2n Report - *Numerical solution of the Schrödinger's equation*

Simulació de Sistemes Nanomètrics - *Nanociència i Nanotecnologia - 22/23*

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1 Description of the problem

I have chosen to make a 1D Particle in a Box with a normal potential barrier in the middle of the box. For this type of problem I have picked the Atomic Units, which I found a Libre text article [1]. In this problem the important units are the Hartrees, the Bohrs and the electron rest mass. The equivalences can be seen in 1. With this units my Schrödinger equation for a numerical integration resolution with D. Truhlar's method has a μ value of 1. Therefore, my equation is 1:

$$\Psi_{i-1} - 2\left[1 + h^2 V_i\right]\Psi_i + \Psi_{i+1} = 2h^2 E \Psi_i \tag{1}$$

Table 1: Equivalences between SI units and AtomicUnits

	SI UNits	More common Units	Atomic Units
Hartrees (H)	$4.35910^{-18}J$	$27.2eV$	$1H$
Bohr (a_o)	$5.29110^{-11}m$	$0.5291nm$	$1a_o$
m_e	$9.10910^{31}kg$	———	$1m_e$

2 Results

I based my code in two Libre Text articles [2] [3]. Therefore I chose a Box dimension of 1 a_o, a Barrier Energy of 100 H and my barrier is placed in the middle and has a dimension of 0.1 a_o.

With this units and using a grid of 500 points I have obtained the energies that can be seen in Figure 1, and their Wave Functions can be seen in Figure 2.

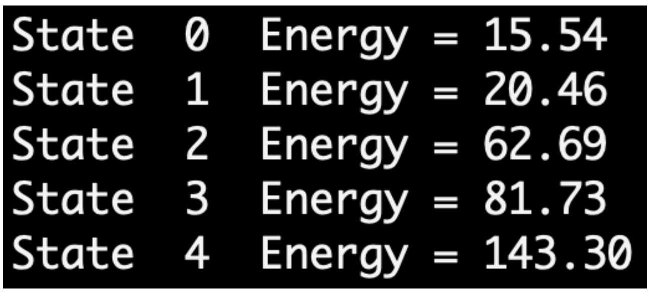

Figure 1: The Energy levels with its corresponding state number $(n-1)$

As we can see in Figure 2 even though the barrier dictates how the electron behaves inside the box, because we can clearly see that this wave functions are not the typical Particle in a Box functions [4], the barrier is thin and energetically low enough to let tunneling happen with barely any difficulty. We can also appreciate that the state $n = 5$ is not affected by the barrier, as the calculus in Figure (1), which say that this state has an energy of $143.3H$, therefore, bigger than the $100H$ barrier.

