|^2$: The probability per unit volume of finding a "particle" at $\vec{r}, t$.

As we can see, squaring the modulus gives us a real, physical interpretation and something we can actually work with. Furthermore, to normalize, we multiply by our volume, so the probability within a cube $d\vec{r}$ becomes:

$$P(\vec{r}, t)d\vec{r} = |\Psi(\vec{r}, t)|^2 d\vec{r}$$

For generality, we write $d\vec{r}$ to refer to a volume irrespective of any coordinate system.

3.3 ‖ Wave Superposition

Now, a key insight in quantum mechanics (and one that carries over from classical mechanics) is that of superposition:

> **Theorem 3.1: Superposition**
>
> If Ψ_1 and Ψ_2 are two allowed waves/states (solutions to some wave equation), then
>
> $$\Psi = c_1 \Psi_1 + c_2 \Psi_2$$
>
> is also allowed, where $c_1, c_2 \in \mathbb{C}$.

We allow the constants to be complex to not eliminate the interference we saw earlier with our double slit experiment.

3.4 Introducing Operators

Now, if we recall classical mechanics, knowing the position and momentum gives us everything we could ever want to know about the system [INSERT TIKZ HERE]. Now, what happens if we try to throw a plane wave into our model? [INSERT TIKZ] We immediately run into a problem: the wave is everywhere. This means that position and velocity are essentially meaningless quantities to us here. So, how do we reconcile this?

3.4.1 de Broglie Relations

Recalling the de Broglie relations that we learned in high school:

> **Theorem 3.2: de Broglie Relations**
>
> For a quantum-mechanical system:
>
> $$E = hf = \hbar\omega \qquad\qquad \hbar = \frac{h}{2\pi}$$
>
> $$p = \frac{h}{\lambda} = \hbar k \qquad\qquad k = \frac{2\pi}{\lambda}$$

This allows us to better understand our system, but we still need to take it one step further.

3.4.2 Enter the Operator

Consider first a 1D particle: [INSERT TIKZ] In this case, we write out our wave function and we get:

$$\Psi = A e^{i(kw - \omega(k)t)}$$

All of our vectors turn into scalars. Rewriting this, we get:

$$\Psi = A e^{\frac{i(p_x x - E(p_x)t)}{\hbar}}$$

This is great and all, but we want information about the momentum and the energy, and they're stuck in the exponent. How do we get them? Easy: take the derivative (with respect to either):

$$-i\hbar \frac{\partial}{\partial x} \Psi = p_x \Psi$$

$$i\hbar \frac{\partial}{\partial t} \Psi = E \Psi$$

If we look at these equations, they look suspiciously like equations with eigenvalues and eigenvectors, so if we consider just the eigenvectors, we get our $\boxed{\text{momentum and energy operators}}$:

> **Definition 3.3 (Momentum and Energy Operators):** e define these operators as such:
>
> $$\text{Momentum} : -i\hbar\frac{\partial}{\partial x}$$
> $$\text{Energy} : i\hbar\frac{\partial}{\partial t}$$

Now, we have another crucial tool that we will use a lot.

3.4.3 | Operators in 3 Dimensions

We can obviously then extend this to three dimensions, where we see that the operators become <u>gradients</u>:

$$i\hbar\frac{\partial}{\partial t}\Psi = E\Psi$$

$$-i\hbar\vec{\nabla}\Psi = \vec{p}\Psi \qquad\qquad \vec{\nabla} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

It's important here to now remember that we have vectors rather than scalars.

3.5 ‖ Probability Density and Normalization

We have all of these cool values, but we need to remember that these need to be normalized for us to deal with them, so we have the following important insight:

> **Insight:** $\boxed{\int_{\text{all space}} |\Psi(\vec{r}, t)|^2 dr = 1}$: The probability that the "particle" is somewhere in space is 1.

We will use this insight a lot.

3.5.1 | Plane Waves are Problematic

Here, though, we already run into an issue: if we throw our plane wave into this equation, we see that the integral goes to ∞, since the wave exists everywhere in space and time. So, plane waves are far too simplistic a description of life.

3.5.2 | Wave Packets and Fourier Transforms

Since we can't use plane waves, we need a type of wave that is localized rather than everywhere-permeating, where we get the *wave packet*: [INSERT TIKZ] Clearly, it's much more difficult to deal with, but we will learn how to work with them. How do we get wave packets? We get them by <u>adding together many plane waves</u> (of different amplitudes and frequencies), with a method that is more commonly referred to as a $\boxed{\text{Fourier Transform}}$. We will learn about how to do this in the next lecture.

Lecture 4 (8/31)

The fourth lecture of Physics 137A was held on **Wednesday, August 31**. It covered wave packets and reviewed the mathematics of the Fourier transform.

4.1 Last Time: Wave Description of Nature

Last lecture, we explained how everything in the world, in the context of quantum mechanics, can be described as a wave and by a wave function. We started with a standard plane wave, described by the expression $e^{i(kx-\omega t)}$, where k is the spatial frequency and ω is the temporal frequency. [INSERT TIKZ] Furthermore, we were given the de Broglie relations, which describe the momentum and energy of such a wave:

$$p = \hbar k \qquad\qquad\qquad k = \frac{2\pi}{\lambda}$$

$$E = \hbar\omega \qquad\qquad\qquad \omega = 2\pi f$$

From this, we see that a large k will imply more momentum, and a large ω will imply more energy.

While this is all well and good, we found that a plane wave doesn't really help us in describing localized phenomena, since it exists everywhere in space and time and we need the integral over all of space to come out to 1. And so, for this, we will need to understand *wave packets*, and this is our goal today: move from plane waves to wave packets.

4.2 Wave Packets

We currently have a plane wave permeating all of space: [INSERT TIKZ] We saw that this plane wave $e^{i(k_1 x - \omega t)}$ is pretty OK at describing the wave at the specific location of interest, but as soon as we move away from it, it becomes exceedingly unhelpful. So, our target is a localized wave packet: [INSERT TIKZ] How can we get this? Well, let's add some more plane waves to our initial one: [INSERT TIKZ] As we can see, we can kill a lot of the terms past our desired localized region with the proper choices of k_n, since the waves will interfere with each other there. So, after adding together a bunch of $e^{i(k_m - \omega t)}$ waves, we get something that's pretty darn close to what we want: [INSERT TIKZ] But, we can't just add these waves together blindly: some waves will. have more of an effect in the sum than others. Because of this, we need to properly weight them. How do we do this? Through *amplitudes*! And so, our sum becomes something more like this:

$$A_0 e^{i(k_1 x - \omega t)} + A_1 e^{i(k_2 x - \omega t)} + A_2 e^{i(k_3 x - \omega t)} + A_3 e^{i(k_4 x - \omega t)} + \dots$$

This as some have already no-doubt guessed, is exactly the beginning of a $\boxed{\text{Fourier Transform}}$.

4.2.1 1D Wave Packet

Let's apply this to our simple 1D wave packet. To do this, let's throw in p and E, so that we can deal with a wave function. So, our wave will look like $e^{i\frac{p_x x - E(p_x)t}{\hbar}}$. Summing over many plane waves gives us our new expression for Ψ:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{i\frac{P_x x - Et}{\hbar}} \phi(p_x) dp_x$$

Here, it's important to realize that we are **integrating over momentum, not space or time**! This is because we are considering snapshots in space and time, for which the momentum will be changing. In this expression, notice that $\phi(p_x)$ is the weight parameter, which plays the role of the amplitudes A_m we saw in the first sum we attempted to construct. Finally, the coefficient in front of the integral is our normalization, since we only want to deal with normalized wave functions.

Now, a small 137A gift: we are going to work through the math of the Fourier transform and review everything necessary to move forward with our study of quantum mechanics.

4.3 Review of Fourier Transforms

Here, we are going to cover all of the mathematics of the Fourier transform that is important for our purposes. We won't be delving into too much specific detail; for that, consult some other reading materials from other courses. Now, let's cover all of the pieces of the transform.

