

# Modern Physics (PHY 3305) Lecture Notes

## Waves and Uncertainty (Ch. 4.4-4.5, 5.1-5.2)

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### Review

tags:  
lecture

- We moved to a description of nature that focuses on the wave nature of matter
  - We know that the *relevant dimensions* of a specific problem will lead to more wave-like or particle-like results
- The wave nature of matter is described by the Shroedinger Wave Equation (SWE) that, like Newton's Laws or Conservation of Energy, is motivated by experimental results and is not derivable from first principles.
- We discussed complex numbers and functions, in preparation for handling the complex wave function allowed by the SWE.
- We discussed the meaning of the wave function - that it represents PROBABILITY PER UNIT LENGTH (or VOLUME in 3-dimensions), referred to as PROBABILITY DENSITY.

### Let us begin with a question about atoms

QUESTION: do atoms radiate energy all the time?

DISCUSSION: why not? After all, classically we think of the electron as going around the atom like a planet orbiting a sun. If its orbiting, its moving and being bent in that orbit by the Coulomb force. There is a place where the charge is, and where it is not - the charge density is changing and thus the electron should be radiating energy like crazy! That's what EM predicts for such motion.

DISCUSSION: what did you learn about the atom in your homework? Can it just be treated classically?

Answer: no. Today, we'll begin to see what happens when we think of the electron not as being in classical orbit around the nucleus, but being BOUND to the nucleus.

We'll begin first by picking up our discussion where we left off and then talking about uncertainty. Then we'll jump into what the SWE teaches us about BOUND STATES.

## The Schroedinger Wave Equation

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

QUESTION: what, exactly, is this equation comparing for the wave function?

DISCUSSION:

- You have a second-derivative with respect to space. This is telling us about the CURVATURE of the wave function in space.
- You have a first-derivative of the wave function with respect to time. This is telling us about the change of the wave function in time.
- So the SWE relates spatial curvature to temporal variation.

## Solutions to the Schroedinger Equation: Plane Waves

The whole game of using the Schroedinger equation is the same as using Newton's laws of motion, or relativity:

- First, identify the players in the system
- Second, identify constraints on the systems - are there boundaries to the problem, are there forces, etc?
- Third, convert the above into math and identify a solution to the equation that satisfies all known constraints
- Fourth, with the solution in hand, compute amplitudes-squared to solve for the measurables in the problem

The first solution we will explore is the wave function describing free particles - particles in constant motion free of external forces. The wave function that describes this situation is:

$$\Psi(x, t) = Ae^{i(kx - \omega t)}$$

where  $A$  is a constant. If we insert this into the Schroedinger Wave Equation, we obtain the following equation:

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

The functional dependence on space and time cancels out, and we conclude that this function obeys Schroedinger's equation for all space and time, provided that  $k$  and  $\omega$  are related as above.

So how do plane waves relate to particles? What happens if we insert:

$$p = \hbar k$$

and

$$E = \hbar\omega$$

We find:

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

Well, if we are describing a classical (low-velocity) particle in motion,  $p = m\nu$  and we find that:

$$\frac{1}{2}m\nu^2 = E$$

Which is just an expression that the energy of a particle whose velocity is much smaller than that of light has energy equal to its kinetic energy. This we already know from classical mechanics.

*The Schrodinger Wave Equation, then, is related to energy conservation and a classical accounting of energy.*

What is the probability of finding the particle at any given place in space or time?

$$\Psi^*(x,t)\Psi(x,t) = A^2 e^{-i(kx-\omega t)} e^{i(kx-\omega t)} = A^2$$

Since  $A$  is a constant, this means that such a particle is equally likely to be found anywhere at any time.

### **Plane Waves as Building Blocks**

What we have here is not necessarily a useful description of a real situation, but rather a building block. The plane wave is a useful construct because we can add many of them together to obtain a description of a real situation. They're like building blocks that we can tweak and combine to get what we want.

The idea of taking a simple wave, and tweaking it and adding it together many times is not a strange idea. For instance, imagine you have a machine that can generate only sine waves. You can make as many sine waves at the same time as you want. You are asked to generate a SQUARE WAVE (see slides). How do you use the sine wave to make something with sharp boundaries, like a square wave?

### **The Uncertainty Principle**

We can now turn for a moment away from the wave function and consider another consequence of the wave nature of the universe. This turns out to be one of the most profound ideas of physics.

