## **Supplemental Documentation for Reviewers**

This documentation is taken directly from a website that is referred to in the Appendix of the submitted article. In order to comply with the blind peer-review guidelines, we have removed the website link from the paper and included the information here instead.

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## Quantum Tunneling Overview

## Introduction

At the heart of quantum mechanics is the idea that matter behaves as both a wave and a particle. Experimental evidence from approximately 1900 through present day shows that as we look more closely at the behavior of very small things, such as molecules, atoms, and fundamental particles, the intuitive classical predictions of how matter should behave are not adequate in predicting the results of experiments. Perhaps the most fundamental reason for this is that these small particles were clasically treated as point-like objects whose position and momentum can be predicted with absolute certainty. It was not until the leading physicists of the early 20th century started toying with the idea that these very small objects may behave as waves at certain times and particles other times that they began predicting the results of experiments.

One of the interesting findings of quantum mechanics is that, due to the wave-like nature of matter, small particles can be found in places that would classically be forbidden. This phenomenon is called "quantum tunneling", and it has allowed for new technologies to be developed throughout the 20th century. Such applications are: the scanning-tunneling microscope, tunneling diodes, tunneling field-effect transistors, and the understanding of radioactive decay (which, for example, powers any nuclear power plant). This phenomenon not only demonstrates the 'strangeness' of quantum mechanics, but also plays a fundamental role in society, and is therefore an important subject in any quantum mechanics course. In the rest of this paper, we describe in greater detail what tunneling is, and how it can be treated mathematically.

## **Basics of Quantum Mechanics**

Energy barriers are ubiquitous in physics. A skate board ramp, an electronic circuit element, a material's emission properties, and much more, can be described with the concept of an energy barrier. For example, a skateboard ramp provides a gravitational energy barrier for the skater, such that while the skater is on the ramp, his/her energy is constrained by the ramp. Similarly, a circuit element can provide an energy barrier for electrons, such that only electrons with a certain energy may cross the circuit element.

Quantum tunneling is a problem that involves an energy barrier. Specifically, this barrier tells us about how a quantum particle (such as an electron or proton or small molecule), can be spatially and temporally located within a region of space. One barrier to consider is the one shown in Figure 1. In this figure, three 'regions' exist in one dimension of space (imagine a very small wire, separated by another wire a distance L away from each other).



Figure 1: Energy Barrier for a Quantum Particle

In considering how the particle behaves near this barrier, we use the most fundamental equation in quantum mechanics: the Schrödinger equation. The Schrödinger equation describes a quantum particle's 'wave function', analogous to how Maxwell's equations describe electric and magnetic fields.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$
(1)

In the Schrödinger equation,  $\hbar$  is a constant, m is the mass of the particle under consideration, V(x) is the energy barrier that the particle will see, E is the energy of the particle, and  $\psi(x)$  is the wave function of the particle. The wave function is really what we want to figure out from this equation. If we know the mass of the particle, the energy of the particle, and the energy barrier that the particle will encounter, we can solve for  $\psi(x)$ , and find what we are looking for. Once we know  $\psi(x)$ , we can calculate many other properties, and essentially know 'everything' there is to know about the system.

Physically, the wave function tells us something about the probability of finding the particle in different locations of space. We know that the particle must be located somewhere in space, and this can be represented in the following way:

$$\int_{-\infty}^{+\infty} \left|\psi(x)\right|^2 dx = 1 \tag{2}$$

This equation states that by taking the absolute value of the wave function, squaring it, and summing that quantity over all space (or in this case, over an infinitely long one-dimensional line), we should find that quantity to be exactly equal to 1. In other words, because the square of the wave function tells us the probability of finding a particle within a given region of space, if we look for the particle in the entirety of space, our probability of finding it is 100%. On the face of it, this equation might not seem to tell us much. However, this property is frequently exploited in quantum mechanics. Since we can never know the position of a particle with 100% accuracy, we are forced to use this relationship and say that the particle will certainly be located somewhere in a select region of space.

## **Basics of Tunneling**

In studying quantum tunneling, we can solve the Schrödinger equation for the energy barrier shown in Figure 1. We know the energy of the barrier throughout all space (V(x)), we can pick an energy (E) for the particle, and we can assume that the particle has some mass that is known (m). With all of this, we can solve for  $\psi(x)$  in each of the three regions.

For Region I and III, V(x) = 0, while in Region II, V(x) is a constant value (we will call it  $V_0$ ). Mathematically, this is written:

$$V(x) = \begin{cases} 0, & \text{for } x < 0 \text{ and } x > L \\ V_0, & \text{for } 0 \le x \le L \end{cases}$$
(3)

At this point, we need to know the energy of the electron (E). There are really three choices for the energy that we care about: the case of  $E > V_0$ , the case of  $E = V_0$ , and the case of  $E < V_0$ .<sup>1</sup> The case of E = 0 is one that the tutorial does not cover, so we do not consider it here.