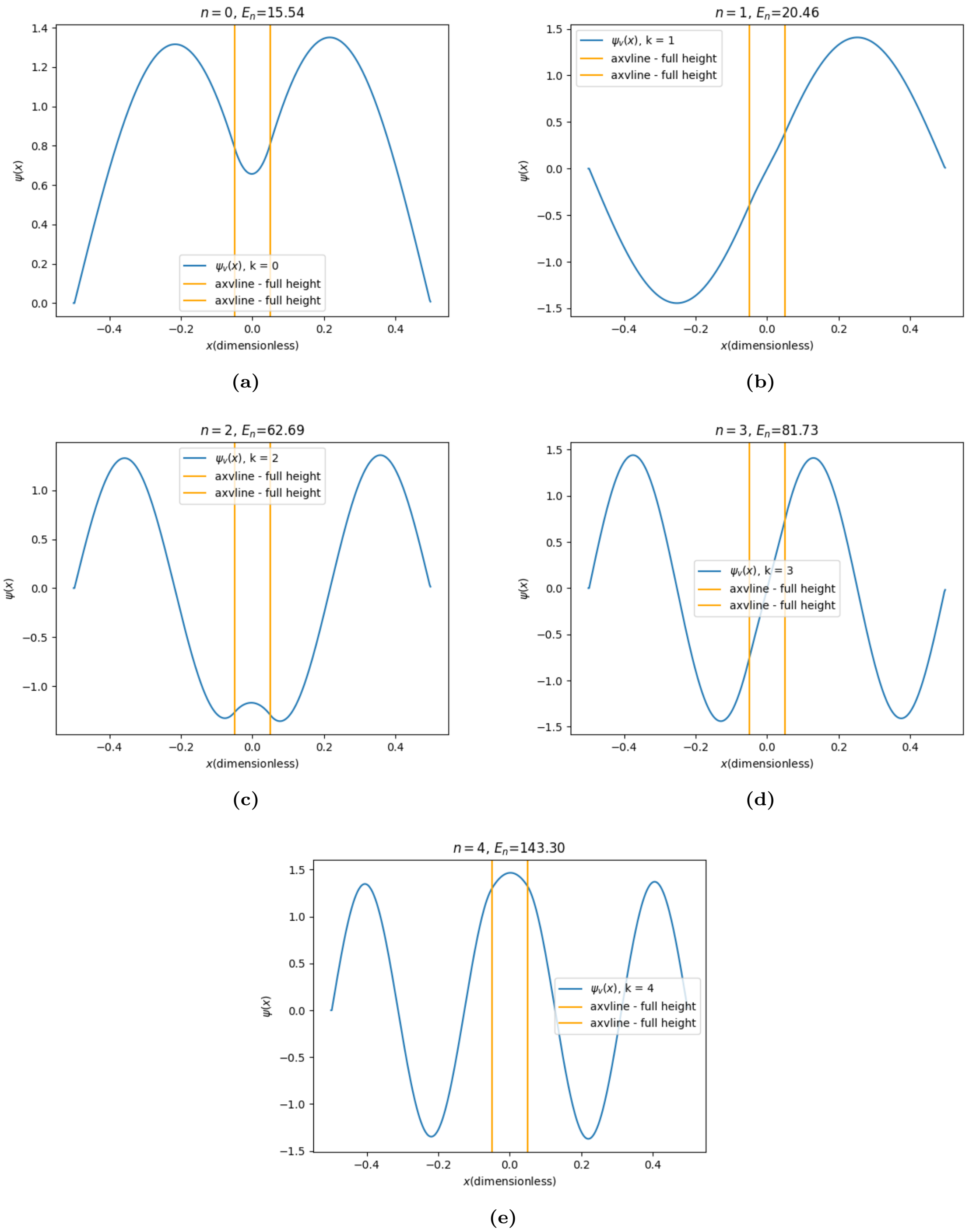

Figure 2: Figures of the different states, in blue we can see the Wave Functions, the vertical orange lines mark where the Energy Barrier is placed.

3 The code

Because of the convenience of the units used the only things I had to modify were the potential and the plots so the vertical lines appeared. This parts can be seen in Figure 3. The entire code can be found in my GitHub repository [5].

```python
#Potential as a function of position
def getV(x,Ebar):
    if (x==xlower) or (x==xupper):
        potvalue = 10000000000
    if (x>-0.05) and (x<0.05):
        potvalue = Ebar
    else:
        potvalue = 0
    return potvalue
```

(a)

```python
#v = int(input("\n Quantum Number (enter 0 for ground state):\n>"))
for v in range(0,5):
        plt.plot(x,psi[v],label=r'$\psi_v(x)$, k = ' + str(v))
        plt.axvline(x = 0.05, color = 'orange', label = 'axvline - full height')
        plt.axvline(x = -0.05, color = 'orange', label = 'axvline - full height')
        plt.title(r'$n=$'+ str(v) + r', $E_n$=' + '{:.2f}'.format(E[v]))
        #plt.axhline(x=-0.05, color = 'orange')
        #plt.axhline(x=0.05, color = 'orange')
        plt.legend()
        plt.xlabel(r'$x$(dimensionless)')
        plt.ylabel(r'$\psi(x)$')
        plt.show()
```

(b)

Figure 3: Modified code

References

[1] "Atomic and molecular calculations are expressed in atomic units, libre text." https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Physical_Chemistry_(LibreTexts)/08%3A_Multielectron_Atoms/8.01%3A_Atomic_and_Molecular_Calculations_are_Expressed_in_Atomic_Units.

[2] "Particle in a box with an internal barrier, libre text." https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Quantum_Tutorials_(Rioux)/09%3A_Numerical_Solutions_for_Schrodinger's_Equation/9.15%3A_Particle_in_a_Box_with_an_Internal_Barrier.

[3] "Another look at the in a box with an internal barrier, libre text." https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Quantum_Tutorials_(Rioux)/09%3A_Numerical_Solutions_for_Schrodinger's_Equation/9.16%3A_Another_Look_at_the_in_a_Box_with_an_Internal_Barrier.

[4] "Particle in a box." https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Quantum_Mechanics/05.5%3A_Particle_in_Boxes/Particle_in_a_1-Dimensional_box.

[5] "Github repository with the code to solve this problem." https://github.com/DaniBedmar/Nanometric-Systems-Simulation/tree/main/Project_02_Schordinger_Equation_Numerical_Solution.