Your Name: ____

Your lab partner(s): ____

Lab 10: Quantum States and Tunneling
(Instructions partially adopted from
http://phet.colorado.edu/en/simulations/keyword/quantumMechanics)

Purpose:

- To visualize plane waves and wave packets and study how they relate to each other
- To investigate the real and imaginary parts and magnitude of a wave function
- To visualize wave functions for constant, step and barrier potentials
- To study how the reflection and transmission probabilities are related to the energy of the wave, the energy of the step or barrier and the width of the barrier
- To visualize wave functions, probability densities, and energy levels for bound states in Square and Harmonic Oscillator potentials
- To investigate what is and is not time-dependent for an energy eigenstate
- To predict how the spacing of energy levels depends on the potential and the particle's mass.

Theory: Consult your class notes and textbook for theoretical explanations of relevant quantum mechanical phenomena. Keep in mind that a wave packet consists of individual waves of different frequencies. Each wave moves with its own phase velocity, v_{ph}. A wave packet moves at the group velocity, v_g. In general, $v_g \neq v_{ph}$.

Procedure: Access the program at http://phet.colorado.edu/en/simulation/quantum-tunneling.
Click on the **Run Now!** button.

I. Introduction to the Program **(the bold text denotes clickable choices)**

1. Click through the pull-down menu called **Potential**, in the right upper corner of the screen, to become familiar with various potentials used in the program.
2. Click on **Reset All**, then click **Yes**. Select the default **barrier/well** potential. Select the first two boxes to show the values for energy and reflection and transmission probabilities. Uncheck the boxes.
3. Select the **plane wave** box. Then, select each box in the **Electron Wave Function form** to observe the displays of the magnitude and real and imaginary parts of the wave function.
4. Click the **Start** button (►) to observe the time dependence of the wave function and probability density. Click the (▌◄◄) button to rewind to t = 0. You can step through a simulation by repeatedly clicking the (▌►) button.
5. The values of the total energy, potential energy and the barrier parameters can be changed by dragging the arrows in the top-most window. These values can be adjusted more precisely within the **Configure Energy** window. Change each of these values and observe how it affects the magnitude of the wave function, as well as the probability density.

Remember: Click the (▌◄◄) button to rewind to t = 0 before each run.

II. A Free Particle

(Unless already opened, access the program at http://phet.colorado.edu/en/simulation/quantum-tunneling. Click on the **Run Now!** button.)

6. **Reset All**. Choose the appropriate potential for a free particle and select the **plane wave**. Select a positive value of E and display the **magnitude**. Vary initial widths of the packet and observe how fast the packet spreads. Answer the following:

   The initially narrower wave packet spreads ____________ than the initially wider one.
   (faster/slower)

   Explain (hint: the initially narrow and wide packets have different distributions of momenta.)

   ____

   ____

III. The Step Potential

(Unless already opened, access the program at http://phet.colorado.edu/en/simulation/quantum-tunneling. Click on the **Run Now!** button.)

In this program, different values of the potential energy can be set for $x < 0$ and $x > 0$ (V_1 and V_2, respectively). We will investigate the step potentials in two different situations:

b) The total energy $E > V_2$ and the particle is free to move into the region $x > 0$
a) The total energy $V_1 < E < V_2$ and the wave function penetrates a limited distance into the classically forbidden region, $x > 0$.

a) *Step-Up Potential*

7. **Reset All**. Select the **step potential**, **wave packet**, and **show reflection & transmission probabilities**. Set the step so that $V_2 > V_1$ (step up). Vary the value of total energy E and explain what happens to the transmission, T, and reflection, R, probabilities.

	Value	Explanation
T		
R		

8. Set $V_1 = -0.80$, $V_2 = +0.20$ and $E = +0.80$. Calculate the wave numbers k_1 (in region $x < 0$) and k_2 (in region $x > 0$). For simplicity, use that $m_e = \hbar = c = 1$.

   k_1 = ______________________ k_2 = ______________________

9. Using your values of the wave numbers, calculate the transmission and reflection probabilities and compare them to the values displayed on the screen. Show your calculations in the table below.

Show your calculations for R and T

$T_{calculated}$ = ____________________ $R_{calculated}$ = ____________________

$T_{displayed}$ = ____________________ $R_{displayed}$ = ____________________

10. Select the **plane wave** and **separate** for the **Incoming/Reflected waves**. Display the **real part** of ψ. Let the simulation run. The **real part** of ψ is:

    ________________________ for x < 0 and ___________________________ for x > 0
    (exponential/oscillatory) (exponential/oscillatory)

11. Reset the time to t = 0 and let the simulation run. After a few "femtoseconds", pause the simulation. Answer the following:

    The wave amplitudes for x < 0 are ________________ than the wave amplitude for x > 0.
    (greater/smaller)

    The wavelength in region x < 0 is _________________ than the wavelength in region x > 0.

    (greater/smaller)

12. Vary the value of E between 0.80 and -0.80. Describe what happens to the real part of ψ, probability density, T, and R in both regions. Record your observations in the table below.