In the case of both  $E > V_0$  and  $E < V_0$ , we first solve for  $\psi(x)$  in each of the three regions separately. The Schrödinger equation is a second-order equation, so every time we solve it, we will have 2 unknown quantities. We have to solve this equation for three different regions in space, so we should expect to have 6 unknown quantities, for which, we will need boundary conditions to pin down. We can start figuring out the boundary conditions by think about two constraints on the wave function. The first of these is:  $\psi(x = 0)_{R1} = \psi(x = 0)_{R2}$  and  $\psi(x = L)_{R2} = \psi(x = L)_{R3}$ , meaning that the wave function must be continuous across the two boundaries (so that there can be no discontinuities in  $\psi(x)$ . The second constraint is that the slope of the wave function across these boundaries must also be the same:  $\psi(x = 0)_{R1} = \psi(x = 0)_{R2}$ 

<sup>&</sup>lt;sup>1</sup>Also note that E can never be less than 0, since in such a case, there is no solution to the Schrödinger equation. We assume that E > 0 for this problem.

and  $\psi'(x = L)_{R2} = \psi'(x = L)_{R3}$ .<sup>2</sup> These two conditions provide 'boundary conditions' for solving the Schrödinger equation given in (1).

In the case of both  $E > V_0$  and  $E < V_0$ , the solutions for  $\psi(x)$  take the same form in Region I and Region III. We skip over the details of solving this, and simply write them here:

$$\psi_{R1}(x) = Ae^{ikx} + Be^{-ikx} \tag{4}$$

$$\psi_{R3}(x) = Fe^{ikx} + Ge^{-ikx} \tag{5}$$

where  $k = \sqrt{2mE/\hbar^2}$ , and we give different amplitudes (A, B, F and G) for the two regions to indicate that the amplitudes may be different across the different regions. Note that these solutions are just sine waves, with one sine wave (the +ikxterm) traveling towards positive x and the other (the -ikx term) traveling towards negative x. A sum of sine waves simply adds to another sine wave, so the wave function in both Region I and Region III looks like a sinusoidal wave.

If we consider the case of  $E > V_0$ , the solution to the Schrödinger equation in Region II takes the same form as (4), but the constant k is slightly different. We can write this solution as:

$$\psi_{R2}(x) = Ce^{ik_2x} + De^{-ik_2x} \tag{6}$$

where  $k_2 = \sqrt{2m(E - V_0)/\hbar^2}$ . The difference between  $k_2$  and k is important, because it tells us something about how the wavelengths in Region I and III compare to the wavelength in region II. Recall that  $k = 2\pi/\lambda$ , where  $\lambda$  is the wavelength of the sine wave. Because  $k_2 < k$ , we should expect that  $\lambda_2 > \lambda$ . Therefore the wave function has a larger wavelength in Region II, so the solution looks slightly different.

In the case of  $E < V_0$ , the solution to the Schrödinger equation in Region II no longer looks like a sine wave. The reason for this is that because  $V_0$  is larger than E, the only acceptable solution in that region takes the form of real exponentials. Thus, we can write the solution in Region II for  $E < V_0$  as:

$$\psi_{R2}(x) = Ce^{\kappa x} + De^{-\kappa x} \tag{7}$$

where  $\kappa = \sqrt{2m(V_0 - E)/\hbar^2}$ . Here, we have a term with exponential decay in x added to a term with exponential increase in x.

At this point, we have solved the solutions to Schrödinger's equation in all of the three regions for the case of  $E > V_0$  and the case of  $E < V_0$ . Here, we summarize our solutions:

<sup>&</sup>lt;sup>2</sup>These two constraints are postulates of quantum mechanics; there is really no other way to explain why we use this.

For  $E > V_0$ :

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & \text{for } x < 0\\ Ce^{ik_2x} + De^{-ik_2x}, & \text{for } 0 \le x \le L\\ Fe^{ikx} + Ge^{-ikx}, & \text{for } x > L \end{cases}$$
(8)

For  $E < V_0$ :

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & \text{for } x < 0\\ Ce^{\kappa x} + De^{-\kappa x}, & \text{for } 0 \le x \le L\\ Fe^{ikx} + Ge^{-ikx}, & \text{for } x > L \end{cases}$$
(9)

As is the process with solving any differential equation, after solving for the general solutions (as we have now done), we must plug in boundary conditions to solve for the unknown quantities. In our situation, we now have 6 unknown quantities (A, B, C, D, F, and G) for both cases of E.<sup>3</sup> So far, we have discussed four boundary conditions: the condition that  $\psi(x)$  must be continuous at both x = 0 and x = L (this gives us two), and the fact that  $\psi'(x)$  must be continuous at both x = 0 and x = L. However, we have 6 unknown quantities, so it seems we need 2 more boundary conditions.

