Problem Set 3

Chemistry 675, Fall 2024

Due Date: September 27, 2024

Relevant Chapter: Levine 2

1. Consider a right-moving particle subject to the potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0 \end{cases} \tag{1}$$

with energy $0 < E < V_0$.

   (a) Draw the potential energy surface making sure to remember axes labels.

   (b) Calculate the wavefunction in all regions of space.

   (c) Determine the reflection and transmission coefficients.

2. Let the wavepacket

$$\Psi(x, t = 0) = \left(\frac{A^2}{\pi}\right)^{1/4} \mathrm{e}^{-a^2(x-L/2)^2/2 + \mathrm{i}k_0 x} \tag{2}$$

describe the state of an electron in a box of length $L = 10$ au where $a = 2$ au and $k_0 = 10$ au.

   (a) Given that the position x must be a length and the argument of an exponent must be unitless, convert L, a, and k_0 to SI units.

   (b) Compute the average momentum of the electron.

   (c) Expand the wavefunction in terms of particle-in-a-box basis states.

   (d) Plot $|\Psi(x,t)|^2$ at several times $0 - 2$ au and describe the motion of the particle.

   (e) Compute the amount of time for a *classical* electron of momentum $\hbar k_0$ to pass from the center of the box to the wall.

   (f) How do the results change for different a?

   (g) How do the results change for different L?

3. Consider a left-moving particle subject to the potential

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq L \\ 0 & x > L \end{cases} \tag{3}$$

   (a) Determine the wavefunction for left-moving particles with energy $E < V_0$ either analytically or computationally with `problemset3.ipynb`.

   (b) Calculate the reflection and transmission coefficients. How do the reflection and transmission coefficients compare to the classical values? Hint: This problem indicates the existence of quantum tunneling.

   (c) Determine the wavefunction for left-moving particles with energy $E > V_0$ either analytically or computationally with `problemset3.ipynb`.

   (d) Calculate the reflection and transmission coefficients. How do the reflection and transmission coefficients compare to the classical values? Hint: This problem indicates the existence of quantum reflection.