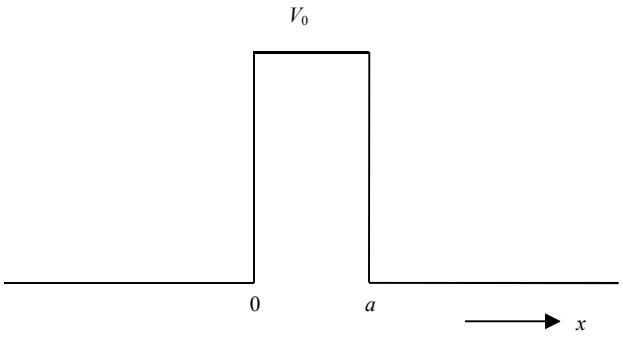
Quantum Chemistry
Exercises 2D

1. Let us consider the following potential.



According to classical mechanics a particle with energy less than the potential barrier would be reflected by the barrier, a particle with energy larger than that of the barrier would be totally transmitted. However, due to tunneling the Quantum Mechanical result is very different. Although tunneling is a purely microscopic effect, it has important consequences for our macroscopic world. For example, tunneling is largely responsible for the decay of radioactive elements. It is also thought to contribute to the high light-to-energy conversion efficiency of photosynthesis. It even has been proposed to play a role in mutation of our DNA. To get an idea of the efficiency for such processes let us calculate transmission of particle through the potential barrier.

a. Divide the problem into three regions and find the general solutions for each of the corresponding Schrödinger equations for the case that $E < V_0$.

b. Write down the boundary conditions assuming that the particle originates from $x = -\infty$.

c. Determine the reflection and transmission coefficients, i.e. the probability that the particle is reflected and transmitted, respectively, by the barrier.

d. OPTIONAL: Solve the same problem for $E>V_0$.

2. In general, one uses the square root of the variance as a measure of the uncertainty in the measurement of a quantity.

For example:

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

For the specific case of the particle in a box, determine σ_x and σ_{p_x} and verify that the product of these two quantities is consistent with the Heisenberg uncertainty principle.

3. Consider an electron in a box with length *a*. At time $t = 0$ the wavefunction is given by:

$$\Psi(x, t = 0) = \sqrt{\frac{30}{a^5}} x(a - x)$$

a. How does the wavefunction evolve with time?

b. How does the probability evolve with time?