To determine the remaining boundary conditions, we must refer to the physical situation that we are dealing with. We are interested in a particle approaching the barrier from either the left side (Region I, moving in the direction of +x) or a particle approaching from the right side (Region III, moving in the direction of -x).

In the first case, we can consider what happens to the particle as it approaches the energy barrier. Starting with the change in V(x) at x = 0, we can have some transmission of the wave function, as well as some reflection of the wave function. Recall that the top equation in (8) and (9) describes the sum of a right-going wave (corresponding to the coefficient A) and a left-going wave (corresponding to B). By saying that the wave is coming from Region I, we are essentially saying that at  $x \to -\infty$ , we are setting the amplitude of A at some constant value. On the other hand, if we were talking about case 2 (the left-going wave), we would be saying that at distance  $x \to +\infty$ , we are fixing G to be a constant value. Therefore, by giving information about where the particle is coming from, we have provided ourselves one more boundary condition, and know everything there is to know about A or G.<sup>4</sup>

If we continue to consider the first case of the wave approaching from Region I, the barrier at x = 0 can allow for some reflection of the wave, and some transmission

<sup>&</sup>lt;sup>3</sup>Note that by unknowns, we are not referring to the energy (E), mass (m), or potential (V(x)), nor anything that depends on those quantities (such as  $k, k_2$ , or  $\kappa$ ). We assume that those quantities are chosen for our given physical situation, and that we now want to watch what happens.

<sup>&</sup>lt;sup>4</sup>It may seem strange to say that A or G is now known, when we haven't set A or G equal to some quantity. But remember that A and G are just constants; we could arbitrarily rename them something else, but it won't make a difference in our calculation at this point.

of the wave. The transmitted wave can then continue to the barrier at x = L, and some of it can be transmitted and some can be reflected back.<sup>5</sup> For the wave that is transmitted to Region III, we can now follow the wave along its path towards  $x \to +\infty$ . This wave never encounters a barrier, and because of this, we can say that there is no reflected wave in this region. Since there is no reflected wave, we know that G in (8) must be 0 (remember that x and k are non-zero, so the only way to get rid of this term altogether is to eliminate G). If we were looking at the case of the wave approaching from the right, we could apply the exact same reasoning and decide that  $A \to 0$ , since the left-going wave in Region I never encounters a barrier to reflect off of.

Let us now summarize what the wave function should look like for these different cases:

For  $E > V_0$ , assume the wave is traveling towards the right. In Region I, we have a sine wave that will be both reflected and transmitted. In Region II, we have another sine wave (this time with a larger wavelength), which will be both transmitted and reflected. In Region III, we have another sine wave with the same wavelength as in Region I, but with no reflection.

For  $E < V_0$ , again assume the wave travels towards the right. Region I looks qualitatively the same as it did for the case of  $E > V_0$ . In Region II, the solution becomes a sum of real exponentials, which is dominated by the exponential decay term. Therefore, the wave function is "dying off" in Region II. This means that in Region III, though the wave function again appears sinusoidal, the amplitude in this region is smaller than in Region I.

Also note that this solution to the wave function is not physically real, since it is not normalized. That is to say that we can not integrage the probability density over all space and come up with a value that is anything but infinite. (Imagine trying to integrate a  $\sin^2(x)$  function over all space. The area under the curve is infinite.) To make this physically real, we would have to use many different solutions to this problem (i.e. many energy values) so that we could sum those different solutions into a wave 'packet', which can be normalized. The reason we use this non-physical situation is because it is simpler and still gives a great deal physical inition into the nature of tunneling.

<sup>&</sup>lt;sup>5</sup>It is common to worry about the reflected wave in Region II going back and transmitting back into Region I, and even worse, some of it bouncing back and forth inside the barrier until it decides to leave at some random time. It might seem like we can't say exactly where the reflected and transmitted waves are going to go for all times. Fortunately, we don't have to worry about this, since the four boundary conditions mentioned earlier take care of this automatically by forcing  $\psi(x)$ and  $\psi'(x)$  to be continuous at x = 0 and L.

