1)

4.11: Plot u vs x obtained from all three solutions and compare to see if there are differences.

Apply the Numerov Algorithm to solve:

$$u"(x) = -4\pi^2 u(x)$$

With $u(0) = 1$ and $u'(0) = 0$. Discuss the accuracy of the result by comparing it with the solution obtained via the fourth degree Runge-Kutta algorithm and with the exact result

2)

4.12: Plot u vs x obtained from the exact solution and from the shooting method and compare to see if there are differences.

Develop a program that applies the fourth-order Runge–Kutta and bisection methods to solve the eigenvalue problem of the stationary one-dimensional Schrödinger equation. Find the two lowest eigenvalues and eigenfunctions for an electron in the potential well

$$V(x) = \begin{pmatrix} V_0 \frac{x}{x_0} & \text{if } 0 < x < x_0 \\ V_0 & \text{elsewhere} \end{pmatrix}$$

Atomic units (a.u.), that is, $m_e = e = h = c = 1$, $x_0 = 5$ a.u., and $V_0 = 50$ a.u. can be used.

3)

In this problem we will solve the one-dimensional time independent Schrödinger equation (Eq. 4.91 in your text) using two different methods. Consider a single electron of mass m_e in one dimension trapped in a potential well of the following form:

It's simplest to use atomic units (a.u.) with Set the potential parameters to be and

a)

Use the code from Chapter 4.9 of the text (which uses the Numerov algorithm with secant method) to find the two lowest eigenvalues and eigenfunctions of the Schrödinger equation with the above potential.

b)

Then develop a program that does the same thing as part a), but with the Runge-Kutta and secant methods.

c)

To compare results from parts a) and b), plot the square of the eigenfunctions versus position for both methods to see if there are differences.

Comment: The solutions to Problem 3 (and variants) are now commonly used in semiconductor device modeling. See, e.g.,

"Basic Semiconductor Physics" S. Hamaguchi, Springer 2017 or J. H. Luscombe et al., Physical Review B 46, 10262 (1992)