That idea is *fundamental uncertainty* about the exact properties of a system, or the exact outcome of an experiment. Recall that in classical physics, the mechanical view of nature posited that if you know the initial conditions of a system you can predict all future behavior of the system exactly. Quantum mechanics offers an alternative, one which experimentation has demonstrated to be true: you cannot know with absolute certainty the outcome of anything, only the spectrum of outcomes.

The wave description of nature already implies uncertainty. For instance, EM waves passing through one or two slits are forced to spread out on the

other side. This spreading out already implies a loss of certainty in the exact properties of a single photon once it passes through the slit.

We can make this more concrete. First, we need to quantify uncertainty, which can otherwise sound like a nebulous business.

DISCUSSION: offer some ideas about how to quantify uncertainty (in general), asking them to draw on their own experiences.

In physics, as in other disciplines, we use the *standard deviation* as a measure of uncertainty. In general, we are interested in knowing how far from a mean value a series of measurements will deviate.

Imagine repeating the same experiment many times. Do you expect the result to be identical every time?

- in laboratories, we're usually concerned with uncertainty introduced by random variation, or by systematic effects in the equipment that alter the results with each measurement (e.g. response to temperature by the equipment, etc.)
- we're going to focus on a more fundamental uncertainty, one which cannot be removed, but the language of the two is the same

We can define the standard deviation as follows: if we are performing repeated identical experiments to measure a quantity,  $Q$ , then in each experiment we will measure a value  $Q_i$ . The MEAN of the measurements is simply

$$\bar{Q} = \frac{\sum_i Q_i n_i}{\sum_i n_i}$$

where  $n_i$  is the number of times a given result  $Q_i$  is obtained.

The STANDARD DEVIATION is defined as:

$$\Delta Q = \sqrt{\frac{\sum_i (Q_i - \bar{Q})^2 n_i}{\sum_i n_i}}$$

Let's think about this, because math and language are usefully connected here. This is a measure of how much measurements differ from the mean value. You compute the distance each individual measurement lies from the mean value, then square it, compute the means of that quantity, and take the square root. This is where the alternative name, root-mean-square, comes from.

We see that it serves its purpose. When measurements cluster very near the mean,  $\Delta Q$  is very small - should all numbers be equal to the mean, it is zero. When the measurements spread out further from the mean,  $\Delta Q$  gets larger and larger. It helps us measure the uncertainty on the mean.

When we talk about uncertainty, now there is a quantitative basis for having that discussion and not just a nebulous meaning of "uncertainty".

### **DISCUSSION: Wave Properties and the Basis of the Uncertainty Principle**

How can we begin to think about how the wave nature of light leads to a fundamental concern about our certainty regarding  $x$  and  $p$ ?

Re-consider the single-slit diffraction experiment. What do we learn from the outcome of the experiment?

(see slides)

As the width increases (that is, we are less certain where the electron or photon is on the other side of the slit), the certainty on the momentum along the x-direction (the spread in the diffraction pattern) decreases.

Inversely, as we become more certain about where the particle is on the other side of the slit by narrowing the slit, we become LESS certain about the momentum along the x-direction (the spread of the diffraction pattern gets larger and larger and larger).

So there appears to be a relationship:

$$\Delta p_x \propto \frac{1}{\Delta x}$$

where  $\Delta x$  represents not CHANGE but UNCERTAINTY in the value of a position measurement (likewise for momentum).

The experiment is not to blame for this effect. This relationship is a consequence of the wave nature of matter.

- INCREASED CERTAINTY IN THE POSITION OF AN OBJECT MEAN DECREASED CERTAINTY IN THE MOMENTUM OF AN OBJECT

One way to see this is to consider what happens if you draw a regular wave and constrain more and more where the wave is - you become less and less certain of the curvature of the wave, which is related to its momentum. In other words, if you constrain the space of your experiment to much less than one full cycle of a wave, how certain are you of the wavelength? Very uncertain.

Let's just lay out the Heisenberg Uncertainty Principle, and then we can discuss why this is and what implications it has:

$$\Delta x \Delta p \geq \hbar/2$$

This is a theoretical limit on the precision with which some familiar quantities can be known simultaneously. Knowing exact place means knowing nothing of momentum:

$$\Delta x \rightarrow 0; \Delta p \rightarrow 0$$

## DISCUSSION

Returning to the business of wave functions, the Uncertainty Principle is a very valuable tool because it allows us to to make estimates of things with complete ignorance of the actual wave function.