4.3.1 Discrete Fourier Transform

Starting with the simplest form, we have the discrete Fourier transform, which can model the behavior of a period function $f(x) = f(x + 2\pi)$, with $x \in [-\pi, \pi]$, as an example. From this, we get our first equation for the transform:

$$f(x) = \frac{1}{2}A_0 + \sum_{n=1}^{\infty}[A_n \cos(nx) + B_n \sin(nx)]$$

Writing this down is no big deal, but the hard part is figuring out these coefficients A_n and B_n. This would be akin to being told the ingredients of coffee and being asked to make a perfect latte: you need the proper proportions of ingredients, not just the ingredients themselves. How do we do this?

Example 4.1: Finding Components of Vectors

Consider a vector $\vec{v} = a\hat{x} + b\hat{y} + c\hat{z}$. How can we find the coefficients a, b, and c? Easy: take the dot product:

$$a = \vec{v}x$$
$$b = \vec{v}y$$
$$c = \vec{v}z$$

We can now apply this to our situation.

As we can see, taking the dot product can give us the components, so why don't we try something similar? This time, instead of taking a dot product, we can integrate. Remember, we hace to pick our "basis vectors" accordingly and normalize the integral. Doing so and putting everything together gives us the full expression with all of the components for the discrete Fourier Transform:

> **Definition 4.1 (Fourier Transform: Discrete Case):** Given periodic function $f(x) = f(x + 2\pi)$ with $x \in [-\pi, \pi]$:
>
> $$f(x) = \frac{1}{2}A_0 + \sum_{n=1}^{\infty} [A_n \cos(nx) + B_n \sin(nx)]$$
>
> $$A_n = \frac{1}{\pi} \int f(x) \cos(nx) dx$$
>
> $$B_n = \frac{1}{\pi} \int f(x) \sin(nx) dx$$

That's it for the discrete Fourier transform. Now, let's write it in terms of exponents.

4.3.2 | Discrete Case: Exponential Form

Having written out the Fourier transform in terms of sin and cos, let's write it out in terms of exponents, since we will be dealing with functions of this form a lot more. Converting everything gives us the following expression:

> **Definition 4.2 (Fourier Transform: Discrete Case with Exponents):** Given the same periodic function:
>
> $$f(x) = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} C_n e^{inx}$$
>
> $$C_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} f(x) e^{-inx} dx$$

It's at this point where we need to introduce a new tool: the *Kronecker delta*.

4.3.3 | Kronecker Delta

For the future, we will define this new function, which looks like this:

> **Definition 4.3 (Kronecker Delta):** Denoted δ_{mn}: $\frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{i(n-m)x} dx = \boxed{\delta_{mn} = \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n \end{cases}}$

This Kronecker delta establishes *orthonormality*, since we want our vectors to be orthonormal. With that, we have finished with discrete Fourier transforms, and we can move on to understand the generalized continuous case.

4.3.4 | Continuous Fourier Transform

In the continuum limit, the sums will become integrals, so our expressions will look like this:

> **Definition 4.4 (Fourier Transform: Continuous Case):** Given the same period function:
>
> $$f(x) = \frac{1}{\sqrt{2\pi}} \int_{0\infty}^{\infty} g(k)e^{ikx}dk$$
>
> Here, $g(k)$ is defined as the **Fourier transform** of $f(x)$.

How do we find the transform $g(k)$? Well, we can then take the *inverse Fourier transform*:

> **Definition 4.5 (Inverse Fourier Transform):** Given $g(k)$:
>
> $$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)e^{-ikx}dx$$
>
> Then, f is defined as the **inverse Fourier transform** of $g(k)$.

These integrals we just saw are commonly referred to as **Fourier integrals**, and we will later learn that these are a special case of a *unitary transform*.

Similarly, we need to understand how the Kronecker delta behaves in the continuum limit.

4.3.5 | Dirac Delta

As was probably surmised, in the continuum limit, the Kronecker delta becomes the much-feared *Dirac delta function*. Let's expand out our integral to see where it comes from:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(x')e^{-ikx'}dx' \right] e^{ikx}dk$$

Manipulating this:

$$g = \int_{-\infty}^{\infty} f(x')\delta(x - x')dx$$

And so, we get our Dirac delta function:

> **Definition 4.6 (Dirac Delta):** Denoted $\delta(x - x')$: $\delta(x - x') = \frac{1}{2\pi} \int_{\infty}^{\infty} e^{ik(x-x')}dx$

Now, this function is very odd and has some pretty weird properties, so let's explore them a bit here.

Since $f(x)$ and $f(x')$ are arbitrary and independent, $\delta(x - x')$ must be 0 if $x \neq x'$, and $\int \delta = 1$ otherwise. These properties need to hold in order for our integral to not fall apart, but these are still difficult to understand. To better comprehend just how a delta function behaves, let's illustrate this with a diagram: [INSERT TIKZ with descriptions] Here, we see that $g(k)$ must be infinitely sharp at exactly one point: k_0. Similarly, this implies that the Fourier transform for a single plane wave will be precisely the δ function. What happens if we add more waves? [INSERT TIKZ] As we can see, the function gains width, and decreases in sharpness. This will lead us nicely into the Uncertainty Principle later on.

This marks the end of the mathematical review. Back to physics!

4.4 ‖ Back to Wave Packets

Recall our 1D wave packet:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{i\frac{p_x x - E(p_x)t}{\hbar}} \phi(p_x) dp_x$$

Now that we have our mathematical tools in place, let's expand this. Suppose $\phi(p_x)$ is a sharp function, but not quite as sharp as a delta function: [INSERT YET ANOTHER TIKZ] As we can see, the added width at the bottom will correspond precisely to increased uncertainty in the measurement of p_x.

4.4.1 │ Stationary Phase Condition

For added simplicity, let $\beta p_x = p_x x - E(p_x)t$. Then, our equation simplifies:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\frac{\beta(p_x)}{\hbar}} \phi(p_x) dp_x$$

Now, let's release the inner mathematician and try to see what is going on. If $\beta(p_x)$ varies, then the exponential component will rapidly oscillate. And, outside p_0, the weight $\phi(p_x)$ goes to 0. The oscillation in the exponent will disappear when β goes to 0. This is referred to as the **stationary phase condition**. Let's try to look for it.

4.4.2 │ Group Velocity

The stationary phase condition, by definition, will be an inflection point, so we need to set the derivative to 0:

$$\left.\frac{d\beta(p_x)}{dp_x}\right|_{p_x=p_0} = 0$$

Computing this gives:

$$x - \left(\frac{d}{dp_x}E(p_x)\right)t = 0 \implies \frac{x}{t} = \left.\frac{dE(p_x)}{dp_x}\right|_{p_x=0}$$

Many will recognize that last expression as the *group velocity*:

> **Definition 4.7 (Group Velocity):** Denoted v_g:
>
> $$v_g = \left.\frac{dE(p_x)}{dp_x}\right|_{p_x=0}$$
>
> Group velocity refers to **how fast the center of the wave packet moves**.

Even though all of the individual waves will most likely be traveling at different speeds, the whole wave packet group will travel at one velocity, which we just derived.

4.4.3 | Phase Velocity

Now, if group velocity is the velocity of the group wave packet, then we also want to find the velocity of any individual wave. To do this, we can find the stationary phase condition for an individual plane wave:

$$e^{i(k_0 x - \omega(k_0)t)}$$

$$\therefore k_0 x - \omega(k_0)t = 0 \qquad\qquad \text{(set phase to 0 for SPC)}$$

$$\therefore \frac{x}{t}\frac{\omega(k_0)}{k_0} = \frac{E(p_0)}{p_0}$$

That last expression is precisely our phase velocity:

> **Definition 4.8 (Phase Velocity):** Denoted v_p:
>
> $$v_p = \frac{\omega(k_0)}{k_0} = \frac{E(p_0)}{p_0}$$
>
> The phase velocity refers to **how fast any individual plane wave is traveling**.

It'll be super crucial to remember the difference between these two different velocity types!

4.5 ‖ Next Time: Dispersion

Now, because of these differences between phase and group velocity, we actually find that, with time, the wave packets will *disperse*. We will build on this next time.

Lecture 5 (9/2)

The fifth lecture of Physics 137A was held on **Friday, September 2**. It covered more on wave packets and built up to the Heisenberg uncertainty principle.

