PHYS-E0412 Computational Physics :: Homework 8

Due date 12.3.2019 at 10 am

Finite-element discretizations of the Schrödinger equation

In this exercise we study finite-element discretization of the Schrödinger equation in one dimensional potential well. Consider the eigenvalue problem

$$\begin{cases} -\frac{1}{2}\psi''(x) + V(x)\psi(x) = \epsilon\psi(x), \quad 0 < x < 1 \\ \psi(0) = \psi(1) = 0 \end{cases}$$

where the potential is given by two cusps

$$V(x) = -150e^{-40(x-0.25)^2} - 50e^{-10(x-0.75)^2}$$

a) Implement a finite-element solver for the eigenvalue problem. (You can use the code skeleton provided with the homework.) How many of the states have negative energy indicating that they are bound to the cusps? Use uniform distribution of the nodes, $x_i = ih$. To calculate the entries of the potential matrix

$$V_{ij} = \int_0^1 \phi_i(x)V(x)\phi_j(x)\,dx$$

you can either use some library routine for numerical integration (see, e.g. `integral` in matlab). If you prefer to implement your own routine use a Gaussian quadrature of high enough order
(`https://en.wikipedia.org/wiki/Gaussian_quadrature`) (3 p.)

b) Plot some of the lowest eigenfunctions. Is the uniform distribution of the nodes optimal? Given a budget of $N = 30$ nodes devise a more effective placement in the interval $[0, 1]$ to approximate the lowest eigenpair. (2 p.)

c) How many hours did you spend working on this exercise?