Modern Physics (PHY 3305) Lecture Notes

Matter in Motion (Ch. 5.8, 6.1-6.3)

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What are Waves Doing?

tags: lecture

We can now turn to step four in solving quantum problems: making predictions from the wave function. This boils down to the following actions:

- Determining "EXPECTATION VALUES" (an average of possible outcomes)
- Defining operators that "act" on the wave function to determine outcomes

Where are you likely to be? Expectation Values

We have already, in our discussion of normalization, talked about how to compute the total probability of finding the particle somewhere in the experiment. To do this,

- we define the probability of finding the particle in an interval dx around a point x as $|\psi(x)|^2 dx$.

If we integrate over all allowed x, we should obtain 1.0 from the integral.

What is we want to know the expectation of finding the particle around a given point, x? We can then instead compute the expectation value of x, defined as:

$$\bar{x} \equiv \int_{\text{all space}} x |\psi(x)|^2 dx$$

This symbol on the left is the symbol for "expectation value." Be careful - although this is mathematically equivalent to computing the average value of a function $f(x)$, we are not computing averages of particle behavior in a system. Rather, we are interested in knowing how likely it is to expect to find the particle in a given region. You can't average a single particle's behavior without watching it continuously, and as we know this changes the parameters of the system.

The expectation value, rather, is strictly defined as follows:

- If the expectation value of a particle is the value we would obtain if were were to begin a particle in state A, find it, start again with a particle in state A, find it again, and so on, repeating the same identical experiment over and over. The expectation value is a number, not a function, since we integrate over x.

By the same logic, the expectation value of the square of the position is:

$$\overline{x^2} \equiv \int_{\text{all space}} x^2 |\psi(x)|^2 dx$$

We are interested in this square because, as in statistical problems, we can use it to define UNCERTAINTY. For instance:

$$\Delta x \equiv \sqrt{\int_{\text{all space}} (x - \overline{x})^2 |\psi(x)|^2 dx}$$

Keep in mind that $\overline{x}$ is a VALUE, not a FUNCTION. This let's us manipulate this equation into a convenient form.

This is a good definition of uncertainty for several reasons:

- The integral is only zero if the integrand is zero
- When the wave function is spread out over space, Δx also become broader and broader

That's a good definition of uncertainty (we have to pick something!).

We can manipulate this now into an easier-to-calculate form by using:

$$(x - \bar{x})^2 = (x^2 - 2x\bar{x} + \bar{x}^2)$$

We get three integrals:

$$\Delta x \equiv \sqrt{\int_{\text{all space}} x^2 |\psi(x)|^2 dx - 2\bar{x} \int_{\text{all space}} x|\psi(x)|^2 dx + \bar{x}^2 \int_{\text{all space}} |\psi(x)|^2 dx}$$

The first integral is just $\overline{x^2}$, the second integral is just $\bar{x}$, and the third is 1 due to normalization. This yields:

$$\Delta x = \sqrt{\overline{x^2} - 2\bar{x}^2 + \bar{x}^2} = \sqrt{\overline{x^2} - \bar{x}^2}$$

So it boils down to just computing two integrals and taking the square root of the differences. We only need two pieces of information:

- The average of the square
- The square of the average

Any function of position can also be inserted, so that we might determine the expectation value of the function for that particle:

$$\overline{f(x)} = \int_{\text{all space}} f(x)|\psi(x)|^2 dx$$

Where are you going? Operators

EXPECTATION VALUES are mathematical tools that allow us to connect the form of the wave functions of OBSERVABLE properties of a quantum system, such as position or momentum. Generally speaking, if you have some quantity Q you want to determine in an experiment, and you want to

predict the expectation from the wave function,

$$\overline{Q} = \int_{\text{all space}} \Psi^*(x,t)\hat{Q}\Psi(x,t)dx$$

$\hat{Q}$ is an OPERATOR - a function that acts on the wave function and represents the act of measuring a property, Q, of the system. $\hat{Q}$ acts on $\Psi(x,t)$, and returns a function which is then multiplied by the complex conjugate of the original wave function to determine the probability of that outcome. Schematically:

- $\hat{Q}\Psi(x,t)$ is the act of making a measurement, which puts the wave function into some definite state
- $\Psi^*(x,t)(\hat{Q}\Psi(x,t)$ is the probability of that outcome, given the original wave function

You then integrate and determine the expectation value for that measurement.