5.1 | Last Time: Wave Description of Matter for Free Particle

From the previous lectures, we want a wavelike description of matter. To accomplish this, we've been playing around with the free particle [INSERT TIKZ] Modeled as a wave, this becomes a wave packet described by the wave function $\Psi(x)$, where $|\Psi(x)|^2$ is the probability density to find the "particle" at x. [INSERT TIKZ] Note that this isn't a plane wave: plane waves go on forever and we want to localize our wave function just where the "particle" is. Despite this, plane waves are just fine for some approximations in the right regions:

> **Example 5.1: Wave Between two Walls**
>
> Here, we have two different functions between two walls. As we can see, for this small approximation, the wave packet and the plane wave are basically the same, so a plane wave (which is much simpler to model) suffices as a decent approximation.

With all of this, we constructed a formula for our wave function:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(i\frac{p_x X - E(p_x)t}{\hbar}\right) \phi(p_x) dp_x$$

As we found, writing out this equation is easy, but the hard part is figuring out the weight ϕ, which we can do with the Fourier transform, a trick which we learned last time.

5.1.1 | Modeling ϕ

As we found, for a single plane wave, $\phi(p_x)$ is a delta function at p_0 [INSERT TIKZ] Adding more plane waves gives us a delta function that spreads out. This is our **first level of approximation**.

5.1.2 | Uncertainties Everywhere

From that model, we can see the following key insight which will become important later on:

> **Insight:** Having no uncertainty in momentum gives no information for position, and having no uncertainty in position gives no information for momentum

This will come up later when we develop the Heisenberg uncertainty principle. Similarly, we had another insight when calculating the phase velocities v_p and group velocity v_g of our wave packet:

> **Insight:** Because each plane wave in the wave packet has a different momentum (and by extension phase velocity, the wave packet will eventually <u>disperse.</u>

With all of these tools, let's continue playing around with the free particle.

5.2 ‖ Playing Around with our Function

Consider some distribution for ϕ which is not quite a delta function: [INSERT TIKZ] Recalling our equations for group velocity, we have

$$v_g = \frac{\partial \omega}{\partial k} = \frac{\partial E}{\partial p}$$

Since we're modeling a particle here, the classical velocity v exactly corresponds to the group velocity v_g:

$$v = v_g = \frac{p_x}{m}$$

So, $\frac{\partial E(p_x)}{\partial p_x} = \frac{p_x}{m}$, which means that

$$E(p_x) = \frac{p_x^2}{2m}$$

This is the exact formula for kinetic energy that we expect in classical mechanics!

5.2.1 | Energy for Plane Wave

In the case of a single plane wave, that means that

$$E(p_x) = \frac{p_0^2}{2m}$$

How can we add more terms to this to get an expression for an actual wave packet that isn't just a delta function? *Taylor expand*!

5.2.2 | Energy for Wave Packet

Taylor expanding our equation gives us:

$$E(p_x) = \frac{p_0^2}{2m} + \frac{p_0}{m}(p_x - p_0) + \frac{(p_x - p_0)^2}{2m}$$

Note that these are the only three terms in the Taylor expansion since the derivative is with respect to p_0. Now, plugging this into our wave function:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(i \frac{p_x x - (E(p_0)t + v_g t(p_x - p_0 + \frac{(p_x - p_0)^2}{2m}t}{\hbar} \right) \phi(p_x) dp_x$$

Note that v_g is simply $\frac{p_0}{m}$. Now, there are a lot of term corrections here, so how can we drop that ugly second-order correction? Well, we can drop it when $\frac{(p_x - p_0)^2 t}{2m\hbar} \ll 1$. This actually gives us something important:

> **Insight:** The second-order correction term gives you information about the dispersion time for the wave packet: for small t, the packet won't disperse, but for a sufficiently large t, the packet will spread out.

Coming back to our wave function:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(i\frac{p_x x - E(p_0)t - v_g t(p_x - p_0)}{\hbar} \right) \phi(p_x) dp_x$$

This is quite a clunky expression. How do we make progress on solving this?

5.2.3 | Adding 1 or Multiplying by 0

One very useful trick that came up a lot in algebra and will make a stunning reappearance here in physics is the trick of **multiplying by** 1 **or adding** 0. In other words, if we add a nice-looking expression that neatly fixes our equation while not actually changing the result, we can have a much easier time. So, let's try adding (and subtracting) $p_0 x$:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(i\frac{p_x x - p_0 x + p_0 x - E(p_0)t - v_g t p_x + v_g t p_0}{\hbar} \right) \phi(p_x) dp_x$$

Now pull out all of the constant terms with respect to dp_x:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p_0 x - E(p_0)t}{\hbar}} \int_{-\infty}^{\infty} \exp\left(i\frac{(p_x - p_0)(x - v_g t)}{\hbar} \right) \phi(p_x) dp_x$$

Notice that we ended up with a plane wave as one of the factors in the front! Similarly, we have thrown all information about our envelope in the exponential! Let's call the new expression in our integral

$$\exp\left(i\frac{(p_x - p_0)(x - v_g t)}{\hbar} \right) \phi(p_x) = \boxed{F(x,t)}$$

Notice what this is:

> **Insight:** The function
>
> $$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(i\frac{p_0 x_0 E(p_0)t}{\hbar} \right) \int_{-\infty}^{\infty} F(x,t) dp_x$$
>
> is a **plane wave modulated by envelope F, moving at speed v_g.**

Calculating the probability density gives us:

$$|\Psi(x,t)|^2 = |F(x,t)|^2$$

The rest has modulus 1, so it disappears.

Now, let's model our distribution. As we can clearly see with the previous graphs for the distribution of ϕ, the distribution of Ψ will look like a <u>Gaussian</u>!

5.3 ‖ Gaussian Wave Packets

As we've discussed before, approximations are key in physics. So, looking at our distribution for ϕ, we see that the best model for it would be that of a Gaussian:[INSERT TIKZ] A Gaussian distribution is then defined as such:

> **Definition 5.1 (Gaussian Distribution):** A distribution of the form
> $$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left[\frac{x-\mu}{\sigma}\right]^2\right)$$

In our case, our ϕ then looks like this:

$$\phi(p_x) = C\exp\left(-\frac{(p_x - p_0)^2}{2(\Delta p_x)^2}\right)$$

So, $|\phi|^2$ falls to $\frac{1}{e}$ for $p_x = p_0 \pm \Delta p_x$.

5.3.1 | Computing Ψ

To proceed, we're going to introduce an important identity from mathematics that we will assume to be given:

> **Theorem 5.1: Integral Identity**
> $$\int_{-\infty}^{\infty} e^{-\alpha u^2} e^{-\beta u} du = \left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}} e^{\frac{\beta^2}{4\alpha}}$$

We could prove this with complex analysis, but we'll just take it to be true. Now, let's go back to $\Phi(x,t)$, but take a snapshot at $t = 0$. Essentially, we are eliminating time dependence here (though on the homework we will re-introduce time dependence to get a full picture of our wave function). With $t = 0$, we can eliminate everything that has a factor of t in it from our expression. This then gives us:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{i\frac{p_x x}{\hbar}}\phi(p_x)dp_x$$

As we can see, in the time-independent case, this is a true Fourier transform of $\phi(p_x)$. As stated before, on the homework, we will put back t to find the full expression for Ψ.

How do we solve this? Just plug it into our identity! Plugging in, we get:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}}C\int \exp\left(i\frac{p_x x}{\hbar}\right)\exp\left(-\frac{(p_x - p_0)^2}{2(\Delta p_x)^2}\right)dp_x = \frac{\pi^{-\frac{1}{4}}}{\sqrt{\alpha}}(\Delta p_x)^{\frac{1}{2}}\exp\left(i\frac{p_0 x}{\hbar}\right)\exp\left(-\frac{(\Delta p_x)^2 x^2}{2\hbar^2}\right)$$

As we can see, this last term is yet another Gaussian! This confirms an important fact:

> **Insight:** The Fourier transform of a Gaussian is also a Gaussian.

