Group Problems #30 - Solutions

Wednesday, November 9

Problem 1 *Constant potential using simulation*

Set up a constant potential in the "Quantum Tunneling" simulation with a plane wave.

(a) Does the phase velocity depend on the difference $E - U$ only, or also on the absolute energy E? Justify your answer with a mathematical expression.

The phase velocity of a traveling wave can be obtained by setting the phase of the traveling wave equal to a constant, and then differentiating with respect to time. In particular, we found that for $E > U$, the plane-wave solutions to the Schrödinger equations are given by:

$$\psi(x,t) = Ae^{i(kx-\omega t)}, \tag{1}$$

where A is the (complex) wave amplitude, k is the wave vector, and ω is the angular frequency of the wave. The phase ϕ of this right-moving plane-wave solution is just the real part of the argument of the exponential, $\phi = kx - \omega t$. Setting this equal to a constant and differentiating gives:

$$\phi = kx - \omega t = constant \implies \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial t}(kx - \omega t) = 0 \tag{2}$$

$$\tag{3}$$

$$\implies \frac{\partial x}{\partial t} = v_\phi = \frac{\omega}{k}. \tag{4}$$

We can use the relationship for kinetic energy, $K = p^2/(2m)$, and conservation of energy, $E = K + U$, to find an expression for the wave vector:

$$k = \frac{\sqrt{2m(E-U)}}{\hbar}. \tag{5}$$

Substituting this into Eqn. 4 and using $\omega = E/\hbar$ gives:

$$v_\phi = \frac{\omega}{k} = \frac{E}{\sqrt{2m(E-U)}}, \tag{6}$$

and we see that the phase velocity depends both on $E - U$ and also on E.

(b) Does the wavelength depend on the difference $E-U$ only, or also on the absolute energy E? Justify your answer with a mathematical expression.

The wavelength can be derived from the DeBroglie relation:

$$p = \frac{h}{\lambda} = \hbar k \longrightarrow \lambda = \frac{2\pi}{k} = \frac{h}{\sqrt{2m(E-U)}}, \tag{7}$$

and we see that λ depends only on the difference $E-U$. This makes sense since the wavelength is directly related to the momentum, which is directly related to the kinetic energy, which is given precisely by $E-U$.

Problem 2 *Step-down potential using simulation*

Set up a step-down potential on the simulation: a plane wave of energy E is incident from the left onto a step-down potential of height U_0. Consider the case when $E = \frac{4}{3}U_0$.

(a) Visually determine the ratio wavelengths, λ_t/λ_i, for these conditions.

The incident wave has $(E-U)_i = \frac{1}{3}U_0$, while the transmitted wave has $(E-U)_t = \frac{4}{3}U_0$. Thus, using Eqn. 7, the ratio of transmitted to incident wavelengths is

$$\frac{\lambda_t}{\lambda_i} = \sqrt{\frac{(E-U)_i}{(E-U)_t}} = \sqrt{\frac{1/3}{4/3}} = \frac{1}{2}. \tag{8}$$

This agrees with the simulation.

(b) Visually determine the ratio of amplitude coefficients, A_t/A_i for these conditions. Is $A_t < A_i$ or vice versa? Why? This requires a bit of thought: what does the amplitude represent (or rather, what does $|A|^2$ represent) in each of the regions?