What are some operators?

Position Operator

This is simply x, as we used in the examples above to determine Δx.

Momentum Operator

There is a derivation of this result in Appendix E of Harris, but we'll state the result:

- $\hat{p} = -i\hbar\frac{\partial}{\partial x}$

Energy Operator

The result is:

- $\hat{E} = i\hbar\frac{\partial}{\partial t}$

Functions of Operators

Functions of the operator are also possible. For example

- $KE = p^2/2m \rightarrow \hat{KE} = \frac{1}{2m}\hat{p}^2 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

The Shroedinger Wave Equation in Operator Form

We may now re-write the SWE in operator form, since the above operators
all appear in the SWE:

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

Where is the Plane Wave going?

We can use this language of operators to answer some basic questions
about wave functions. Let's consider the plane wave - a particle traveling
free of forces. Originally, we wrote down a plane wave that looked like this:

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

How do we know what direction it's traveling in? Is it going forward (in the
positive x-axis direction) or backward? We can use the momentum operator
to tell us!

$$\hat{p}\Psi(x,t) = \left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t) = A(k)\hbar e^{i(kx-\omega t)} = (\hbar k)\Psi(x,t)$$

So from this we find that the momentum returned by the operator is:

$$p = \hbar k$$

Which is positive! Aha, so we can then easily write down the formula for a

wave function traveling in the NEGATIVE x-direction:

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

We will now immediately apply this to a real-world problem: a free particle suddenly encountering a barrier.

Plane Waves and Square Barriers

A *barrier* is here defined as a region where the potential energy suddenly increases over its value in other parts of space.

Demonstrate the creation of a barrier using the PhET simulator for quantum waves

- In the *PhET* simulator for quantum tunneling, begin by setting the kinetic energy of the wave (green line) to something like 0.75. Set the barrier potential to zero. Set the simulator to use plane waves.
- You should have a plane wave traveling from left to right unaffected in its behavior. The probability of finding the wave should everywhere be 1.0.
- Now, slowly raise the barrier. Discuss and describe the effect on the plane wave when the barrier is STILL less than its kinetic energy.
- *DIscuss* what the class expects to happen when the barrier is raised above the kinetic energy. Appeal to previous discussions of potential wells to guide their answers.
- Now, raise the barrier potential above the kinetic energy. See if their predictions came true.

- Switch to a wave packet - this will allow you to really visualize the motion of the matter wave, its probability, and then make quantum measurements.
- Make a quantum measurement. This is equivalent to "applying the position operator" and determining where the particle is (say, by sending in a photon or "looking" for the particle to strike some detector medium and interact with it in a well-defined location). See if the particle is ever found beyond the barrier.

A wave packet is simply the sum of a number of plane waves, with different contributions from plane waves of different frequencies:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)e^{i(kx-\omega(k)t)}dk$$

A few important things come out of this discussion:

- Left of the barrier ($x < 0$), where the particle originates, the wave function has two components: the initial incident forward-going plane wave, and a reflected part that is backward going. Thus:

$$\Psi(x,t)|_{x<0} = Ae^{i(kx-\omega t)} + Be^{-i(kx-\omega t)}$$

- We can define the REFLECTION COEFFICIENT as the ratio of the intensities of these two waves:

$$R = \frac{|B|^2}{|A|^2}$$

- On the right side of the barrier ($x > L$), there is only a forward-going component - the transmitted wave. This is given by

$$\Psi(x,t)|_{x>L} = Fe^{i(kx-\omega t)}$$

- The TRANSMISSION COEFFICIENT is then defined as

$$T = \frac{|F|^2}{|A|^2}.$$

The sum of $R + T = 1$ is a physical requirement on the problem, since the particle has to be found SOMEWHERE.

Simplifying Tunneling Problems

The discussion of Tunneling in Harris is lengthy and detailed. You are STRONGLY encouraged to read through this. However, in class I only emphasize the simplified case where the barrier is wide.