5.3.2 | Arriving at the Heisenberg Uncertainty Principle

In other words, this means that $\boxed{\Psi(x) \text{ looks like a Gaussian}}$: [INSERT TIKZ] This time, Ψ falls to $\frac{1}{e}$ of the maximum at $x = \pm \Delta x$. Rewriting this, we have another crucial identity:

> **Theorem 5.2: Heisenberg Uncertainty Principle: Equivalence Case**
>
> $$\Delta x = \frac{\hbar}{\Delta p_x}$$

This is the famed Heisenberg Uncertainty Principle that we were searching for! Notice that for a Gaussian wave packet, it's an equality. This is the *minimum amount of uncertainty*. Every other wave packet will have a bigger uncertainty. We may prove this later, but it's hard. And so, we have that the Gaussian wave packet is the minimum uncertainty state:

> **Definition 5.2 (Minimum Uncertainty State):** The state where uncertainty is minimized (as name suggests).

So, for a non-Gaussian wave function, we can rewrite this principle into a form we all know and love:

> **Theorem 5.3: True Heisenberg Uncertainty Principle**
>
> $$\Delta p_x \Delta x \geq \hbar$$

5.4 ‖ Heisenberg Uncertainty Principle: What does it Mean?

And so, we have calculated the space part of our wave function, and we will calculate the time part on the homework. Now, before we can move on with the rest of quantum mechanics, it is important for us to answer this question completely and correctly: *what does the Heisenberg uncertainty principle mean?* Trying to unpack the inequality gives us this insight into the meaning of this simple expression:

> **Insight:** If you measure $\Psi(x)$ and measure it to an accuracy of $\Delta x = a$, then that means that immediately measuring p will have some uncertainty Δp which must be larger than equal to $\frac{\hbar}{\Delta x}$.

Notice the simultaneity condition for these measurements: the wave function will change with time, so this doesn't necessarily have to hold if one were to wait some amount of time before taking the measurement for p. But, in our case, where we are still dealing with instantaneous measurements, then this will hold.

5.4.1 | Proving the Heisenberg Uncertainty Principle

How did Heisenberg prove his principle? With the help of a special tool: the *Heisenberg microscope*:

Example 5.2: Heisenberg Microscope

The following is a model for the microscope: [INSERT TIKZ] As we can see, we have an emitter passing electrons one at a time through a double slit. As we know from wave mechanics, this will produce an interference pattern on the back panel. However, we want to see inside of this, so we must illuminate the box with some gamma rays of wavelength λ_γ. This will then deflect the path of some of the electrons by some error $\Delta p_{e^{-1}}$ and some angle $\Delta\theta$. Now, if we want to resolve which slit a given electron came from, we must have that

$$\lambda_\gamma < d$$

Now, from our de Broglie relations, $p_\gamma = \frac{h}{\lambda_\gamma}$. Plugging this in, we have the following:

$$\Delta p_{e^{-1}} \approx \frac{h}{\lambda_\gamma} \geq \frac{h}{d}$$
$$\therefore d\Delta p_{e^{-1}} \geq h$$
$$\therefore \Delta\theta \approx \frac{\Delta p_{e^{-1}}}{p_{e^{-1}}} = \frac{h}{pd} = \frac{\lambda_e}{d}$$
$$\therefore L\Delta\theta = \lambda_{e^{-1}}\frac{L}{d}$$

The takeaway here is that trying to measure the momentum loses the interference pattern. And so, this uncertainty principle must hold.

Lecture 6 (9/7)

The sixth lecture of Physics 137A was held on **Wednesday, September 7**. It covered a final review on wave packets and introduced the Schrodinger equation and Hermiticity.

6.1 Last Time: Waves and Wave Packets

What have we learned so far? So far, we have learned that everything is a wave. Why do we say this? We say it, because a wave description of matter is a more accurate and all-encompassing description than our previous particle model. Case in point: the double slit experiment. That experiment seems to definitively confirm that waves are the best description. Now, we had two different types of waves that we could use: plane waves and wave packets.

Plane waves are everywhere, meaning that they are merely an approximation. While they're bad over large intervals, they are pretty decent over certain intervals.

Secondly, wave packets are localized collections of many plane waves. Specifically, we have been considering wave packets that are localized in **space** and **momentum**. Then, the Heisenberg uncertainty principle gave us that

$$\Delta p_x \Delta x \geq \hbar$$

Heisenberg illustrated this principle with the *Heisenberg microscope* thought experiment, explored last time.

6.2 Localization in Energy and Time

We explored localization in space and momentum, but we could also think about a wave packet being localized in **frequency** and **time**. In other words, we can think of it as a snapshot in time.

6.2.1 Another Uncertainty Relation

Now, with what we discovered, we see that, should our wave packet be localized in time and frequency, this means that we need another uncertainty relation for these two quantities. And so, we have the following:

> **Theorem 6.1: Uncertainty Relationship for Time**
>
> $$\Delta E \Delta t \geq \hbar$$
>
> We write it this way, because $E = \hbar \omega$

Now, this relationship does look nice, but how can we confirm that it's actually accurate? Well, let's see why this works.

6.2.2 | Model of the Atom

Now, we're going to illustrate why our uncertainty principle works:

Example 6.1: Bohr Atom

Consider a simplified model of the standard Bohr atom: [INSERT TIKZ] Here, the electron has two possible states: a **ground state** and an **excited state**. The electron can reside in the ground state for as long as it desires, because there is no lower energy state for it to drop down to. However, when it's in the excited state, it will have some decay half-life. What do we mean by this? Well, at any given moment, the electron has some chance of dropping down to the ground state, and averaging out over a long time gives us a general curve which can help us predict after what time we can expect there to be a roughly 50% chance that the electron has decayed into the lower state.

Can we predict when this decay will happen? No, quantum mechanics won't let us. But we can average to get some half-lifetime τ.

Now, if we consider the uncertainty in the energy, we see that the higher energy level will actually have some width to it (since we don't actually know the exact energy), and this uncertainty will be equal to $\Delta E = \frac{\hbar}{\tau}$.

In the ground state, the decay time is essentially infinite, so the uncertainty in the energy is practically negligible. However, in the excited state, we will have some decay time τ_e, with a corresponding uncertainty in the excited energy $\Delta E_e = \frac{\hbar}{\tau_e}$. In other words, the emission will have some width: [INSERT TIKZ]

Now, let's take it a bit further and examine some more details about this uncertainty, specifically with what happens when an electron does jump down to a lower energy state:

Example 6.2: Fluorescent Lights

Consider some fluorescent tube: [INSERT TIKZ] How does it work? Well, the edges are blasted with some electricity, and the gas inside heats up and glows a specific light frequency as a plasma. But why does the whole tube light up when just the edges are excited?

Well, when electrons jump to lower states, they release photons. So, when the atom releases a photon, Newton tells us that the atom must have some recoil in the opposite direction: [INSERT TIKZ] But still, how can the next atom in the chain absorb emitted light coming from a different atom if it ends up recoiling? Because the recoil is small compared to the line width! This means that we get *resonant absorption.*

Notice that this doesn't apply for nuclei or gamma rays, since the line width then becomes small compared to the recoil. There is actually one case when the nuclei can absorb: when the entire lattice recoils. [INSERT TIKZ] When the lattice recoils, the recoil will then be distributed over many particles in the lattice, and so the recoil will once again fall into the limit of being shorter than the line width, hence resonant absorption.

This is actually the famous **Mössbauer Effect**!

With that, we're done with waves and wave packets. Now it's time to move on to the Schrödinger equation.

6.3 ‖ The Schrodinger Equation

Now, we can move on to understanding one of the most important equations in not just quantum mechanics, but in physics as a whole.

6.3.1 │ How do We Find Wave Functions?

We have good expressions for the wave function, but our biggest problem right now is actually finding this wave function. We've been told what it is and what it looks like, but we can't actually find it for some given parameters. We need something akin to Newton's Second Law of Motion, but just for waves.

6.3.2 │ Equations for Wave-Equation for Quantum Mechanics

This wave equation must satisfy a few important conditions:

- Linear (permits superposition): waves can be added
- Should reproduce ("agree" with) classical physics
- Boundary conditions

To review what these mean, we firstly want to be able to add waves with our equation, which means it must be linear. Secondly, we don't want any previously-established laws of physics to break with this new equation, so the other laws must still be satisfied. Finally, our equation must satisfy some important boundary conditions. Let's look at those a bit more in-depth here.

