EEE434/591: Quantum Mechanics

Homework set #5

1. Following the steps outlined in the class that describe the shooting method, write a code for calculating the energy levels in a 1D confining potential of arbitrary shape. You are not required to write a routine for the energy search, but you can detect an eigenvalue if you take a small enough energy mesh and plot the error function f as a function of energy. The zeroes of f will signal that an energy eigenvalue has been obtained. Once you have detected where the eigenvalues are located, you can integrate the 1D Schrodinger equation and obtain the corresponding eigenfunctions for the bound states in the well. The parameters of the well which you need to simulate are the following ones: well height V_0=0.8 eV and well width W=3 nm. For the effective electron mass use $m=6\times10^{-32}$ kg. Submit the listings of the code that you have written for this homework problem.

2. SCHRED solves self-consistently the 1D Poisson equation coupled with the 1D Schrödinger equation, for the purpose of electrostatic modeling of MOS capacitors. This exercise will help you to become familiar with SCHRED. You are required to model a MOS capacitor with oxide thickness t_{ox}=4 nm and the following two values of the substrate doping: $N_A=10^{16}$ cm^{-3} and $N_A=10^{18}$ cm^{-3}. Use metal gates and T=300 K. Assume complete ionization of the impurity atoms. The applied bias on the gate equals to V_G=1 V. For each of the subsrate doping densities use both semiclassical and quantum-mechanical charge description (use 5 as maximum number of subbands for each subband ladder corresponding to either Δ_2 or Δ_4 band) of the electron density in the triangular potential well. For each simulation run, plot the following:

   (a) Conduction band profile and the electron density.

   (b) When using quantum-mechanical charge description, plot the wavefunctions that correspond to the bound states in the triangular potential well.

   Also answer the following questions:

   (c) How does the energy separation between the bound states in the well varies with doping. Why?

   (d) Explain the differences in the electron density distributions obtained by using the semiclassical and quantum-mechanical model.

   (e) How does the average distance of the carriers from the interface changes when we use quantum-mechanical charge description rather than semiclassical (Maxwell-Boltzmann statistics). What implications will this parameter have on MOSFET operation? (You do not need to answer the last portion of this question if you do not have the required background in semiconductor devices).