## References

- [1] Taylor, J.R., Zafiratos, M.D., and Dubson, M.A. (2003). Modern Physics for Scientists and Engineers. Addison-Wesley. ISBN-10: 013805715X
- [2] Krane, K.S. (2012). Modern Physics, 3rd Ed. Wiley. ISBN-10: 1118061144.
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## **Tutorial: Quantum Tunneling**

### PART A: CLASSICAL PARTICLE

A ball of mass *m* rolls to the right on a flat, frictionless surface with total energy E = 3mgh. The ball soon encounters a sloped surface and rolls up to height 2h. After, the ball rolls back



down the ramp, always staying in contact with the surface.

- 1) Is the total energy of the ball as it rolls from 0 to 3L increasing, decreasing, or staying the same?
- 2) Sketch the kinetic energy, gravitational potential energy, and total energy of the ball between 0 and 3L. Scale your graph with multiples of mgh.

3) Is the amount of time the ball spends between L and 2L greater than, less than, or equal to the amount of time it spends between 0 and L? How does it compare to the amount of time it spends between 2L and 3L? (Ignore the time the ball spends on the ramp.)

4) Now imagine that we take a photograph of the ball at some random time. Is the probability of finding the ball between 0 and L greater than, less than or equal to the probability of finding it between L and 2L? Why?

## PART B: SOLUTIONS TO SCHRÖDINGER'S EQUATION

The time-independent Schrödinger equation is given by:

$$\frac{-\mathbf{h}^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E_{TOT}\psi(x)$$

This can be rewritten as:

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{h^2} (E - V)\psi = \frac{2m}{h^2} (V - E)\psi$$

1) If E < V, will the solutions to Schrödinger's equation be real exponentials or complex exponentials? [Hint: Is the quantity on the right-hand side positive or negative in this case?]

2) Write down the most general solution to Schrödinger's equation for the case when E < V.

3) If E > V, will the solutions to Schrödinger's equation be real exponentials or complex exponentials? [Again, consider whether the right-hand side is positive or negative.]

4) Write down the most general solution to Schrödinger's equation for the case when E > V.

## PART C: ELECTRON IN A WIRE $(E > V_{\theta})$

Consider an electron with total energy E moving to the right through a very long smooth copper wire with a *small* air gap in the middle:



Assume that the work function of the wire is  $V_{\theta}$  and that V = 0 inside the wire.

1) If  $E > V_0$ , draw a graph of the electron's potential energy in all three regions. Also draw a dashed line indicating the total energy of the electron.

2) In each of the three regions, are the solutions to Schrödinger's equation real exponentials or complex exponentials? Write down a solution for each of the three regions corresponding to an electron traveling to the right.

**Region I:** 

**Region II:** 

**Region III:** 

3) How does the kinetic energy of the electron compare in each of the three regions? Rank the kinetic energies in the three regions  $(KE_1, KE_2 \& KE_3)$  from high to low.

4) How does the deBroglie wavelength of the electron compare in each of the three regions? Rank the wavelengths in the three regions  $(\lambda_1, \lambda_2, \lambda_3)$  from largest to smallest. If the wavelength is not defined in a particular region, then say so.

**5)** How does the amplitude of the electron's wave function compare in each of the three regions? [Hint: think about  $|\psi(x)|^2$  what tells you in terms of probabilities].

6) With this information in mind, sketch the *real part* of the electron's wave function in all three regions:



### PART D: ELECTRON IN A WIRE (E < V)

Consider the same situation as in **Part C**, but now the total energy E of the electron is *less than* the work function  $V_{\theta}$ .

1) If  $E < V_0$ , draw a graph of the electron's potential energy in all three regions. Also draw a dashed line indicating the total energy of the electron.

2) In each of the three regions, are the solutions to Schrödinger's equation real exponentials or complex exponentials? Write down a solution for each of the three regions corresponding to an electron traveling to the right.

**Region I:** 

**Region II:** 

**Region III:** 

3) How does the kinetic energy of the electron compare in each of the three regions? Rank the kinetic energies in the three regions  $(KE_1, KE_2 \& KE_3)$  from high to low.

4) How does the deBroglie wavelength of the electron compare in each of the three regions? Rank the wavelengths in the three regions  $(\lambda_1, \lambda_2, \lambda_3)$  from largest to smallest. If the wavelength is not defined in a particular region, then say so.

5) How does the amplitude of the electron's wave function compare in each of the three regions? [Hint: think about  $|\psi(x)|^2$  what tells you in terms of probabilities]. Explain what physical meaning we can make from the shape of the wave function in Region II.

6) With this information in mind, sketch the *real part* of the wave function for this electron:



7) Using the solution to #6, what conclusions can you make about the possible position of the particle? How is this different than a classical particle in the same situation? Can you offer an explanation of why classical objects (people) don't exhibit the same property, called tunneling?