When:	Describe what happens in both regions	Explain
0.20 < E		
E = 0.20		
- 0.80 < E < 0.20		
E = - 0.80		
E < - 0.80		

b) *Step-Down Potential*

13. Create a "step down" potential by setting V_1 = + 0.20 and V_2 = - 0.80. Set E = 0.80. Repeat the previous steps to answer the following:

    - The wave amplitudes for x < 0 are _______________ than the wave amplitude for x > 0.
      (greater/smaller)

    - The wavelength in region x < 0 is _______________ than the wavelength in region x > 0.
      (greater/smaller)

    - The transmission and reflection probabilities are:

      T = __________________________ R = __________________________

    - How do the values for T and R compare to those for the "step up" potential? Explain.

      ____

IV. The Barrier Potential

(Unless already opened, access the program at http://phet.colorado.edu/en/simulation/quantum-tunneling. Click on the **Run Now!** button.)

14. Select the **barrier potential** with the width of 5.0. Display the **real part** of the **plane wave**. Choose **separate** for the **Incoming/reflected waves**. Set $V_1 = -0.80$, $V_2 = +0.50$ and $V_3 = -0.40$. Vary the value of E and describe what happens to the probability density, T and R in each of the three regions. Record your observations in the table below.

When:	Describe what happens in all three regions	Explain
$0.50 < E$		
$-0.40 < E < 0.50$		
$E = -0.40$		
$-0.80 < E < -0.40$		

15. Set $E = +0.80$. Vary V_1, V_2 and V_3. Describe what happens to the probability density, T and R in all three regions. Record in the table below.

When:	Describe what happens in all three regions	Explain
V_1 increases		
V_2 increases		
V_3 increases		

V. The Square Well Potential

(Unless already opened, access the program at http://phet.colorado.edu/en/simulation/bound-states. Click on the **Run Now!** button.)

Energy values for the square well are discrete. They are determined by the boundary conditions on the wave functions. At the edges of the well the decaying wave functions of the classically forbidden regions are smoothly joined to the oscillating solutions in the well. Simpler boundary conditions (i.e., the solutions go to zero at the boundary) are exact for an infinitely deep well and are an approximation for the finite well.

16. Select the **Square** well potential and click on the **Configure Potential** button to change the well parameters. The parameters can also be changed by sliding the three arrows on the screen. Set the parameters as follows: offset 0, height 9 eV and width 1 nm. Select 1.00 m_e for the particle's mass. Display the **real part** of the **Wave Function**.

    a) How many energy levels exist within the well? __________

       Does the distance between adjacent energy levels increase or decrease as n increases?

       ____

b) Quantized total energy levels can be selected by clicking on the level (the green line will turn red and the energy value will be displayed). Click on each of the quantized levels and record energy values in the table below. Using the infinite well formula, calculate and record energies for each value of n.

value of n	E_n (eV) calculated for the infinite well	E_n (eV) for the finite well, read off the screen
1	0.373	0.30

For a given value of n, E_n for the infinite well is ___________ than E_n for the finite well
(greater/smaller)

Explain why this is the case: ____

c) What are the *approximate* boundary conditions for a particle in a finite square well (that is, how much is ψ at the boundaries)? (Hint: keep in mind the exact boundary conditions for an infinite well.)

____

17. Change the **offset** of the well to -5.0 eV. Change the energy height.
Does the number of energy levels increase or decrease with the increased well depth?

____

The lowest energy, E_1, becomes ____________ negative, as the well depth increases.
(more/less)

18. Repeat the previous step, this time changing the well width. Write your answers below.
Does the number of energy levels increase or decrease with the increased well width?

____

The lowest energy, E_1, becomes ____________ negative, as the well width increases.
(more/less)

Explain both observations (Hint: how does E_n depend on L?):

____

____

VI. The Harmonic Oscillator

(Unless already opened, access the program at http://phet.colorado.edu/en/simulation/bound-states. Click on the **Run Now!** button.)

The simplicity of the harmonic oscillator makes it useful in understanding more complex systems, often found in nature, in which a system in a state of stable equilibrium is displaced slightly and subsequently oscillates about that equilibrium.

19. Select the **Harmonic Oscillator** potential and display the **real part** of the **Wave Function**. Set the **offset** to zero and **frequency f** to 5 $(fs)^{-1}$. As n increases, the distance between adjacent energy levels:

    ____
    (increases/decreases/stays the same)

    Explain why: ____

20. Vary the angular frequency ω and answer the following.

    As ω increases, the spacing between adjacent energy levels _________________
    (increases/decreases)

    Explain why: ____

21. Click on each of the energy levels and record energy values in the table below. Expand the table as needed. Using the formula for the energy of the harmonic oscillator, calculate and record energies for each value of n.

value of n	$E_n = h \cdot f$ (eV) (calculated)	E_n (eV) (read off the screen)
0	1.64	1.64

22. For the ground state, **probability density** is the greatest

    ____
    (near equilibrium/at classical turning points)

    As n increases, the **probability density** becomes greater

    ____
    (near equilibrium/at classical turning points)

    This means that for greater energies, the particle spends more time

    ____
    (near equilibrium/at classical turning points)