Visual Quantum Mechanics

Prepared for Contemporary Physics by

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- Glossary

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1. Wavelength−Momentum Relation

The diffraction of electrons indicates that we need to develop a system for describing the wave behavior of small objects. From observation we learn that the wavelength of an object is related to its momentum. The relationship is given by

$$Wavelength = Planck's\ Constant \div Momentum,$$

or

$$\lambda = \frac{h}{p},$$

where h is Planck's Constant (6.63E−34 J s = 4.14E−15 eV s), named for Max Planck.

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2. Schrödinger's Equation

When considering objects as small as electrons, the equivalent to Newton's Laws is an equation which was originally written down by Erwin Schrödinger. This equation cannot be derived from any fundamental law but is based on several well established principles of physics. The basic ingredients in Schrödinger's Equation are:

1. The equation which relates the wavelength of an object to its momentum,
2. Conservation of energy,
3. Knowledge about how waves, such as water waves, behave, and
4. Accounting for forces which act on the object by using changes in potential energy.

Once the equation is set up for a particular situation, someone with an advanced math background or a computer can solve the equation. The result is a mathematical relation called a wave function.

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3. Wave Functions

A wave function has a variety of features including an amplitude, a wavelength; and nodes. The square of the amplitude can be used to describe the probability of the object being at each point in space. Thus, the wave function offers us an equivalent to an equation which relates distance, velocity, acceleration and time for larger objects.

However, the wave function is not identical to results obtained using equations such as *Force* = *mass* × *acceleration*. With a result which comes from Newton's Laws, we obtain precise information about the location of the object at any future time. All we need to know are the forces acting on it, its present location, and its present velocity; all other information regarding the future motion of the object is then determined. Schrödinger's Equation, on the other hand, can only provide us with information about the probability of finding the object in each location at some future time. We can state that the probability of finding the object at each point is high or low, but we can never say with certainty where the object will be at a future time.

The study of the behavior of small objects such as electrons by using Schrödinger's Equation is usually called Quantum Mechanics.

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4. Probability Basics

An object's wave function is related to the probability of finding the object at a given location. A graph of the *square* of the wave function illustrates the range of locations accessible to the object and the probability of its being at each location within that range.

The total probability that the object is "somewhere" is 1. The area under a probability versus position curve must therefore equal 1. For the wave function shown here, the probability of the object being somewhere between locations x1 and x2 is equal to the area of the small rectangle under the probability curve bounded by x1 and x2.

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5. Potential and Kinetic Energy Diagrams −−Large Objects

When we work with Newton's Laws, we frequently write down the forces acting on an object. Then, we use the forces to predict how the object will behave at any future time. However, we could equally well develop ideas of motion by starting with energy as the fundamental idea. In situations that we encounter while studying quantum concepts, we generally find energy the easier concept to use.

As an example of using energy to describe motion, consider a small cart moving on a level, very low−friction surface. If we ignore the friction entirely, then the cart always has whatever energy it had at the beginning of its motion. No potential energy exists in this case, so the total energy is equal to the kinetic energy; the potential energy is zero. A simple graph or diagram describes this situation.

In a real situation, even on an air track, the cart does not go on forever. Instead, it strikes the end of the track and turns around. With a perfect collision at the end of the track, the cart would have the same kinetic energy before and after the collision with the end; only the direction would change. However, during the collision the cart's speed decreases to zero. Plotting kinetic energy versus distance, we get another diagram.

Looking at the end of the track, we see what happens during the collision. The flexible steel springs on the cart and track bend. This process increases the elastic potential energy, resulting in a different diagram.

We can combine kinetic, potential, and total energies for this situation into a single diagram.

Consider the question: For each value of kinetic energy, how far will the metal on the ends compress? The first step in our answer is to draw the potential energy diagram for the situation. It looks like the first of the three diagrams above. The high sides indicate that the potential energy gets very large at the ends of the track. Now pick a value for kinetic energy. What is the furthest location to the left that the cart will reach? Why?

Now we add a magnet on the track and on the cart so that the magnets attract. Look at the kinetic energy diagram for the cart. The total energy does not change, so the potential energy must be as shown here. For most situations, we can draw a potential energy diagram by following similar reasoning patterns.

