Department of Electronics & Communications Engineering

ETE/ICE 470 LAB – Applied Numerical Methods

Lab Project

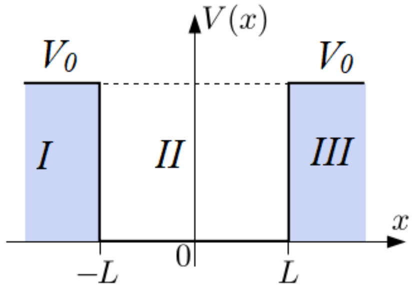
Course Code: ETE/ICE 470 LAB
Teacher's Initial: SMRC
Deadline: Sept 25, 2020

Semester: Summer'20
Section: 1 (One)
Full Marks: 100

(All the questions must be answered. Symbols have their usual meanings.)

Finite Well Problem – Consider a Quantum Particle trapped in a Finite Potential Well whose potential profile is given below.

$$V(x) = \begin{cases} 0 & -L \leq x \leq L \\ V_0 & \text{otherwise} \end{cases}$$



The wave-function $\psi(x)$ of the particle with energy E follows the following time independent Schrodinger Equation guided by some boundary conditions given below.

$$\frac{d^2}{dx^2}\psi(x) + \frac{2m(E - V(x))}{\hbar^2}\psi(x) = 0$$

Boundary conditions –

$$\begin{aligned} &\psi_I(-L) = \psi_{II}(-L) \qquad &&\psi_{II}(L) = \psi_{III}(L) \\ &\psi'_I(-L) = \psi'_{II}(-L) \qquad &&\psi'_{II}(L) = \psi'_{III}(L) \\ &\psi_I(-\infty) = \psi_{III}(\infty) = 0 && \end{aligned}$$

Where, $\psi_I(x)$ is the wave-function in the Region-I and so on. The prime denoted the first derivative w.r.t the position, x. Assume, $m = 9.11 \times 10^{-31}$ kg, $\hbar = 1.0546 \times 10^{-34}$ Js, $L = 8$ nm and $V_0 = 5.5$ eV.

Using **Finite Difference Method (FDM)** [1,2] in **Python**, determine the followings.

1. An array containing all the allowed values of energy levels E within the well. From this result, mention the value of the ground energy (min E) and valence energy (max E). Show the energy levels in the same plot as the potential $V(x)$. **[30]**

2. Generate the wave-functions (normalized) corresponding to each energy level and plot at least three wave-functions including the ground state. Take $-1.5L \leq x \leq 1.5L$ as the plot window. Also, you can take the FDM mesh size as per your convenience. **[40]**

3. Also, elaborately discuss how you have modeled the ordinary differential equation in FDM scheme and mention the corresponding FDM matrix you have built to solve this problem prior to the python code. **[30]**

Submission Guideline:

1. Upload your project report (.pdf), python code (.py or .ipynb), resulting plots (.png or .jpg) and 'Read-me' file (if necessary) in your drive folder.
2. Set the sharing option of the drive folder as 'Anyone with the link can view' and create the link.
3. Submit the link in the Canvas Portal of project submission. Note that, there is only one submission attempt.

Deadline: Sept 25, 2020 (11:59 PM, GMT +6:00)

Important Notes:

1. Only Canvas submission is acceptable. The project files sent to me via email or any other social networking sites without my permission won't be accepted for assessment.
2. No late submission will be accepted except in the case of any verified medical issue. You have to inform me at least one week ago and submit an application with proper attachment of medical documents along with your guardian's signature and contact number.
3. Copying or Cheating of any kind is strictly prohibited, if found, all parties concerned will be given 'null' without any consideration.
4. Copying code from any online platform (GitHub, Stack Overflow etc.) will also be considered as 'Copying' and will be dealt in the same way mentioned in (3).
5. The texts of your report pdf must be in selectable form, if found in non-selectable scan form, that text-block will not be assessed and if found matched to someone's text, will be considered as 'Copy'.

References

[1] Finite Difference Schemes and the Schrodinger Equation – by Jonathan King & Pawan Dhakal, University of Dartmouth, Washington, USA.

[2] Theoretical aspects of Finite Difference Method - Wikipedia