The classical wave equation has two derivatives in space and two derivatives in time. This means that we must impose two boundary conditions for us to get some kind of expression. However, this is bad news for us, because classically, we only need one boundary condition in order to invoke Newton's Second Law. So, our new wave equation should only have *one time derivative to satisfy causality.*

Let's now construct this wave equation!

6.3.3 │ Schrödinger Equation: the 1D Free Particle Case

Firstly, let's consider the system we've been trying to understand for a while: a free particle in one dimension. [INSERT TIKZ] So, this system is then described by a wave function

$$\Psi(x,t) = Ae^{i\frac{p_x x - Et}{\hbar}}$$

Now, recall ten that we can write energy as

$$E = \frac{p_x^2}{2m}$$

Substituting some expressions into the terms gives us our dispersion relation:

$$\boxed{\omega = \frac{\hbar k^2}{2m}}$$

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Now, remember operators? We had the following note before:

$$\frac{\partial \Psi(x,t)}{\partial t} = A(-i\omega)e^{i(kx-\omega t)} = -i\omega\Psi = -\frac{i}{\hbar}E\Psi$$

Taking two derivatives in space, we similarly get:

$$\frac{\partial^2}{\partial x^2}\Psi(x,t) = -k^2 A e^{i(kx-\omega t)} = -\frac{p_x^2}{\hbar}\Psi = -\frac{2Em}{\hbar^2}\Psi$$

We have two Es, so let's group the equations together and solve to get this very crucial equation:

Theorem 6.2: Schrödinger Equation for Free Particle in 1 Dimension

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)$$

Now, if we think of those original terms in front of the Ψs as operators, we have our momentum and energy operators as before:

$$\hat{E} = i\hbar\frac{\partial}{\partial t}, \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

But, this is only for a free particle in one dimension, so we have to add in potential energy and the other dimensions. More correctly, we need to take into account a force that can be derived from a potential.

6.3.4 | Correcting the Equation

What types of forces can be derived from a potential? **Conservative forces**! They then are described as the gradient of some potential:

Definition 6.1 (Conservative Force): Recalling from mechanics, this refers to a force that can be derived from a potential, which makes work done independent of a path.

So, consider some conservative force:

$$\vec{F}(\vec{r},t) = -\vec{\nabla}V(\vec{r},t)$$

Here, V is our potential. Writing this out in terms of operators, we have:

Definition 6.2 (Potential Operator):

$$\hat{V}(\vec{r},t)\Psi(\vec{r},t) = V(\vec{r},t)\Psi(\vec{r},t)$$

Here, $\hat{V}$ is our **potential operator**.

Throwing this all together, we get:

Theorem 6.3: Schrödinger Equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r},t)\right]\Psi(\vec{r},t)$$

This is exactly the equation that Erwin Schrödinger wrote down in 1926. This equation is super important, and you should remember it for the rest of your life.

> **Insight:** Notice that the first term in the brackets of the equation corresponds exactly to the **kinetic energy** component, whilst the second term in the bracket sum is the **potential**. Finally, the entire expression in the bracket is exactly the **Hamiltonian Operator** $\hat{H}$.

> **Definition 6.3 (Hamiltonian Operator):** Denoted $\hat{H}$: $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r}, t)$

In other words, at its most basic, the Schrödinger equation is simply an equation of <u>energy conservation</u>. Let's now talk about some properties of these operators.

6.4 ‖ Properties of Ψ, $\hat{H}$

Firstly, we have our most important property: probability conservation:

$$\int_{\text{All Space}} |\Psi(\vec{r}, t)|^2 d\vec{r} = 1$$

Now, let's derive *hermiticity*. Taking the derivative here gives:

$$\frac{\partial}{\partial t} \int_{\text{All Space}} |\Psi(\vec{r}, t)|^2 d\vec{r} = 0$$

An important thing to remember here:

> **Insight:** Never listen to mathematicians! You can move derivatives anywhere! Everything is smooth. If it weren't, life would be discontinuous.

Notice that $|\Psi|^2$ is actually a different way of writing $\Psi^*\Psi$. So, throwing that in gives:

$$\frac{\partial}{\partial t} \int_{\text{All Space}} |\Psi|^2 d\vec{r} = \int_{\text{All Space}} \Psi^* \left(\frac{\partial \Psi}{\partial t}\right) + \int_{\text{All Space}} \left(\frac{\partial \Psi^*}{\partial t}\right) \Psi d\vec{r}$$

Now, let's substitute in our operators:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \hat{H}\Psi(\vec{r}, t)$$

$$-i\hbar \frac{\partial}{\partial t} \Psi^*(\vec{r}, t) = \left[\hat{H}\Psi(\vec{r}, t)\right]^*$$

So, throwing this all in gives:

$$\int_{\text{All Space}} \Psi^* \left(\frac{\partial \Psi}{\partial t}\right) + \int_{\text{All Space}} \left(\frac{\partial \Psi^*}{\partial t}\right) \Psi d\vec{r} = \frac{1}{i\hbar} \int_{\text{All Space}} \left[\Psi^*(\hat{H}\Psi) - (\hat{H}\Psi)^*\Psi\right] d\vec{r} = 0$$

$$\therefore \int_{\text{All Space}} \Psi^*(\hat{H}\Psi) d\vec{r} = \int_{\text{All Space}} (\hat{H}\Psi)^* \Psi d\vec{r} = \int_{\text{All Space}} \Psi^* \hat{H}^* \Psi d\vec{r}$$

Since this integral we've been calculating is arbitrary for any surface, we have then:

> **Theorem 6.4: Hermiticity**
>
> $$\hat{H} = \hat{H}^*$$

Here, $\hat{H}$ has a special name:

> **Definition 6.4 (Hermitian Operator):** Denoted $\hat{H}$.

And so, we have derived Hermiticity. This gives us this important fact:

> **Insight:** E must be real number always.

We will continue with this and with expectation values next time.

Lecture 7 (9/9)

The seventh lecture of Physics 137A was held on **Friday, September 9**. It covered more on the **Schrödinger equation** and introduced **Hermiticity and the commutator**.

7.1 ‖ Last Time: Schrödinger Equation Describes Conservation of Energy

Last lecture, we tried to better understand the Schrödinger equation by modeling it as an equation that, like Newton's Second law with conservation of momentum, basically describes the conservation of energy for a wave function. We noted that total energy can be written as the sum of some kinetic energy KE and some potential energy PE. These energy components were then defined by their separate operators, where total energy was described by the *Hamiltonian operator* $\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$, kinetic energy was described by the *momentum operator* $\frac{\hat{p}^2}{2m}\Psi = \left(-i\hbar\frac{\partial}{\partial x}\right)^2\Psi$, and finally the potential energy was described by a *potential operator* $\hat{V}\Psi$. So, in the end, the equation became:

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}(x)\right]\Psi = E\Psi$$

Notice that the Hamiltonian and momentum operators are unique and will remain the same for all cases of the wave function Ψ. However, the potential operator $\hat{V}$ is not unique, so we will spend roughly a third of the course figuring out different cases for this operator.

We also started on Hermiticity:

$$\int |\Psi(\vec{r},t)|^2 d\vec{r} = 1$$

$$\therefore \frac{\partial}{\partial t}\int |\Psi(\vec{r},t)|^2 d\vec{r} = 0 = \int \Psi^*\left(\frac{\partial\Psi}{\partial t}\right) + \left(\frac{\partial\Psi^*}{\partial t}\right)\Psi d\vec{r}$$

We need to generalize the * here, since it won't always be just the complex conjugate. But we need something new if we want to substitute Schrödinger into this. So, our generalization (from linear algebra) becomes the **adjoint**. For scalars, it will remain the complex conjugate, but for matrices, it will be the conjugate transpose. We will, typically, use † to denote the adjoing (a "dagger").

7.2 ‖ Substituting in Schrödinger

Now, substituting in the Schrödinger equation:

$$\frac{1}{i\hbar}\int\left[\Psi^*(\hat{H}\Psi) - (\hat{H}\Psi)^*\Psi\right]d\vec{r} \rightarrow \boxed{\hat{H} = \hat{H}^*} \tag{7.1}$$

This gives us the Hermitian operator (the adjoing is equal to the normal).