## **Tutorial: Quantum Tunneling with PhET Simulation**

#### Part A: Classical Particle

A ball of mass *m* rolls to the right on a flat, frictionless surface with total energy E = 3mgh. The ball soon encounters a sloped surface and rolls up to height 2h. After, the ball rolls back down the ramp, always staying in contact with the surface.



- 1) Is the total energy of the ball as it rolls from 0 to 3L increasing, decreasing, or staying the same?
- 2) Sketch the kinetic energy, gravitational potential energy, and total energy of the ball between 0 and 3L. Scale your graph with multiples of mgh.

3) Is the amount of time the ball spends between L and 2L greater than, less than, or equal to the amount of time it spends between 0 and L? How does it compare to the amount of time it spends between 2L and 3L? (Ignore the time the ball spends on the ramp.)

4) Now imagine that we take a photograph of the ball at some random time. Is the probability of finding the ball between 0 and L greater than, less than or equal to the probability of finding it between L and 2L? Why?

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#### PART B: Quantum Particle with E > V (Using PhET sim)

 Observe the plot of the wave function for plane wave solutions for the case where E > V. Where does the time-dependent oscillation come from mathematically? Describe how the frequency of oscillation changes as you change E.

2) Now widen the width of the wire gap (where V > 0) to 3.5 dashed-lines wide. How does the wavelength of the wave function in this region compare to the wavelength in the region to the left? How about to the region on the right? Lastly, how do the wavelengths in the regions on the left and right compare to each other?

3) What does your answer to (2) tell you about the kinetic energy of the particle in each of these three regions? Be sure to discuss this with your group members.

4) Now refer back to the classical particle case. How does the kinetic energy of the classical particle from L to 2L relate to the kinetic energy wave function in the air gap? What does this say about the relationship between wavelength and kinetic energy?

5) Now let's look at the amplitude of the wave function. What does the amplitude of  $\psi$  (or  $|\psi|^2$ ) tell you?

6) If we were to make a measurement of position of the particle, would we be more likely to find it in the region to the left of the air gap or in the air gap (for now ignore the region to the right of the air gap)?

7) In this case of E > V, explain how measurements of position for a quantum particle compare to taking a photograph of a classical particle.

### PART C: Classical Particle with E < V

Now imagine that the same ball from PART A has an initial total energy of E = 1.5 mgh, while the height of the hill remains at 2h.

1) What happens to the ball as it starts to go up the hill? Is it possible for the ball to be found between L and 2L? How about between 2L and 3L?

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#### PART D: Quantum Particle with E < V

1) Now, using the PhET sim, decrease the size of the wire gap to 1 dashed-line wide and increase the height of the potential energy line all the way to the top. What type of function do you see in region 1 and 3 (e.g. sinusoidal, exponential growth, exponential decay, linear, quadratic, etc)?

2) What type of function is shown inside the wire gap (e.g. sinusoidal, exponential decay, exponential growth, linear, etc.)? Hint: It might be more obvious if you look at the wave function when the air gap is very wide... but return to 1 dashed-line wide for the next question!

3) How do the wavelengths of the wave function on the left and right of the air gap compare to each other? What does that tell you about the kinetic energy of the particle in each of those regions?

4) Now refer back to PART C with the classical particle. How does the kinetic energy of the classical particle in regions 2 and 3 compare to the kinetic energy of the quantum particle in regions 2 and 3?

5) What does the amplitude of  $\psi$  (or  $|\psi|^2$ ) tell you about finding a particle in regions 2 or 3?

6) If we were to make a measurement of the particle's position with E < V, which region would we be most likely to find it in? Compare this to the case of the classical particle.

## PHYS 3220 PhET Quantum Tunneling Tutorial

#### Part I: Mathematical Introduction

Recall that the Schrödinger Equation is  $i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t)$ . Usually this is solved by first assuming that  $\Psi(x,t) = \psi(x)\phi(t)$ , from which we obtain the solution  $\phi(t) = e^{-iEt/\hbar}$  and are left with the following equation to solve for the spatial dependence:

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

1. Consider a potential region such as the one shown in the figure below. Given that  $E > V_0$ , write down a general solution of the Schrödinger Equation for each region. Define any constants that will simplify your solution.



2. How many boundary conditions are needed to completely specify this situation?

3. If a right-going plane wave with amplitude A originating from  $x \to -\infty$  is incident upon the barrier, what simplifications can be made in your above equations? Which of your unspecified constants (if any) are now specified completely?

4. What are the remaining boundary conditions for this system? (A simple mathematical formula or explanation in words are both acceptable.)