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6. Drawing Potential Energy Diagrams

Potential energy diagrams will be used to describe the forces which act on small objects. They will form the basis of our solutions to Schrödinger's Equation. Thus, the first rule for obtaining wave functions is:

> **Draw a diagram of the potential energy versus position for the object.**

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7. Potential Energy Diagrams –– Small Objects

As an example consider an electron which is moving through empty space and then enters a metal. When it enters the metal, it interacts with the electrons in lots of atoms. These interactions slow the electron, so its kinetic energy decreases. Because the total energy does not change, the potential energy of the electron must increase while the kinetic energy is decreasing. The electron experiences a sudden change in kinetic and potential energies when it enters the metal. Thus, the potential energy diagram will reflect a rapid change at that boundary.

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8. Determining Wavelengths ––General

Because the wavelength of an object is associated with its momentum, we can find a relation between wavelength and kinetic energy. The first step is to establish a relation between kinetic energy and momentum. Both kinetic energy and momentum are related to the speed of the object. Thus, we can relate the kinetic energy to the momentum as follows:

$$Kinetic\ Energy = \frac{1}{2}\ Mass \times (Speed)^2$$

$$Momentum = Mass \times Speed$$

$$\Longrightarrow Kinetic\ Energy = \frac{(Momentum)^2}{2 \times Mass}$$

or

$$KE = \frac{1}{2}mv^2$$

$$p = mv$$

$$\Longrightarrow KE = \frac{p^2}{2m}$$

Then, we can use these equations with the wavelength–momentum relation to write the wavelength in terms of the kinetic energy.

$$Wavelength = Planck's\ Constant \div \sqrt{2 \times Mass \times Kinetic\ Energy}$$

or

$$\lambda = \frac{h}{\sqrt{2m(KE)}}$$

We can use this equation for any object. To describe an electron using units of electron volts (eV) for energy and nanometers (nm) for wavelength, the equation above becomes

$$Wavelength = \sqrt{1.5\ nm^2 \cdot eV\ /\ Kinetic\ Energy}$$

or

$$\lambda = \sqrt{\frac{1.5\ nm^2 \cdot eV}{KE}}$$

We can use this result to find the wavelength of the wave function in each region of potential energy. In general we will not calculate the exact number for the wavelength. Instead, we will want to know how the wavelength in one region compares to that in another. For that comparison we can use the equation above to note that

as the kinetic energy goes **up** *the wavelength goes* **down** *and*

as the kinetic energy goes **down** *the wavelength goes* **up**.

Looking at the equation, we can also see that the kinetic energy must be positive for the wavelength to have any meaning. If the kinetic energy is negative, we get the square root of a negative number. That gives us a meaningless wavelength. Thus, we can use this result only for positive kinetic energies. That is: when the total energy is greater than the potential energy.

This discussion leads to our second rule for obtaining solutions to Schrödinger's Equation:

> **When the total energy is greater than the potential energy, determine the wavelength of the wave function by using the relation between the wavelength and the kinetic energy.**

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9. Determining Wavelengths –– Example

As an example, use the potential energy for an electron entering a metal. Here, we repeat the earlier diagram but include a dotted line to indicate the total energy of the electron.

To determine the kinetic energy of the electron we look at the difference between the total energy and the potential energy. As shown in the next figure, the kinetic energy on the left side is about four times greater than that on the right side of the edge of the metal.

So, we conclude that the wavelength on the left side will be about one–half of that on the right side. The approximate wave function looks like the one in this figure.

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10. Wave Functions at Boundaries

When drawing wave functions at changes in potential energy, we make a smooth connection between the wave functions in the two regions. This type of connection comes from an understanding that it would be difficult to make sense of different probabilities of finding the electron if we approach the boundary from different directions. For example, suppose that this wave function could be possible. The probability distribution, given by the square of this wave function, looks like this.