CHAPTER 7. LECTURE 7 (9/9)

> **Theorem 7.1: Hermitian Operator Properties**
>
> The Hermitian operator is associated with two things:
> - Real eigenvalues
> - Observables (needs to be a measurable quantity)

Now, let's do something with equation 7.1. Substitute the spatial part of the Schrödinger equation into equation 7.1 (assume a real-valued $\hat{V}$):

$$\cdots = \frac{i\hbar}{2m} \int \left[\Psi^*(\nabla^2 \Psi) - (\nabla^2 \Psi^*)\Psi \right] d\vec{r} = \cdots$$

Now, use the vector identity for the Laplacian: $\nabla^2 x = \vec{\nabla} \cdot \vec{\nabla}(x)$:

$$\cdots = \frac{i\hbar}{2m} \int \vec{\nabla} \cdot \left[\Psi^*(\vec{\nabla} \Psi) - (na\vec{b}la\Psi)^*\Psi \right] d\vec{r} = \cdots$$

Now, call the integrand $\vec{j}$:

$$\cdots = - \int \vec{\nabla} \cdot \vec{j} d\vec{r}$$

Use Stokes' Theorem:

$$\frac{\partial}{\partial t} \int |\Psi(\vec{r}, t)|^2 d\vec{r} = - \int \vec{j} \cdot d\vec{s}$$

Here, s refers to our surface over which we're integrating. Now, if integrals are equal, the integrands should be equal. So, we can invoke an important identity from E&M:

$$\boxed{\frac{\partial}{\partial t} p(\vec{r}, t) + \vec{\nabla} \cdot \vec{j}(\vec{r}, t) = 0}$$

> **Insight:** If we examine this qualitatively, $\vec{\nabla} \cdot \vec{j}$ tells you what the "flow" of $\Psi^*\Psi$ is at any given point.

And so, we can give $\vec{j}$ a new definition:

> **Definition 7.1 (Probability Current):** Denoted $\vec{j}$; describes flowing probability for a wave function.

Notice that if Ψ were real-valued, then the flow $\vec{\nabla} \cdot \vec{j}$ would always be 0. That would be quite boring.

This completes the introduction to the Schrödinger equation. Now, how do we get rid of Ψ to calculate things? For this, we need to introduce the <u>expectation value</u>.

7.3 | Expectation Value

Firstly, let's consider classical mechanics.

7.3.1 | Classical Mechanics Version

In classical mechanics, the <u>mean value</u> is equal to

$$\langle r \rangle = \int r P(\vec{r}, t) d\vec{r}$$

Here, $P(\vec{r}, t)$ refers to probability. This is the classical version, so let's now translate this into the quantum version.

7.3.2 | Quantum Version

In quantum mechanics, we have $P = |\Psi|^2$. So...

> **Definition 7.2 (Expectation Value):** For some wave function Ψ, we define the **expectation value** of an operator $\hat{r}$ as
> $$\langle \hat{r} \rangle = \int \Psi^* \hat{r} \Psi \, d\hat{r}$$

Here, we substitute the operator $\hat{r}$, since $\hat{r}\Psi = \vec{r}\Psi$. So, in disguise, before, we were really calculating the expectation value of the *identity operator*:

$$\Psi^* \Psi = \Psi^* 1\!\!1 \Psi$$

Now, let's calculate some expectation values for our operators:

> **Theorem 7.2: Expectation Values for Energy and Momentum Operators**
>
> $$\left\langle \hat{V}(\vec{r}, t) \right\rangle = \int \Psi^* \hat{V} \Psi \, d\vec{r}$$
> $$\boxed{\langle \hat{p} \rangle} = \int \Psi^* \hat{p} \Psi \, d\vec{r} = \boxed{-i\hbar \int \Psi^*(\vec{r}, t) \vec{\nabla} \Psi(\vec{r}, t) d\vec{r}}$$

A quick aside for homework assignment and exams:

> **Insight:** Always write your thoughts down first; you get partial credit points just for that, and it's usually not too difficult to figure out the rest of the solution from there!

7.4 ‖ How to Work with Hermitian Operators

Is the momentum operator hermitian? Yes. But...

> **Insight:** $\hat{p}$ is Hermitian, but $\hat{p} = -i\hbar\vec{\nabla}$; it's important to remember that we need to multiply by Ψ to see this hermiticity.

What about the product of Hermitian operators? Is that Hermitian? **No**. These operator can't be interchanged, since operators usually *do not commute*. For example, $\hat{x}\hat{p}_x$ is not Hermitian (check other lecture notes for full derivation). For another example, let's consider something from classical physics: translation and rotation. This clearly isn't Hermitian, since first rotating and then moving will send you to a different place than first moving and then rotating: these don't commute.

7.4.1 | Enter the Commutator

How do we figure out if they commute? For this, we simply need to calculate the commutator:

> **Definition 7.3 (Commutator):** Denoted $[\vec{A}, \vec{B}]$: $[\vec{A}, \vec{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

We literally just compute these two separate operator combinations and subtract them. If the commutator evaluates to 0, then $\hat{A}$, $\hat{B}$ commute. If the commutator evaluates to anything else, then $\hat{A}$, $\hat{B}$ don't commute.

> **Insight:** What does it mean to commute? It means that the properties we're measuring *don't correlate.*

In other words, things that commute can be measured simultaneously, since measuring one thing will not affect the result of the other measurement. By contrast, things that don't commute can't be measured simultaneously, since our measurements will affect each other.

Going back to our above case, $[\hat{x}, \hat{p}_x] \neq 0$, which we can confirm by calculating:

$$[\hat{x}, \hat{p})_x] = \hat{x}\hat{p}_x - \hat{p}_x\hat{x}$$

Both sides of the equation are operators, so let's throw in Ψ on both sides:

$$[x, p_x]\Psi = \left[x\left(-i\hbar\frac{\partial}{\partial x} \right) + i\hbar\left(\frac{\partial}{\partial x} \right)x \right]\Psi = \qquad \text{(critical to get the signs right)}$$

$$= -i\hbar x\frac{\partial\Psi}{\partial x} + i\hbar\left[\Psi + \frac{\partial\Psi}{\partial x} \right] = i\hbar\Psi \qquad \text{(distribute)}$$

That last equation can trip a lot of people up: don't forget the product rule!

So, $\boxed{[\hat{x}, \hat{p}_x] = i\hbar \neq 0}$. Hence, this product is not Hermitian.

> **Insight:** $i\hbar$ is a super important quantity that will pop up a lot!

7.4.2 | Significance of These Operators

Confirming this fact is great, but what is the significance of these non-commutative operators? Well, consider the *harmonic oscillator*. SHO has kinetic energy KE and potential energy PE, so you can always write a system in terms of some harmonic oscillator. So, these operators will be used to describe everything going forward, since we can define everything in terms of the commutator.

> **Insight:** So, given a pair of operators, always start by calculating their commutator.

More on this next week!

Lecture 8 (9/12)

The eighth lecture of Physics 137A was held on **Monday, September 12**. It covered **solving the Schrödinger equation and eigenfunctions**, as well as reviewing the expectation value.

8.1 Last Time: Waves are Complex and The Commutator

Last week, we established that waves must be inherently complex (otherwise the gradient of the probability current would simply always be 0, which would make for a boring universe). We also introduced the *commutator* to determine whether or not operators commute and, by extension, if their product is Hermitian. This essentially, qualitatively, boils down to understanding what operations are independent of each other and hence can be measured simultaneously.

8.1.1 This Week: Eigenfunctions and Solving Schrödinger

With this in mind, we want to now generalize the concept of Hermitian operators through *eigenfunctions*.

8.2 Solving Schrödinger

Now, we can proceed with solving the Schrödinger equation. Recalling from last time, we have the following equation that we want to solve:

> **Definition 8.1 (Time-Dependent Schrödinger Equation):** Time-dependent case of the Schrödinger equation:
> $$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \left[\underbrace{-\frac{\hbar^2}{2m}\nabla^2}_{KE} + \underbrace{\hat{V}(\vec{r})}_{PE}\right]\Psi(\vec{r},t)$$

We now want the general solution to this equation, so let's do it!

8.2.1 Stationary States

To solve for specific states, we're essentially just looking for *separate/stable/eigen solutions* (all different ways of saying the same thing). We will refer to these as **stationary states**:

> **Definition 8.2 (Stationary State):** State solution of the form:
>
> $$\Psi(\vec{r}, t) = f(t)\Psi(\vec{r})$$
>
> Essentially, one that looks like a standing wave.

