# Device Simulation Laboratory

# (EE5195)

Problem Sheet-III

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Choose appropriate grid spacing. You may as well want to change the grid spacing and see the effects

Q.1:- Use finite difference method to solve the Schrodinger's equation for a particle in a 1D box with mass same as that of an electron and well width of 10 nm. Use 101 points for discretization. Plot the energy values vs the eigenvalue number and compare it with the analytical results. Also plot the probability distribution for eigenvalues 1 and 25. Instead of 101 points, use 1001 points for discretization and redraw the plots. What effect do you see? Also check if the wavefunction you are getting is normalized.

Q.2:- The radial wavefunction for an electron inside the H atom can be given by

$$Ef(r) = \left( -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + U(r) + \frac{l(l+1)\hbar^2}{2mr^2} \right) f(r)$$

Use the finite difference method to find out the energy of the 1s & 2s levels. Plot the radial probability as a function of the radius for the mentioned energy levels. Can you obtain the bohr's radius from these graphs? Compare the value of bohr's radius you obtain from these graphs to the analytical value. Also check if the wavefunctions you are getting are normalized.

Q.3:- Consider a finite potential well with $\alpha_0 a = \pi/4$. Use graphical method to solve for the energy value of an electron subjected to this potential well. Assume that the well is 1 nm wide. Use the finite difference method to solve for the energy of the electron and compare the result with the graphical method. Also plot the wavefunction of the electron obtained using the finite difference method. Is the wavefunction normalized?