If we approach this boundary from the left, we obtain the probability marked as A. However, if we approach from the right we get a different probability (B) at the boundary. A different value occurs depending on which way we approach the boundary, yet it is the same boundary. Two different values for the probability at the same point would be meaningless. So, we have another rule, called the smoothness condition, for drawing wave functions:

> **The wave function must be smoothly connected at all points including boundaries where the potential energy changes.**

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11. Constraints on the Wave Function: An Infinite Potential Example

In many conditions, the physical situation will lead to constraints on the wave function. As an example consider an idealized situation in which the motion of an electron is restricted to a box. To be certain that the object cannot get out of this box, we imagine that the box has infinite forces on the edges. Infinite forces lead to infinite potential energies at the edges of the box. The potential energy diagram is shown here.

If the object cannot get out of this box, we know that the probability of finding the electron outside the box must be zero. That leads us to the conclusion that the wave function is zero outside the box. Because of the smoothness condition, wave functions inside the box must approach zero as they get near to the edges of the box. These nodes at the edge of the box represent a constraint on the wave function.

With this constraint in mind, we will create some wave functions for the object in this box. Inside the box the potential energy is zero, so the kinetic energy is equal to the total energy. First, we will pick an energy and see what we get. The process will be easier if we use numbers with units of electron−volts and nanometers. In particular, we will use a length of 0.2 nm for our box.

As a starter, we will see what happens with a kinetic energy of 6 eV. Calculating the wavelength we have:

$$Wavelength = \sqrt{\frac{1.5\ nm^2 \cdot eV}{KE}}$$
$$= \sqrt{\frac{1.5\ nm^2 \cdot eV}{6\ eV}}$$

$$\Longrightarrow \lambda = 0.5\ nm$$

The wavelength here is two and a half times the length of the box. Drawing this wave within the boundaries of the box gives a picture which looks like this.

This wave function has problems because it cannot meet the constraints of going to zero on the edges of the box. Thus, we must eliminate this wave function as one of the possibilities.

Based on this experience, it makes some sense to work backwards from the way we have been. Sketch waves that fit in the box, then determine the energies which will match those waves. Waves which meet the zero condition at the edge and the smoothness condition are similar to standing waves on a string. The following diagram shows several possibilities for these wave functions.

With the constraint that the wave function must be zero on the edges of the box, only certain wave functions are allowed in the box. These wave functions must have wavelengths such that they fit in the box. Just as the standing wave on a string, the wave functions which fit can have wavelengths equal to half the length of the box, the length of the box, one and a half times the length of the box, twice the length of the box, and so forth.

Because the energy of a wave is related to its wavelength, such an object is allowed to have only certain energies. Since only certain values of energy result in allowed wave functions, these systems are said to be "quantized." Thus, the name "quantum mechanics" is associated with systems which have only certain values of energy. We see evidence for this quantization of energy in the light emitted by atoms.

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12. Constraints on the Wave Function: A Finite Potential Example

The example of the infinite potential energy at the edge of a well is not very realistic, but it does give us a result that connects nicely with what we see in atoms. To see if the same idea holds when we become more realistic, we consider a box with a potential energy which is less than infinite. The potential energy diagram for this situation is shown in the following figure.

To determine the wave functions, we will need to think through what could happen. First, we know the results for an infinite potential energy. Suppose that the potential energy were just a little less than infinite. (Say, infinity – 2, whatever that means.) We would not expect much change in the wave functions from the infinite potential energy, because the potential energy is only slightly less. We also know that the object will have a low probability of being in locations which are very far away from the box.

Studies of waves tell us that when the potential energy changes as in this case, the wave function decreases to zero quickly in the region of large potential energy. Thus, one possibility is for the wave function to look similar to standing waves inside the box but to decrease to zero quickly as it leaves the box. These wave functions are shown in the following figure.

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13. Decreasing Wave Functions –– Qualitative

In regions where the total energy is less than the potential energy, the amplitude of the wave function decreases. Further away from the boundary where the potential energy changes, the probability of the object being located there decreases. However, in the region where the total energy is less than the potential energy, the probability of finding the object is not always zero.

We would also expect that, for a given total energy, the rate of decrease should depend on the size of the potential energy. If the potential energy is large, the object should be more restricted than if it is small. The results show that this does occur as illustrated here.