5. Using this information, do your best to make a plot of the wave function for the case of  $E > V_0$ .



- 6. In the graph that you just drew, did you account for the wavelength and amplitude differences in the three regions? (Don't change your graph, just think about it!)
  - (a) Rank the magnitude of the wavelengths for the three regions.

(b) How do you expect the amplitude to compare across the three regions? Give a brief qualitative explanation.

#### Part II: Plane Wave of $E > V_0$ using PhET sim

Download the Tunneling PhET sim, found at: http://phet.colorado.edu/sims/quantum-tunneling/ quantum-tunneling\_en.jar. Play with the sim for a bit, and then switch to "Plane Wave" mode to answer the following questions.

# Notice: For this tutorial, you may find it very useful to switch between using the "Separate" and "Sum" representations on the sim!!!

- 1. Comparing your findings in Part I to the sim:
  - (a) What are the main differences between your plot of the wave function and what is shown?

(b) Do your predictions for wavelength and amplitude agree with what you see? If not, why were your predictions wrong?

- 2. You should be able to see the wave function in Region 1 bob up and down.
  - (a) What causes this? (You might find the 'Notice' at the top of the page helpful!)

(b) List *all* parameters that you can adjust to eliminate this "bobbiness." Is there only one way to do this, or are there several different ways?

- 3. Play with the sim and maximize the amount of transmission to Region 3.
  - (a) What parameters affect the amount of transmission in this region? List them all. Again, is there only one way to maximize the amount of transmission, or are there multiple ways?

(b) How does the case of maximum transmission compare to "eliminating the bobbiness" in region 1? Give a brief qualitative explanation of why this is the case.

(c) Often times the probability of transmission is denoted by the variable T, and takes the following form:

$$T = \frac{1}{1 + \frac{V_0 \sin^2(k_2 L)}{4E(E - V_0)}}$$

According to this equation, what condition must be satisfied for maximum transmission to occur?

(d) How many variables does the Transmission probability depend on (don't forget to think about what  $k_2$  depends on)? Does this account for everything you found in 3a?

4. Is there any way to set up the sim such that there is a time-dependence in the probability density? Use the fact that  $\Psi_{\text{region }j} = A_j e^{i(k_j x - \omega_j t)} + B_j e^{-i(k_j x + \omega_j t)}$  to justify your answer.

- 5. (a) Based on your result from 4, which regions can show sinusoidal probability densities in the spatial dependence?
  - (b) Is there any way to make Region 3 have a sinusoidal probability density?
  - (c) Under what conditions can you have a sinusoidal probability density?

## Part III: Case of $E < V_0$

1. For the case of  $E < V_0$ , write down the most general solutions to the Schrödinger Equation for each of the three regions. Define any constants that help simplify your answers.

2. This time, assume that a left-going plane wave with *fixed amplitude* originating from  $x \to +\infty$  is incident upon the barrier. Which variables are now "fixed" or completely specified? List the remaining boundary conditions using a simple mathematical expression.

3. Do your best to plot  $\psi(x)$  vs. x across all three regions.



#### Using the sim for $E < V_0$

1. What parameters can you adjust to maximize the amount of transmission to Region 1 in the sim? List all of the possible ways.

2. (a) When  $E < V_0$ , is there any way to completely eliminate the reflected wave in Region 3?

(b) Assuming that the potential barrier,  $V_0$ , has *some* finite width, is there any way to get 100% transmission in this case? Why is this the case?

3. Looking at the wave function in the potential barrier, is there any similarity to the case of  $E > V_0$ , where there was a reflected wave and a transmitted wave? Is the full wave function a sum of solutions or just one particular solution?

## **Build a Molecule Computer Sim**

#### Learning Goals:

- 1. Describe the difference between a molecule name and chemical formula.
- 2. Distinguish between the coefficient and subscript in a chemical formula.
- 3. Use pictorial representations of molecules to generate chemical formulas.

#### First Tab

- 1. Make a molecule:
  - a. How do you know you made a molecule? \_\_\_\_\_

\_\_\_\_\_

- b. Write the **name** of some molecules you made (ex. Water).
- 2. Molecule Names and Chemical Formulas:
- a. Compare the name and chemical formula for some molecules:

| Molecule Name | Drawing | Chemical Formula |
|---------------|---------|------------------|
|               |         |                  |
|               |         |                  |
|               |         |                  |
|               |         |                  |
|               |         |                  |
|               |         |                  |
|               |         |                  |

5

#### Second Tab

#### 3. Make Many

a. Fill all the collection boxes and then complete the questions for each Goal.