So, we have the ansatz solution and the equation. What do we do? As always, <u>substitute</u>!

$$i\hbar\Psi(\vec{r})\frac{d}{dt}f(t) = \left[-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + \hat{V}(\hat{r})\Psi(\vec{r})\right] * f(t)$$

Notice here that we have the full derivative, so we will not use the partial derivative notation. Now, we need to <u>separate the variables</u>. Divide by $f(t)\Psi(\vec{r})$ to compartmentalize:

$$i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = \frac{1}{\Psi(\vec{r})}\left[-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + \hat{V}(\vec{r})\Psi(\vec{r})\right]$$

In the separable case, these need to be independent, which means that $\boxed{\hat{V} \text{ has to be independent}}$. Time-dependent potential operators exist, but they are much harder to deal with, so we'll largely avoid them for now.

8.2.2 | Time-Independent Schrödinger Equation

Now that we have this, *set both sides equal to E*, and solve piece-by-piece. Starting with the time piece first:

$$i\hbar\frac{d}{dt}f(t) = Ef(t) \implies f(t) = \boxed{Ce^{-i\frac{Et}{\hbar}}}$$

This solution looks like a plane wave! Notice that $f(t)$ will then never change for our wave functions, since this is a simple derivative independent of everything else. Now, the space part:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r})\right]\Psi(\vec{r}) = E\Psi(\vec{r})$$

This expression is completely time-independent, and we actually give it its own name:

> **Definition 8.3 (Time-Independent Schrödinger Equation):** Time-independent case of the Schrödinger equation:
>
> $$\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r})\right]\Psi(\vec{r}) = E\Psi(\vec{r})$$

Notice one big problem: <u>we can't solve this</u>. Why not? <u>We don't know $\hat{V}$</u>! If $\hat{V}$ were 0, then we have our *free particle* case (which we have already solved), but we want the general case now.

8.2.3 | Eigenfunctions and Eigenstates

Now, we need to quickly define what we mean by eigenfunction, since this term has been coming up a lot recently:

> **Definition 8.4 (Eigenfunction):** Similar to eigenvectors, an **eigenfunction** is one that is preserved under a corresponding **eigenvalue** like so:
>
> $$\hat{H}\Psi_E = E\Psi_E$$
>
> Here, Ψ_E deotes the eigenfunction with eigenvalue E.

In the definition, we wrote down the eigenfunctions of the Hamiltonian operator, but it applies in general for eigenfunctions. Moving on, the eigen functions of the Hamiltonian operator $\hat{H}$ are essentially the **stationary states with time dependence** $e^{-i\frac{Et}{\hbar}}$.

But how do we solve for the eigenfunction Ψ_E? We solve the Time-Independent Schrödinger Equation!

> **Insight:** As a note, this is where quantization will come in, since we need speific pairs Ψ, E, meaning that only certain energy states will be allowed, hence energy is quantized.

8.2.4 | Solving Time-Independent Schrödinger Equation

We want $\left\langle \hat{H} \right\rangle$, which we began to do last week. Essentially, this means that we need to weigh with the probability over all space. To calculate mean value of something, we weight it with the probability of finding it at a particular point, and then integrate over all space. Places with smaller probabilities have little-to-no impact, while places with higher probabilities comprise most of the average value calculation.

> **Insight:** Also, remember the following: the time derivative gives **energy**, the space derivative gives **momentum**, and $\Psi^*\Psi$ gives **probability**.

With this, we have:

$$\left\langle \hat{H} \right\rangle = \int \Psi^*(\hat{H})\Psi d\vec{r}$$

Bu, there's a problem with this: we need to specify Ψ, since our wave function will change for different cases. Let's try Ψ for a stationary state:

$$\left\langle \hat{H} \right\rangle_{\Psi_E} = \int \Psi_E^* E\Psi_E d\vec{r} = E \int \Psi_E^*\Psi_E d\vec{r} = \boxed{E} \checkmark$$

We will denote which Ψ we are interested in for the mean calculation with the subscript shown above. Notice what this has just told us:

> **Insight:** For an eigenfunction, the average value is just the energy!

So, to find all possible values of (stable) energies in a system, we simply need to calculate all possible eigenfunctions Ψ.

So, let's quickly calculate this probability density:

$$P(\vec{r}, t) = |\Psi_E(\vec{r}, t)|^2 = |f(t)\Psi_E(\vec{r})|^2 = |\Psi_E(\vec{r})|^2$$

Why can we write this? Well, $f(t)$ will cancel out with its conjugate. So, we're left with the following extremely important insight:

> **Insight:** Probability density is independent of time!

This is extremely important and something we will use a lot going forward.

8.3 Solving Quantum Problems

Now, let's write a prescription for describing a quantum system.

1. **Specify $\hat{V}(\vec{r})$.**

   This happens in two ways:

   a) It's given to us in the problem, or

   b) You have to model the system and then write the corresponding $\hat{V}$.

   We will spend a bunch of time figuring out different cases for the latter option.

2. **Solve Time-Independent Schrödinger Equation**

   This gives us $\Psi_E(\vec{r})$, and the corresponding E (in other words, eigenfunctions and their corresponding eigenvalues).

3. **Throw in Time Dependence:** $\Psi_E(\vec{r}, t) = \Psi_E(\vec{r})e^{-i\frac{Et}{\hbar}}$.

   But, this is the stationary solution; a general solution will be a **combination of all possible ones**. In other words, we're finding the *basis vectors* through these eigenfunctions, meaning that the general solution will be a linear combination of all of these basis vectors.

4. **General Solutions Are a Combination of $\Psi_E(\vec{r}, t)$** (eigenfunctions).

   > **Insight:** Notice: if we consider eigenfunctions as our basis vectors, they have to be <u>orthonormal</u>

And so, we postulate the following:

> **Insight:** E, Ψ_E found by solving the Schrödinger Equation gives us all possible energies E.

Let's confirm this with some math.

8.3.1 Math Time

Considering this, we then write this expression:

$$\Psi(\vec{r}, t) = \sum_E C_E(t)\Psi_E(\vec{r})$$

> **Insight:** This will be pretty much all of the rest of 137A: finding all eigenfunctions and corresponding energies E, then summing over all E for varying potentials $\hat{V}$!

Now, how do we find the coefficients? From last week, we saw that we use the *inner product*.

> **Definition 8.5 (Inner Product):** Generalization of the dot product. **Inner products** are operations satisfying the following properties:
> - **Positivity**: $\langle x, y \rangle \geq 0$
> - **Definiteness**: $\langle x, y \rangle = 0 \implies x = y$
> - **Additivity in First Slot**: $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$
> - **Homogenaity in First Slot**: $\langle \alpha x, y \rangle = \alpha \langle x, y \rangle$
> - **Conjugate Symmetry**: $\langle x, y \rangle = \overline{\langle y, x \rangle}$
>
> Most will remember this from linear algebra. In normal Euclidean space, vectors have the traditional *dot product.*

So, in our case, taking the inner product means multiplying by some $\Psi_{E'}$ (important to use a different index!) and integrating:

$$\int \Psi_{E'}^*(\vec{r})\Psi(\vec{r},t)d\vec{r} = \sum_E C_E \int \Psi_E^* \vec{r} \Psi_E(\vec{r})d\vec{r}$$

Notice that the integrand on the right is simply the Kronecker Delta, since thse are orthonormal. This, then, will only not vanish when $E' = E$, in which case the integral evaluates to 1. Hence, we get:

$$\sum_E C_E \int \Psi^* E(\vec{r})\Psi_E(\vec{r})d\vec{r} = C_{E'}(t)$$

And so, we have our general solution:

$$\Psi(\vec{r},t) = \sum_E \underbrace{C_E(t=0)}_{\text{Orientation of vector @ } t=0} \Psi_E(\vec{r})e^{-i\frac{Et}{\hbar}}$$

$$C_E = \int \Psi_E^*(\vec{r})\Psi(\vec{r},t=0)d\vec{r}$$

Notice that this implies that

$$\boxed{\sum_E |C_E|^2 = 1}$$

This makes perfect intuitive sense, since it has to be somewhere at some energy.

