Problem 1

Particle in a well that is infinite on one side and finite on the other

Let’s first write the Hamiltonian of the System:

\[ H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \]

with

\[ V(x) = \begin{cases} \infty & x < 0 \\ -V_0 & 0 < x < a \\ 0 & x > a \end{cases} \]

First we find the eigenfunctions for this Hamiltonian, i.e. we solve the eigenvalue problem for the Hamiltonian:

\[ H\phi(x) = \epsilon \phi(x) \]

We will concentrate at the beginning in find the solution only for bound states that is states with an energy \( \epsilon \) that is \( -V_0 < \epsilon < 0 \). This assumption does not change the way we write the eigenvalue problem in the three different regions of space but it allows us to know the sign of the coefficient of the wavefunction in the eigenvalue problem. This sign allows us to distinguish oscillatory from exponentially decaying solutions.

For \( x < 0 \) the eigenvalue problem is

\[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \infty \phi(x) = \epsilon \phi(x) \]

This equation can be solved just for \( \phi(x) = 0 \)
For $0 < x < a$ the eigenvalue problem is \[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V(x) \right] \phi(x) = E\phi(x) \]
that can be rewritten as \[
\frac{\partial^2}{\partial x^2} \phi(x) + \frac{2m}{\hbar^2} (V(x) + E) \phi(x) = 0 .
\] Introducing \( k^2 = \frac{2m}{\hbar^2} (V(x) + E) \) the general solution to this differential equation is \( \phi(x) = A e^{ikx} + B e^{-ikx} \) with A, and B representing two generic complex numbers.

For $x > a$ the eigenvalue problem is \[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right] \phi(x) = E\phi(x) \]
that can be rewritten as \[
\frac{\partial^2}{\partial x^2} \phi(x) + \frac{2m}{\hbar^2} E \phi(x) = 0 .
\] Introducing \( \rho^2 = -\frac{2m}{\hbar^2} E \) the general solution to this differential equation is \( \phi(x) = C e^{\rho x} + D e^{-\rho x} \) with C, and D representing two generic complex numbers.

The general form of our solution is:

\[
\phi(x) = \begin{cases} 
0 & x < 0 \\
A e^{ikx} + B e^{-ikx} & 0 < x < a \\
C e^{\rho x} + D e^{-\rho x} & x > a
\end{cases}
\]

this is the general expression of the solution of the eigenvalue problem. Varying the parameter A, B, C, and D one can obtain an infinite number of function. Only few of those have a real meaning. In fact to obtain the subset of this equation that can actually represent a solution of the Schrodinger equation and thus be a basis for the representation of a generic wavefunction of a particle in this potential well we need to impose some physical conditions.

First the wavefunction cannot go to infinity since otherwise it would not be normalizable. So we have to impose C=0

Second the wave function is continuous. So we have to impose that \( \psi(x=0) = 0 \) and

\[
\left( A e^{ikx} + B e^{-ikx} \right)_{x=a} = \left( D e^{-\rho x} \right)_{x=a}
\]

Third if the step in the potential barrier is not infinite the first derivate of the wave function is continuous. That is:

\[
\frac{\partial}{\partial x} \left( A e^{ikx} + B e^{-ikx} \right)_{x=a} = \frac{\partial}{\partial x} \left( D e^{-\rho x} \right)_{x=a}
\]

Before solving the equation let us comment on this third condition. It derives directly from the eigenvalue problem:
\[
\frac{\partial^2}{\partial x^2} \phi(x) + \frac{2m}{\hbar^2} (V_0 + E) \phi(x) = 0
\]