- Discuss atoms and ground states. Does the uncertainty principle explain why there are minimum energies that electrons in atoms (e.g. hydrogen) can have?
- Absolute rest: is that a problem (e.g. being at rest causing wavelength to be infinite)?

The grain of sand problem:

By visual inspection, we can establish that a 1 mg grain of sand is not moving to within 550 nm, the average wavelength of visible light.

(a) what is the minimum uncertainty on its velocity? If it were moving at that speed, how long would it take to travel the smallest distance perceivable, 1 micron?

- Apply the uncertainty principle:  $\Delta p_x \Delta x \geq \hbar/2$ . We know the upper bound on the uncertainty on the position, 550 nm, so we can solve for the lower bound on the momentum uncertainty:  
 $\Delta p_x \geq 9.59 \times 10^{-29} \text{ kg} \cdot \text{m/s}$ . The uncertainty on momentum is small because Planck's constant is small. If Planck's constant were larger, "quantum" behavior would become more and more apparent.  
**QUESTION: does the uncertainty on this grain's momentum correspond to relativistic or non-relativistic speeds?** To answer, use  $\Delta p_x = m \Delta v_x$  and we find that  $\Delta v = 9.59 \times 10^{-23} \text{ m/s}$ , VERY non-relativistic. So that's consistent with classical physics. How long would it take to go 1 micron? ANSWER: 3.3 million centuries. SAFE!

(b) A wavelength of 1 nm would be small enough to ensure particle behavior in everyday circumstances. How fast would the grain of sand have to move to have such a wavelength?

- Here we apply de Broglie's relationships,  $\lambda = \hbar k = h/p$ . We can solve for speed from momentum, and find:  $v = 6.63 \times 10^{-19} \text{ m/s}$ . A tiny object can appear absolutely stationary yet have a wavelength that is safely small and thus leading to particle behavior in the classical sense.
- Discuss energy and time. Is there a corresponding uncertainty principle? How might we arrive at it?
- Uncertainty in three dimensions: they are disconnected from one another (each dimension has its own principle). Thus  $\Delta p_y$  and  $\Delta x$  can simultaneously be very small.

## The Limitation of Knowledge



Let's summarize the limitations that quantum mechanics place on our knowledge.

- The equations describing particles and forces (we'll add forces later) can be very precisely stated
- The wave function encodes all of the properties of matter
- The wave function, by its nature, prevents us from knowing both momentum and position (or energy and time) precisely at the same time.

Discuss the two slit experiment again

- The wave function of an electron is  $\Psi_A$ , as established by experiment A (the slits). We detect the electron at B, and there we measure its position. But this only establishes  $\Psi_B$ , rather than measuring anything about  $\Psi_A$ . In order to know the properties of matter, we have to measure matter. Trying to figure out which slit the electron passes through necessarily changes  $\Psi_A$ , and prevents the coherent interference of the electron wave with itself when we do not know through which slit it passes.

The modern interpretation of all of this, the Copenhagen Interpretation, states that we do not know the position or momentum of a particle until a measurement is made. Prior to that measurement, the particle does not have a location - the wave function only tells us the probability of finding it in one place or another.

DISCUSSION: other interpretations of quantum mechanics

## **Bound States**

DISCUSSION: What is a "bound state"?

Bound states are simply cases where a particle's motion is restricted by a force (a wall counts as a force). The motion is restricted to a finite region of space.

- What are examples of "bound states"?

- mass on a spring (Hooke's law) - for a perfect spring, regardless of the energy of the mass it is restricted to a finite region of movement
- gas in a box
- ball rolling between two steep hills
- etc.

We will attack some seemingly over-simple problems involving objects bound under various conditions. These are not pointless examples. Rather, they are the basis of solving real problems. To understand the "hopelessly complicated" we must understand the simple. In addition, many problems are too complex to solve exactly, but models can be made (simplified circumstances) that do not fully explain the situation but give insight and a lot of answers.

Again, we start with the SWE:

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

We have discussed plane waves:

$$\Psi(x, t) = Ae^{i(kx - \omega t)}$$

which are one solution to the equation. Substituting this solution, we obtain:

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

Questions:

- What is the quantity  $\hbar^2 k^2 / 2m$ ? Answer: kinetic energy of a particle
- What is  $\hbar\omega$ ? Answer: total energy of a particle

We can then write this as a suggestive equation:

$$(KE)\Psi(x, t) = (E)\Psi(x, t)$$

and we recover that statement that SWE has something to do with classical energy accounting.

