

# 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

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

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

$$\Psi(x, t = 0) = \left(\frac{A^2}{\pi}\right)^{1/4} e^{-a^2(x-L/2)^2/2 + ik_0x} \quad (2)$$

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 right-moving particle subject to the potential

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

- (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.