If we assume the abrupt discontinuity in the position of space: \( x_i = a \) is just the limit for \( \varepsilon \to 0 \) of a function \( V_\varepsilon(x) \) that varies from the values \(-V_0\) and 0 in an interval of space \( \varepsilon \) without ever going to infinity then we can write the eigenvalue problem as follows:

\[
- \frac{\partial^2}{\partial x^2} \phi(x) = \frac{2m}{\hbar^2} (V_\varepsilon(x) + E) \phi(x)
\]
given an interval of \( \pm \eta \) around \( x_i = a \) we can integrate both sides of the equations deriving:

\[
- \frac{d}{dx} \phi(x_i + \eta) + \frac{d}{dx} \phi(x_i - \eta) = \int_{x_i-\eta}^{x_i+\eta} \frac{2m}{\hbar^2} (V_\varepsilon(x) + E) \phi(x) dx
\]

The value of the function that is integrated in the right side of the equation is always finite (even for \( \varepsilon \to 0 \)), thus for \( \eta \to 0 \)

\[
0 = \int_{x_i-\eta}^{x_i+\eta} \frac{2m}{\hbar^2} (V_\varepsilon(x) + E) \phi(x) dx
\]

That is for \( \eta \to 0 \) it is always true that \(- \frac{d}{dx} \phi(x_i + \eta) + \frac{d}{dx} \phi(x_i - \eta) = 0\). The first derivative of a wavefunction of a particle in a potential that does not go to infinity is always continuous.

Now back to our conditions from the second condition we get:

A+B=0 \quad B=-A

And \( (Ae^{ika} + Be^{-ika}) = (De^{-pa}) \) that knowing that B=-A can be rewritten as

\[
\sin(ka) = \frac{D}{2iA} e^{-pa}
\]

The third condition can be written as: \( (Aike^{ika} - Bkae^{-ika}) = -(D \rho e^{-pa}) \) with B=-A

we can write

\[
\cos(ka) = -\frac{D \rho}{2iA \ ka} e^{-pa}
\]
These last two equations can have a solution for A and D just if

\[ \tan(k a) = -\frac{k a}{\rho} \]

that is

\[ \tan(k(E) a) = -\frac{k(E)a}{\rho(E)} \]

only for some particular values of E that we index as \( E_n \).

For those particular values we can find, using the normalization condition the values of A, B and D and write the generic expression of the eigenstates \( \varphi_{E_n}(x) \) of this problem.

Each given eigenstate will have to have a temporal dependence and to solve the Schrodinger equation in order to be a possible wavefunction of our system.

What this means is that we can write the wavefunction using the separation of variables:

\[ \psi_{E_n}(x,t) = \varphi_{E_n}(x) \zeta(t) = \varphi_{E_n}(x) \zeta_{E_n}(t) = \varphi_{E_n}(x)e^{-\frac{E_n t}{\hbar}} \]

This is just one possible wave function of the system, a generic wavefunction of the system needs to be written as the linear combination of all the wave functions:

\[ \psi(x,t) = \sum_n C_n \varphi_{E_n}(x)e^{-\frac{E_n t}{\hbar}} \]

Let us try to understand what happens to this function with time, an easy way of visualizing this is to try to “see” the shape evolution of the function with time. The real and imaginary part of the function behave in identical ways so we will look just at the real part.

\[ \text{Re}(\psi(x,t)) = \sum_n \text{Re}(C_n) \text{Re}(\varphi_{E_n}(x)) \cos\left(\frac{E_n t}{\hbar}\right) \]

For a given eigenstate the wavefunction will be \( \text{Re}(\psi_{E_n}(x,t)) = \text{Re}(\varphi_{E_n}(x)) \cos\left(\frac{E_n t}{\hbar}\right) \)

At a given time the shape of the function is given by \( \text{Re}(\varphi_{E_n}(x)) \) and \( \cos\left(\frac{E_n t}{\hbar}\right) \) is just a coefficient that controls the amplitude of the function.

The different orthogonal components (the eigenstates) of our function

\[ \text{Re}(\psi(x,t)) = \sum_n \text{Re}(C_n) \text{Re}(\varphi_{E_n}(x)) \cos\left(\frac{E_n t}{\hbar}\right) \]

have a coefficient in front of them that does not vary with time and another one that does. The frequency of the time variation of this second coefficient changes depending on the specific eigenvalue. This means that the shape of the function changes with time.