| Goal: 4H <sub>2</sub>                 |  |  |
|---------------------------------------|--|--|
| Draw it!                              |  |  |
|                                       |  |  |
| What does the big '4' in $4H_2$ mean? |  |  |
| What does the little '2' in 4H2 mean? |  |  |

| Goal: 2CO <sub>2</sub>                             |  |  |
|--|--|--|
| Draw it!   |  |  |
|  |  |  |
| What does the big '2' in $2CO_2$ mean?             |  |  |
| What does the little '2' in 2CO <sub>2</sub> mean? |  |  |

| Goal: 20 <sub>2</sub>                                |  |  |
|--|--|--|
| Draw it!   |  |  |
|  |  |  |
| What does the big '2' in $2O_2$ mean?                |  |  |
| What does the little $_{2}$ in 20 <sub>2</sub> mean? |  |  |

| Goal: 2NH <sub>3</sub>  |  |  |
|---|--|--|
| Draw it!  |  |  |
|   |  |  |
| What does the big '2' in $2NH_3$ mean?                          |  |  |
| What does the little ' <sub>3</sub> ' in 2NH <sub>3</sub> mean? |  |  |

#### Third Tab Challenge

4. What's the biggest molecule you can make?

- a. Molecule Name: \_\_\_\_\_
- b. Chemical formula:

5. Can you make a molecule that can be broken into smaller molecules?

- a. Big molecule **name**: \_\_\_\_\_
- b. Big molecule **chemical formula**:
- c. Smaller molecule **names**: \_\_\_\_\_
- d. Smaller molecule chemical formulas:

## **Build a Molecule Pre-Lab (Statistics)**

**1.** We use symbols to represent atoms.

- a. What is the chemical symbol for the atom Hydrogen?\_\_\_\_\_
- b. What is the chemical symbol for atom Oxygen?\_\_\_\_\_
- c. What is the chemical symbol for the atom Carbon?\_\_\_\_\_

|    |           | Ν  | N %   |
|----|-----------|----|-------|
| 1a | Correct   | 43 | 74.1% |
|    | Incorrect | 12 | 20.7% |
|    | N/A       | 3  | 5.2%  |
| 1b | Correct   | 44 | 75.9% |
|    | Incorrect | 12 | 20.7% |
|    | N/A       | 2  | 3.4%  |
| 1c | Correct   | 39 | 67.2% |
|    | Incorrect | 17 | 29.3% |
|    | N/A       | 2  | 3.4%  |

About 3/4 of the students could write the correct chemical symbols from the element names.

**2.** We use chemical formulas to represent individual molecules and groups of molecules. Write the chemical formula below each molecule or groups of molecules





|    |                   | Ν  | N % |
|----|-------------------|----|-----|
| 2a | Correct           | 33 | 57% |
|    | Name, not Symbols | 14 | 24% |
|    | other             | 10 | 17% |
|    | N/A               | 1  | 2%  |

|    |                   | Ν  | N % |
|----|-------------------|----|-----|
| 2b | Correct           | 37 | 64% |
|    | Name, not Symbols | 14 | 24% |
|    | other             | 7  | 12% |
|    | N/A               | 0  | 0%  |

| c. |  |  |
|----|--|--|

|    |                   | Ν  | N % |
|----|-------------------|----|-----|
| 2c | Correct           | 29 | 50% |
|    | Name, not Symbols | 0  | 0%  |
|    | other             | 24 | 41% |
|    | N/A               | 5  | 9%  |



|    |                   | Ν  | N % |
|----|-------------------|----|-----|
| 2d | Correct           | 31 | 53% |
|    | Name, not Symbols | 24 | 41% |
|    | other             | 2  | 3%  |
|    | N/A               | 1  | 2%  |



|    |                   | Ν  | N % |
|----|-------------------|----|-----|
| 2e | Correct           | 0  | 0%  |
|    | Name, not Symbols | 15 | 26% |
|    | H8, all or part   | 28 | 48% |
|    | Other             | 10 | 17% |
|    | N/A               | 5  | 9%  |

#### **3.** Try it!

| Draw CO <sub>2</sub>   |  |
|------------------------|--|
|                        |  |
|                        |  |
| Draw 2H <sub>2</sub> O |  |
|                        |  |
|                        |  |
| Draw 3N <sub>2</sub>   |  |
|                        |  |
|                        |  |
|                        | Draw CO <sub>2</sub><br>Draw 2H <sub>2</sub> O<br>Draw 3N <sub>2</sub> |

|       |                | Count | Column N % |
|-------|----------------|-------|------------|
| Pre3a | 2 O, 1 C       | 43    | 75%        |
|       | Other          | 7     | 12%        |
|       | N/A            | 7     | 12%        |
| Pre3b | 2 separate H2O | 14    | 24%        |
|       | 2 H, 2 O       | 17    | 29%        |
|       | Other          | 21    | 36%        |
|       | N/A            | 6     | 10%        |
| Pre3c | 3 separate N2  | 10    | 17%        |
|       | 3 N Together   | 18    | 31%        |
|       | other          | 18    | 31%        |
|       | N/A            | 12    | 21%        |