8.3.2 | Final Trick: Expectation Value Calculation

For our final trick, we will do the expectation value calculation for the general state:

$$\left\langle \hat{H} \right\rangle_\Psi = \int \Psi^*(\vec{r},t)\hat{H}\Psi(\vec{r},t)d\vec{r}$$

Always remember to specify the wave function for which you are calculating the average value. Notice, now, that we don't know Ψ, but remember that we can act $\hat{H}$ on some specific Ψ_E. Since we can write Ψ as a linear combination of a bunch of Ψ_E's, let's consider Ψ as a sum of such Ψ_E's:

$$\left\langle \hat{H} \right\rangle_\Psi = \int \Psi^*(\vec{r},t)\hat{H} \underbrace{\Psi(\vec{r},t)}_{\sum_E C_E e^{-i\frac{Et}{\hbar}}\Psi_E(\vec{r})}$$

Now, see how we've rewritten the second part of our integral. Notice that we can do the same for the conjugate, but these are <u>independent</u>, so we can't use the same index!

$$\therefore \left\langle \hat{H} \right\rangle_\Psi = \int \underbrace{\Psi^*(\vec{r},t)}_{\sum_{E'} C_{E'}^* e^{i\frac{E't}{\hbar}}} \hat{H} \underbrace{\Psi(\vec{r},t)}_{\sum_E C_E e^{-i\frac{Et}{\hbar}}\Psi_E(\vec{r})}$$

And so, putting these together, we have:

$$\left\langle \hat{H} \right\rangle_\Psi = \sum_E \sum_{E'} C_{E'}^* C_E e^{-i\frac{(E-E')t}{\hbar}} E \underbrace{\int \Psi_{E'}^*(\vec{r})\Psi_E(\vec{r})d\vec{r}}_{\text{Kronecker Delta again!}}$$

Once again, this doesn't vanish only when $E = E'$, so we have:

> **Theorem 8.1: Expectation Value of Hamiltonian Operator**
>
> $$\boxed{\left\langle \hat{H} \right\rangle_\Psi = \sum_E |C_E|^2 E}$$

This is super important, so we've enclosed it in a theorem.

8.4 | That's All We Need (Mostly)!

With this, we have learned basically all of the quantum mechanics we need for the next month. We will spend that next month calculating these expectation values, figuring out eigenfunctions, summing over these eigenfunctions, and solving the time-independent and time-dependent Schrödinger Equations for varying $\hat{V}$s. We will start on these generalized solutions for $\hat{V}$ on Wednesday.

Lecture 9 (9/14)

The ninth lecture of Physics 137A was held on **Wednesday, September 14**. It explored the solutions to the Schrödinger equation given some potential $V(x)$.

9.1 ‖ Last time: Solutions to the Schrodinger Equation

Last time, we talked about how we should interpret solutions to the Schrödinger equation, and specifically we derived how energy eigenstates evolve in time:

$$\psi_E(\vec{r}, t) = \psi_E(\vec{r}) e^{-iEt/\hbar}$$

where ψ_E satisfies the equation $\hat{H}\psi_E = E\psi_E$. Further, we also now know that a general state can be written as a superposition of eigenstates:

$$\psi(\vec{r}, t) = \sum c_E \psi_E(\vec{r}) e^{-iEt/\hbar}$$

Here, we use the generalized position vector $\vec{r}$: the Schrödinger equation is valid for all space (since we're not limited to 1D quantum mechanics in the most general case), as we'll see later.

9.2 ‖ Different Types of Energies

Now let's look at how $V(x)$ changes the nature of our solutions. Consider the following potential

[insert tikz here]

Now recall the 1D Schrödinger equation:

$$\left[-\frac{\hbar}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi_E(X) = E\psi_E(x)$$

There are four different cases that we need to explore here for a given energy E:

- Case 1: $E < V_{min}$
- Case 2: $E > V_{min}$, $E < V_-$
- Case 3: $E > V_-$, $E < V_+$
- Case 4: $E > V_+$

Case 1

We rearrange the Schrödinger equation to see this a little better:

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar}\left(V(x) - E\right)\psi(x)$$

And so here, we get that $V(x) - E > 0$, and so therefore $\frac{d^2\psi}{dx^2}$ and $\psi(x)$ now have the same sign! But this means that there aren't any normalized functions that have that property (as they are exponentials), so we conclude that no such solutions can exist.

Case 2

We know from the previous case that any time $V > E$, then we get exponential solutions. This is still true in our second case, except there are now regions where $E > V$. Here, as we've seen in the case of the free particle, will generate oscillatory solutions. To combine these two together, we enforce the condition that ψ must be a continuous quantity for all x.

> **Insight:** This restriction of continuity actually means that only specific functions solve the Schrödinger equation, and these functions correspond to specific energies (we'll see this later). This is the *fundamental* reason why energy levels are quantized!

Lecture 10 (9/16)

The fifth lecture of Physics 137A was held on **Friday, September 16**. It covered

Lecture 11 (9/19)

The fifth lecture of Physics 137A was held on **Monday, September 19**. It covered

Lecture 12 (9/21)

The fifth lecture of Physics 137A was held on **Wednesday, September 21**. It covered

Lecture 13 (9/23)

The fifth lecture of Physics 137A was held on **Friday, September 23**. It covered

Lecture 14 (9/26)

The fifth lecture of Physics 137A was held on **Monday, September 26**. It covered

Lecture 15 (9/28)

The fifth lecture of Physics 137A was held on **Wednesday, September 28**. It covered

Lecture 16 - Guest Lecture (9/30)

The fifth lecture of Physics 137A was held on **Friday, September 30**. It covered

Lecture 17 (10/3)

The fifth lecture of Physics 137A was held on **Monday, October 3**. It covered

Lecture 18 (10/5)

The fifth lecture of Physics 137A was held on **Wednesday, October 5**. It covered

Lecture 19 (10/7)

The fifth lecture of Physics 137A was held on **Friday, October 7**. It covered

Lecture 20 (10/10)

The fifth lecture of Physics 137A was held on **Monday, October 10**. It covered

Lecture 21 (10/12)

The fifth lecture of Physics 137A was held on **Wednesday, October 12**. It covered

Lecture 22 (10/14)

The fifth lecture of Physics 137A was held on **Friday, October 14**. It covered

PART II

POST-MIDTERM

Lecture 23 (10/21)

The fifth lecture of Physics 137A was held on **Friday, October 21**. It covered

Lecture 24 (10/24)

The fifth lecture of Physics 137A was held on **Monday, October 24**. It covered

Lecture 25 (10/26)

The fifth lecture of Physics 137A was held on **Wednesday, October 26**. It covered

Lecture 26 (10/28)

The fifth lecture of Physics 137A was held on **Friday, October 28**. It covered

Lecture 27 (10/31)

The fifth lecture of Physics 137A was held on **Monday, October 31**. It covered

Lecture 28 - Guest Lecture (11/2)

The fifth lecture of Physics 137A was held on **Wednesday, November 2**. It covered

Lecture 29 (11/4)

The fifth lecture of Physics 137A was held on **Friday, November 4**. It covered

Lecture 30 (11/7)

The fifth lecture of Physics 137A was held on **Monday, November 7**. It covered

Lecture 31 (11/9)

The fifth lecture of Physics 137A was held on **Wednesday, November 9**. It covered

Lecture 32 (11/14)

The fifth lecture of Physics 137A was held on **Friday, November 14**. It covered

Lecture 33 (11/16)

The fifth lecture of Physics 137A was held on **Wednesday, November 16**. It covered

Lecture 34 (11/18)

The fifth lecture of Physics 137A was held on **Friday, November 18**. It covered

Lecture 35 (11/21)

The fifth lecture of Physics 137A was held on **Monday, November 21**. It covered

Lecture 36 - Guest Lecture (11/28)

The fifth lecture of Physics 137A was held on **Monday, November 28**. It covered

Lecture 37 - Guest Lecture (11/30)

The fifth lecture of Physics 137A was held on **Wednesday, November 30**. It covered

Lecture 38 (12/2)

The fifth lecture of Physics 137A was held on **Friday, December 2**. It covered

PART III

MISCELLANEOUS

Closing Remarks