Computational Science 2

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Seminar
Exercises

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Exercise 6 (30.06.2016):

Numerical solution of the Schrödinger equation

from ***An Introduction to Computer Simulation Methods***,
Chapter 16, Problems 16.5-8

a) Modify `SchroedingerApp` to find the eigenvalue associated with a given number of nodes. How is the number of nodes related to the quantum number? Test your program for the infinite square well. What are the values of Δx need to determine E_1 to two and three decimal places, respectively? Add a method to normalize ϕ. Display the first five normalized eigenstates.

b) Find the first five eigenstates and eigenvalues for the potential

$$V(x) = \begin{cases} 0 & \text{for } -a \leq x \leq 0 \\ V_0 & \text{for } 0 < x \leq a \\ \infty & \text{for } |x| > a \end{cases} \tag{1}$$

with $a = 1$ and $V_0 = 1$. Does your result for E_1 depend on the starting value of $d\phi/dx$?

c) Determine the effect of a small perturbation on the eigenstates and eigenvalues of the infinite square well. Place a small rectangular bump of half-width b and height V_b symmetrically about $x = 0$. Choose $b \ll a$ and determine how the ground state energy and eigenstate change with V_b and b. What is the relative change in the ground state energy for $V_b = 10$, $b = 0.1$ and $V_b = 20$, $b = 0.1$ with $a = 1$. Let ϕ_0 denote the ground state eigenstate for $b = 0$ and let ϕ_b denote the ground state eigenstate for $b \neq 0$. Compute the value of the overlap integral $\int_{-a}^{a} \phi_b(x)\phi_0(x)dx$. This integral would be unity if the perturbation were not present (and the eigenstate was properly normalized). How is the change in the overlap integral related to the relative change in the energy eigenvalue? Compute the ground state energy for $V_b = 20$ and $b = 0.05$. How does the value of E_1 compare to that found for $V_b = 10$ and $b = 0.1$?

d) Modify `Schroedinger` to make use of symmetric potential boundary conditions for the harmonic oscillator $V(x) = (1/2)x^2$. Start the solution at $x = 0$ using appropriate initial conditions for even and odd quantum numbers and find the first four energy eigenvalues such that the wave function approaches zero for large values of x. Because the computed $\phi(x)$ will diverge for sufficiently large x, we seek values of the energy such that a small decrease in E causes the wave function to diverge in one direction, and a small increase causes the wave function to diverge in the opposite direction. Initially choose $x_{max} = 5$, so that the classically forbidden region is sufficiently large so that $\phi(x)$ can decay to zero for the first few eigenstates. Increase x_{max} if necessary for the higher energy eigenvalues.

e) Repeat for the linear potential $V(x) = |x|$. Describe the differences between your results for this potential and for the harmonic oscillator potential.

f) The finite square well potential is given by

$$V(x) = \begin{cases} 0 & \text{for } |x| \leq a \\ V_0 & \text{for } |x| > a \end{cases} \tag{2}$$

Choose $V_0 = 10$ and $a = 1$. How do you expect the value of the ground state energy to compare to its corresponding value for the infinite square well? Compute the ground state eigenvalue and eigenstate by determining a value of E such that $\phi(x)$ has no nodes and is approximately zero for large x. What is the total number of bound excited states? Why is the total number of bound states finite?