### Extending the SWE to include forces

How might we extend the SWE to include forces?

DISCUSSION: forces and potentials, potential energy, etc.

- we can only assign potentials to conservative forces (e.g. gravity, Coulomb but not friction).
- our extension will only work for things like the electrostatic force

Answer: add a potential energy term to the equation:

$$(KE + U(x))\Psi(x, t) = (E)\Psi(x, t)$$

which leads us to the guess that:

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

DISCUSSION: In classical physics, how do we determine the outcome of motion?

- Answer: solve the force equation,  $\vec{F} = m \frac{d^2 \vec{r}}{dt^2}$  for  $\vec{r}(t)$ , given knowledge of the external force
- For the SWE, we must solve the equation for  $\Psi(x, t)$ , given knowledge of  $U(x)$ . That is the task at hand in any problem.

This equation is dependent on both space and time. We'll learn a trick now to help solve problems.

## Stationary States: Separation of Variables

Our first step is to separate the space and time parts of the wave into separate functions, multiplied times one another:

$$\Psi(x, t) = \psi(x)\phi(t)$$

This is an assumption, but making it allows us to try to simplify the problem and test our solutions. It does reduce the generality of our solutions, but its advantage is a practical one: these special solutions are often of great interest (and utility!).

We can now re-write the SWE:

$$-\frac{\hbar^2}{2m}\phi(t)\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x)\phi(t) = i\hbar\psi(x)\frac{d\phi(t)}{dt}$$

and then re-order the terms to achieve separation:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt}$$

Consider the following case of this equation:

*What happens at  $(x, t) = (x_1, t_2)$  when the wave function at  $(x, t) = (x_1, t_1)$  allows the SWE to hold?*

In that case, since the left side is constant, the right side must also be constant and thus the SWE has a right-side which is constant:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + U(x) = i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = C$$

In other words, since the left side does not change the right-side cannot either, regardless of the value of  $t$ .  $C$  is the "separation constant".

This would fail is  $U = U(x, t)$ .

Let us now consider each part of the equation separately.

**Stationary States: the temporal part,  $\phi(t)$**

This is:

$$i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = C$$

or

$$\frac{d\phi(t)}{dt} = -\frac{iC}{\hbar}\phi(t)$$

**NOTA BENE: Eqn. 5-6 in Harris is MISSING the minus sign!**

A solution to this equation is:

$$\phi(t) = e^{-i(C/\hbar)t}$$

What does all this mean? Write the solution in terms of the Euler Equation:

$$e^{-i(C/\hbar)t} = \cos((C/\hbar)t) - i\sin((C/\hbar)t)$$

We see that  $C/\hbar$  represents a pure frequency (e.g.  $2\pi f$ ). That means  $C = 2\pi\hbar f = \hbar\omega = E$ .

This means that when we separate variables, we are in fact FOCUSING ON STATES WITH **WELL-DEFINED** ENERGIES. The separation constant IS that energy.

According to the separation of our original wave function, we can now write:

$$\Psi(x, t) = \psi(x)e^{-i(E/\hbar)t}$$

for the wave function. We haven't considered interactions with the potential yet, so  $\psi(x)$  is still general and unsolved-for.

DISCUSSION: what is the probability density of this wave function?

Answer:

$$\Psi^*(x, t)\Psi(x, t) = \left(\psi^*(x)e^{i(E/\hbar)t}\right) \left(\psi(x)e^{-i(E/\hbar)t}\right) = \psi^*(x)\psi(x)$$

- Is there time dependence in the probability?
  - No - it disappears under the case we can separate space and time components of the wave function
  - The properties of such objects do not change in time - they are "stationary states"
- What are the implications for, say, electrons in an atom?
  - The electron is bound by the coulomb force to the atom. That potential is time independent. Classically, as it whizzes around the nucleus it should be losing energy. But quantum mechanics says that's not the case: it tells us that the electron can appear in many places around the atom ( $\psi(x)$ ), but its energy is constant and well-defined. The electron is not orbiting, in the classical sense, but rather in a probability cloud around the nucleus. If the probability density is constant, the charge density is constant, and if the charge density is constant, EM tells us it radiates no energy.

Wild stuff, a beautiful description of exactly what is observed about atoms.

**Stationary States: the spatial part,  $\psi(x)$**

We cannot say anything specific about  $\psi(x)$  without  $U(x)$ , so that is where we shall go next. There are few simple cases for  $U(x)$ , but we'll start with them now and see what they teach us about nature.