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14. Decreasing Wave Functions –– Quantitative

To put some numbers on the rate of decrease of the wave function in regions where the total energy is less than the potential energy, we introduce some approximations based on wave motion. First, we introduce a characteristic length, l, with which we describe the decrease:

$$Length = Planck's\ Constant \div \sqrt{2 \times Mass \times (Potential\ Energy - Total\ Energy)},$$

or

$$\ell = \frac{h}{\sqrt{2m(PE - TE)}}$$

When we use the electron–volt and nanometer units, we obtain an equation similar to the one we used for wavelength.

$$\ell = \sqrt{\frac{1.5\ nm^2 \cdot eV}{PE - TE}}$$

We use this length as a unit to measure the decrease of the wave function's amplitude. The basic (approximate) rule is that when we move six times l in a region where PE > TE the amplitude of the wave function decreases to one–third of its value (see figure).

We can apply this rule to determine how much the wave function decreases in any region where the total energy is less than the potential energy.

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15. Rules For Drawing Wave Functions

- **A.** Draw a diagram of the potential and total energies.
- **B.** Look for constraints on the wave function.
    - **1.** The wave function is zero when the potential energy is infinite.

    - **2.** The wave function oscillates when the total energy is greater than the potential energy.
    - **3.** The wave function decreases when the total energy is less than the potential energy.
- **C.** Relate the situation to similar situations with wave functions
- **D.** The wave function must connect smoothly at a boundary where the potential energy changes.
- **E.** In different regions where the wave function oscillates, use the kinetic energies to determine the relative wavelengths.
- **F.** In regions where the wave function is decreasing, use the potential and total energies to determine the approximate rate of decrease.
- **G.** Draw the wave function.
- **H.** Interpret the wave function by squaring it to determine the probability of the object being in different regions of space.

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Appendix: Newton's Laws

Newton's Laws are three simple laws of motion developed by Isaac Newton in the late seventeenth century. As a group, they provide a single theory with which to explain an enormous range of observations.

1. When the net force acting on an object is zero, the object's momentum does not change.

2. The net force acting on an object is equal to the product of the object's mass and its acceleration. This relationship can also be expressed by the following equation:

Net force = *mass* × *acceleration*.

3. Every applied force results in a reaction force on the applier. This reaction force is equal in magnitude but opposite in direction to the applied force.

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Glossary

Wavelength

The distance between successive crests, troughs, or identical parts of a wave. (See figure.)

Wavelength–Momentum Relation

$$Wavelength = Planck's\ Constant \div Momentum$$

Momentum

The product of an object's mass and its velocity.

$$Momentum = Mass \times Speed$$

Energy

The ability to exert a force.

Amplitude

For a wave or vibration, the maximum displacement on either side of the equilibrium (midpoint) position. (See figure.)

Kinetic energy

Energy of motion, described by the relationship

$$Kinetic\ Energy = \frac{1}{2}\ Mass \times (Speed)^2$$

Electron volt (eV)

In atomic and nuclear physics, it is the most commonly used unit of energy, related to the joule by 1eV = 1.6021E−19

Nanometer (nm)

A unit of length equal to 10E−9 meter. Atoms have a radius of 0.1 to 0.2 nm.

Potential energy

The stored energy that an object possesses because of its position with respect to other objects.

Node

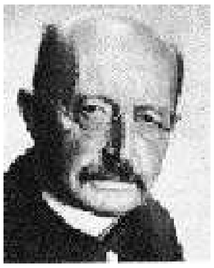
Point of zero amplitude in a standing wave. Antinodes are points of maximum amplitude.(See figure.)

Standing wave

A stationary wave pattern formed in a medium when two sets of identical waves pass through the medium in opposite directions.

Smoothness condition

The wave function must be smoothly connected at all points including boundaries where the potential energy changes.



Max Planck

Max Planck, 1858−1947, German physicist, professor at Berlin and president of the Kaiser Wilhelm Society for the Advancement of Science (now the Max Planck Institute). Planck made significant contributions to thermodynamics before he became involved with the problem of blackbody radiation. He was a very conservative scientist, and he regarded his quantization postulate as "an act of desperation." Planck received the Nobel Prize in 1918.

Erwin Schrödinger

Erwin Schrödinger, 1887−1961, Austrian theoretical physicist, professor at Berlin and at Vienna. One of the founders of the new quantum mechanics, he received the Nobel Prize in 1933.

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