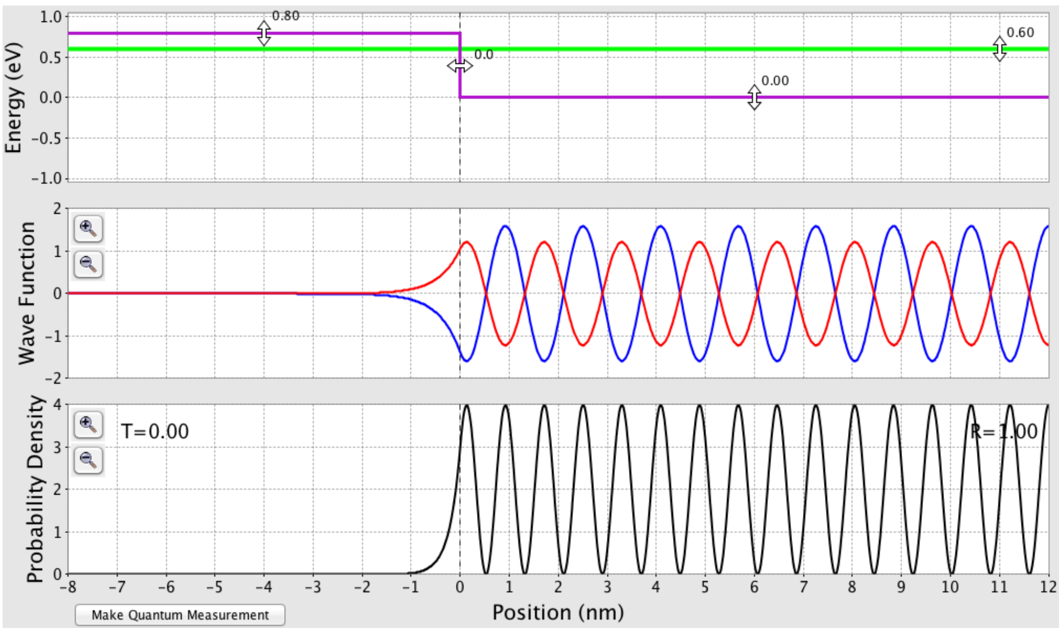
I estimate $A_t/A_i = 0.7$. This makes sense since the particles within the beam represented by the plane wave speed up after transmission past the step, and thus they spread out. Since $|A|^2 = \rho(x)$, where ρ is the particle density (number per unit length, in this case), then when they speed up, they are farther apart and A should decrease.

(c) Now make $E = \frac{3}{4}U_0$ and make the wave incident from the right (i.e., return to a step-up potential). Look at the real part of the wavefunction only and let the simulation evolve in time. To the left of the step, does the wavefunction increase or decrease with x? Why?

The wave function either increases or decreases exponentially depending on the phase of the wave at the step. In particular, the wave function always approaches zero exponentially: if the wave function is negative, then it increases exponentially toward zero; if the wave function is positive, then it decreases exponentially toward zero. This is shown in the figure below.

(d) What does the probability density look like to the left and right of the step? Why?

The probability density oscillates to the right of the step since the reflected wave interferes perfectly with the incident wave (note that the reflection coefficient is 1). The probability density decays exponentially to zero to the left of the step. This is shown in the figure below.