## **Build a Molecule Post-Lab (Statistiscs)**

**1.** We use chemical formulas to represent individual molecules and groups of molecules. Write the chemical formula below each molecule or groups of molecules.

| N N 9   | ó                            |  |
|---|------------------------------|--|
| 1a Correct 50 88  | %                            |  |
| Name, not Symbol 5  | %                            |  |
| a. Other 1 2  | %                            |  |
| N/A 1 2   | %                            |  |
|   | N                            | N %  |
| 1b Correct  | 38                           | 67%  |
| HOH HOH Name, not Symbol  | 4                            | 7%   |
| b. Molecular Formula, no coefficient                                | 3                            | 5%   |
| other   | 9                            | 16%  |
| N/A   | 3                            | 5%   |
|   | Ν                            | N %  |
| 1c Correct  | 36                           | 63%  |
| Name, not Symbol  | 4                            | 7%   |
| Molecular Formula, no coefficient                                   | 5                            | <b>9%</b>                                  |
| O6 as all or part of answer   | 7                            | ' 12%                                      |
| Other   | 5                            | <i>\$</i> 9%                               |
| N/A   | (                            | ) 0%                                       |
|   | Ν                            | N %  |
| 1d Correct  | 40                           | 70%  |
| Name, not Symbol  | 2                            | 4%   |
| Molecular Formula, no coefficient                                   | 1                            | 2%   |
| a. N6 as all or part  | 9                            | 16%  |
| Other   | 4                            | 7%   |
| N/A   |                              | 00/  |
|   | 1                            | 2%   |
|   |                              | 2%   |
| 1a Correct  | 1<br>N                       | 2%<br>N %                                  |
| 1e Correct  | 1<br>N<br>36                 | 2%<br>N %<br>63%                           |
| 1e Correct<br>Name, not Symbol<br>Molocular Formula, po coofficient | 1<br>N<br>36<br>3            | <u>N %</u><br>63%<br>5%                    |
| <b>HHHHHHHHHHHHH</b>  | 1<br>36<br>3<br>4            | <u>N %</u><br>63%<br>5%<br>7%              |
| H H H H H H H H H H H H H H H H H H H                               | 1<br>36<br>3<br>4<br>11<br>3 | <u>N %</u><br>63%<br>5%<br>7%<br>19%<br>5% |

#### 2. Try it!

| a. Draw 2CO <sub>2</sub>  |  |
|---------------------------|--|
| b. Draw 3H <sub>2</sub> O |  |
| c. Draw 4N <sub>2</sub>   |  |
| d. Draw $2NH_3$           |  |

|    |                   | Ν  | N % |
|----|-------------------|----|-----|
| 2a | 2 separate CO2    | 43 | 74% |
|    | 1 CO2             | 3  | 5%  |
|    | 2C, 2O together   | 3  | 5%  |
|    | Other             | 9  | 16% |
| 2b | 3 separate H2O    | 39 | 67% |
|    | Separate H2O      | 8  | 14% |
|    | 3H, 2O together   | 7  | 12% |
|    | Other             | 3  | 5%  |
|    | N/A               | 1  | 2%  |
| 2c | 4 separate N2     | 45 | 78% |
|    | Separate N2       | 5  | 9%  |
|    | 4 N together      | 4  | 7%  |
|    | Other             | 3  | 5%  |
|    | N/A               | 1  | 2%  |
| 2d | 2 separate NH3    | 39 | 67% |
|    | Separate NH3      | 2  | 3%  |
|    | 2 N, 3 H together | 5  | 9%  |
|    | Other             | 10 | 17% |
|    | N/A               | 2  | 3%  |

#### 3. Molecule Names vs. Chemical Formulas

- a. Give an example of a molecule name: \_\_\_\_\_
- b. Give an example of a chemical formula:
- c. What is the difference between a molecule name and a chemical formula?

|    |                 | Ν  | N % |
|----|-----------------|----|-----|
| 3a | Correct         | 46 | 81% |
|    | Incorrect       | 11 | 19% |
|    | N/A             | 0  | 0%  |
| 3b | Correct         | 49 | 86% |
|    | Incorrect       | 8  | 14% |
|    | N/A             | 0  | 0%  |
| 3c | Correct         | 19 | 33% |
|    | Formula Correct | 9  | 16% |
|    | Name Correct    | 1  | 2%  |
|    | Other           | 28 | 49% |
|    | N/A             | 0  | 0%  |