- What does it mean to be a "wide barrier"?
  - The condition for a wide barrier is that the length, L, of the barrier be SIGNIFICANTLY LARGER than the penetration depth of the wave function in the barrier,

$$1 << \frac{L}{\delta} = \alpha L = \frac{\sqrt{2m(U_0 - E)}}{\hbar} L$$

In that case, the transmission probability holds a much simpler form than the general one discussed in Harris:

$$T = 16 \frac{E}{U_0} \left(1 - \frac{E}{U_0} \right) e^{-2L\sqrt{2m(U_0 - E)}/\hbar}$$

The Application of Quantum Tunneling

Let's close today's lecture with a discussion of APPLICATIONS of the quantum tunneling phenomenon. We've already mentioned on of these in class a few times, so we'll start with that:

The Scanning Tunneling Electron Microscope (see slides)

- A tip is brought very close to a sample surface (within 4-7 angstroms)
- The wave functions of the electrons on the tip and those on the surface overlap
- as the tip is scanned over the surface, the height between the tip and surface changes
- This changes the potential barrier
- The changes in potential barrier create changes in probability of tunneling electrons from tip to sample, and vice versa
- This leads to changes in tunneling current, which are read out and interpreted as changes in surface features in the material.

Alpha Decay (Nuclear Decay)

Alpha decay is the emission by an atom of a Helium Nucleus (2 protons and 2 neutrons, total electric charge +2e). It happens spontaneously to unstable nuclei like that of Uranium-238 (U238 decays to Thorium 234 and an alpha particle). Why?

- Classically, the energy of the alpha particle was predicted to be 35 *MeV* once ejected from the nucleus. This is because it would take at least this much energy to overcome the strong nuclear force holding together the nucleus and thus escape from the nucleus.
- Experimentally, the energy of alpha particles was found to be much less - 4-5 *MeV*. Why?
- Quantum mechanics offers the answer: you don't HAVE to have 35 *MeV* to escape the nucleus. You just need to have energy and run into the potential barrier (basically, the outer diameter of the nucleus) sufficient numbers of times to tunnel out of the nucleus with a finite probability.
- Calculation of decay rates of the nucleus using tunneling agree perfectly with the experimentally observed values for nuclear decay rates to alpha particles and other nuclei.

The explanation of alpha decay was a triumph of quantum mechanics.

The Tunnel Diode

- Works by designing a conducting device with an irregular material interface that prevents the free passage of conduction elections through the material.
- At zero voltage, the barrier presented by the material interface is tunneled symmetrically by particles from either direction
- With voltage applied, the barrier becomes asymmetric (with overall potential on one side of the barrier higher than on the other). Tunneling proceeds moreso in one direction then the other, and this happens instantaneously
- This is useful in high-frequency electronics, where you otherwise have to rely on slow, thermal effects to obtain the same non-linear current behavior through a device.

The Tunnel Junction - SQUIDS

There is a far more useful device than a tunnel diode: a SQUID. This consists of two superconductors separated by an insulating barrier. This configuration is known as a JOSEPHSON JUNCTION.

- Superconductivity is described by the long-distance pairing of electrons in a solid.

- In the Josephson Junction, PAIRS of electrons tunnel through the barrier
- These junctions are the basis of a class of electronics devices known as *SQUIDs* - Superconducting *QUantum* Interference Devices.
- The SQUID combines two Josephson Junctions, and makes the relationship between the electron pairs very sensitive to things like magnetic fields - even very weak ones.
- *SQUIDs* are therefore excellent devices for detecting weak/small magnetic fields, as from the human heart and brain. *SQUIDs* can detect fields as small as 5×10^{-18}T (refrigetator magnets are about 0.01T and organic magnetic fields are at the level of 10^{-9}T.)

Next Time

- The Discovery of Spin (Ch. 8.1-8.3)
- Coming Soon (after the break):
    - Statistical Mechanics, or "What Happens When a Bunch of Subatomic Particles Can Do Things"
    - *Solid-State* Physics: quantum mechanics and structure of atomic matter
    - Nuclear Physics: quantum mechanics and the structure of the nucleus
    - Particle Physics: quantum mechanics, relativity, and the origin and fate of the cosmos