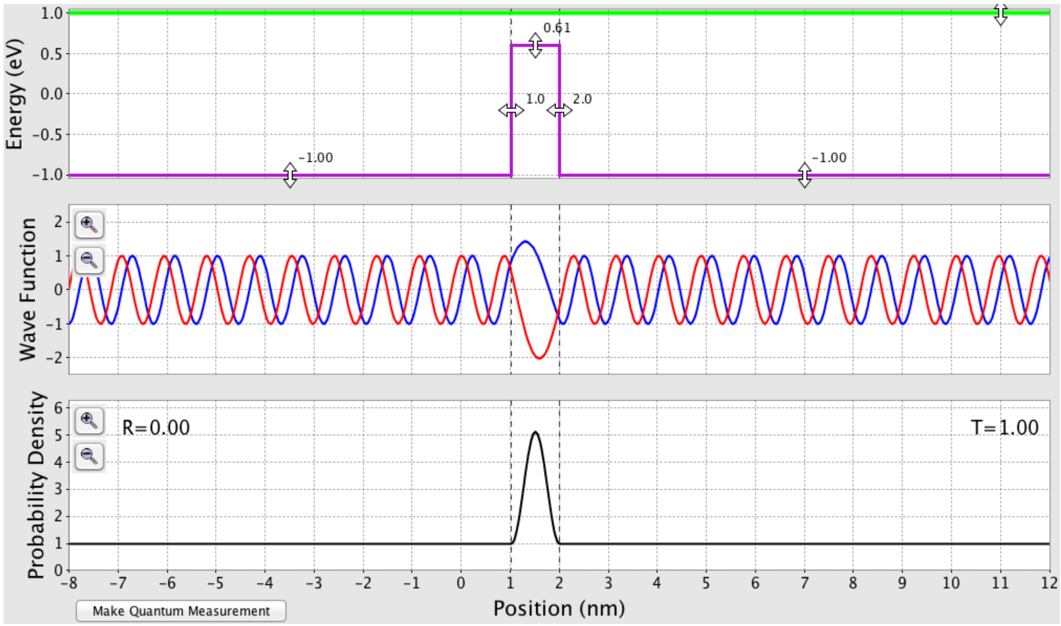


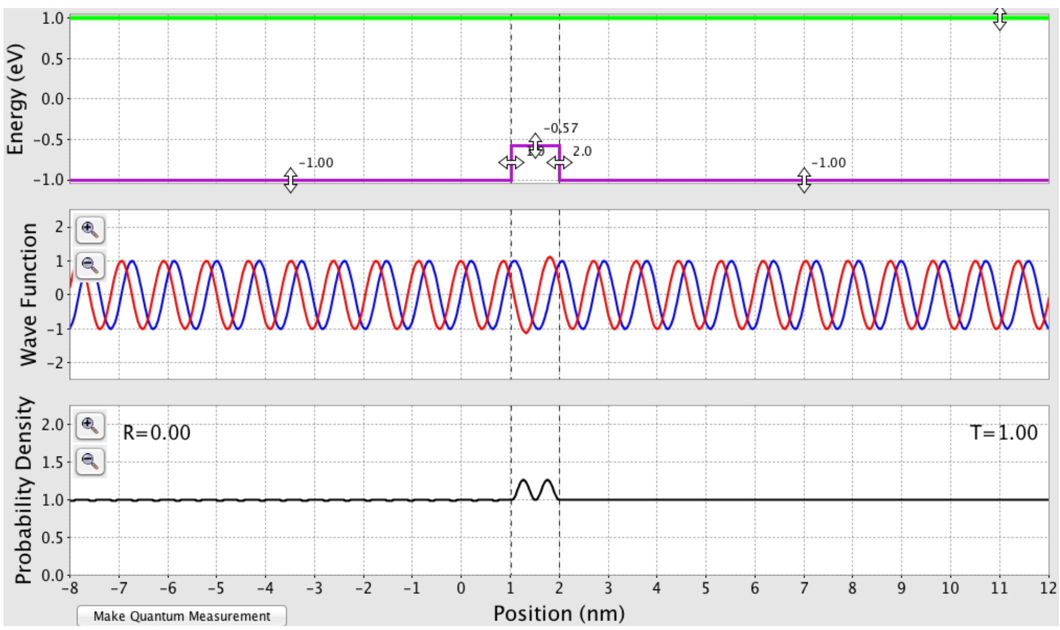
Problem 3 *Potential barrier using simulation*

Set up a potential barrier of width $L = 1$ nm, and set the total energy of the particle to $E = +1.0$ eV. Set the base of the potential barrier to $U_L = U_R = -1.0$ eV, where U_L and U_R are the values of the potential to the left and right of the barrier.

(a) Using the simulation, find the values for the height of the barrier that correspond to resonant transmission. How many different barrier heights correspond to resonant tunneling for these conditions?

There are two barrier energies corresponding to resonant transmission in this case: $U = 0.61$ eV and $U = -0.57$ eV (see below). The barrier "height" should be referenced to the value of potential energy on either side of the barrier (-1.0 eV in this case), so the two barrier heights are 1.61 eV and 0.43 eV. Note that for a barrier energy of $U = 0.61$ eV, exactly one half-wavelength fits into the region spanned by the barrier, while for a barrier energy of $U = -0.57$ eV, exactly two half-wavelengths fit into this region. In this case, it is not possible to find a barrier height with more than two half-wavelengths within the barrier region.





(b) Calculate the barrier heights corresponding to resonant tunneling under these conditions by setting the transmission coefficient to unity, $\mathcal{T} = 1$, or equivalently, the reflection coefficient to zero, $\mathcal{R} = 0$. Do these agree with the values obtained using the simulation?

From the notes (lecture 30) we have:

$$E - U = \frac{n^2 \pi^2 \hbar^2}{2mL^2} = n^2 \frac{\pi^2 (\hbar c)^2}{2mc^2\, L^2} = n^2 \frac{\pi^2 (197 \text{ eV nm})^2}{2(511 \times 10^3 \text{ eV})\, L^2} \tag{9}$$

$$\tag{10}$$

$$= n^2 \times 0.38 \text{ eV}, \tag{11}$$

where n is a positive integer, $L = 1$ nm is the barrier width, and we have used the mass of an electron $m_e c^2 = 511$ keV. (Note that there is no reason to think that the simulation uses the electron mass, but it appears that it does!) The smallest value of $E - U$ (i.e., the highest barrier for resonant tunneling) occurs for $n = 1$. Using this, we calculate $E - U = 0.38$ eV, which agrees with $U = 0.61$ eV to within roundoff error. Using $n = 2$, we find $E - U = 4 \times 0.38 = 1.52$ eV, which agrees with $U = -0.57$ eV, again to within roundoff error.