1. Finite Difference Method (100 pts) – Requires Programming

In class, we solved *analytically* the "particle in a box" (or "quantum well") problem to get the quantized energy levels of electrons in a confining potential. Remember that we first had to guess the solution of the differential equation (i.e., Schrödinger equation) with a certain general form (e.g., plane or sinusoidal waveforms with some unknown constants) which seemed to satisfy the Schrödinger equation. This approach is the simplest and somewhat effective, but if your initial guess happens to be not too good, then you are unlikely able to solve it. Now let's solve the same problem *numerically* at this time by means of finite-difference method that we learned in class.

1-1. (20 pts) Construct a ***N*** by ***N*** Hamiltonian matrix by applying the following conditions, in a similar way that we did in class. For this problem (1-1), you are not required to run the simulation. Just write down your answer. Show your work to get the full credit.

- Select a one-dimensional discrete lattice with ***N*** points spaced by ***a***
- Apply the boundary condition of $\psi(x = 0) = \psi(x = \boldsymbol{N}+1) = 0$
- Set $U(x) = 0$ for $0 < x < \boldsymbol{N}+1$

1-2. (60 pts) Use any available mathematical package like MATLAB to find the eigenvalues and the corresponding eigenvectors for the "electron in a box" problem that you just modeled in 1-1. Because your Hamiltonian is a ***N*** by ***N*** matrix, you should get ***N*** pairs of eigenvalues and eigenvectors. Take ***N*** (# of mesh) = 100 and ***a*** (mesh spacing) = 1e-10 (m) for your simulation.

(a) Plot the numerically obtained eigenvalues (in eV) as a function of eigenvalue number ***n***. ***n*** is the integer number that ranges from 1 to ***N***. For example, if you obtain ***N*** number of eigenvalues, ***n*** = 1 indicates the first set of eigenvalue and eigenfunction, ***n*** = 2 means the second eigenvalue and eigenfunction, etc. (20 pts)

(b) Plot the "analytical" eigenvalues ($E_{\boldsymbol{n}}$ as a function of ***n***), using the equation, $E_{\boldsymbol{n}} = h\_bar^2\pi^2\boldsymbol{n}^2/2\boldsymbol{m}\boldsymbol{L}^2$ where $\boldsymbol{L} = (\boldsymbol{N}+1)\boldsymbol{a}$, together with the result obtained in (a). In other words, overlap your answer in (b) with that in (a). h_bar is the reduced Planck constant. (5 pts)

(c) Describe how well your numerical result in (a) matches the analytical result in (b). (5 pts)

(d) Plot ψ^2 (squared eigenvector) for eigenvalue numbers ***n*** = 1, 2, 10, and 50. (20 pts)

(e) Use the result of (d) to explain any observation you made in (c). (10 pts)

1-3. (20 pts) Re-write your Hamiltonian (don't need to run the simulation again. Just write your answer) when

(a) the periodic boundary condition is applied, i.e., $\psi(x = 0) = \psi(x = \boldsymbol{N})$ and $\psi(x = 1) = \psi(x = \boldsymbol{N}+1)$. (10 pts)

(b) What about the potential energy U(x) is not zero any more, i.e. $U(x) = U_0$ for $0<x<\boldsymbol{N}+1$? What is your new Hamiltonian? (10 pts)