PHYS/ENGP 3170/6170
Computational Physics and Engineering
Spring 2021

Assignment #7: Quantum Eigenvalues in One Dimension
Due: Wed, Apr 28 11:59 pm

Readings: LPB 7.1-7.3

We are looking at bound states of a quantum well defined by $V(x)=V_1$ for $|x|<a$ and $V(x)=V_2$ otherwise, working in units $\hbar=2m=a=1$. As shown in class, the eigenvalues corresponding to even solutions of the Schrödinger equation are given by solutions of $f(E)=k\tan(k) - r = 0$, where $k=\mathrm{sqrt}(E-V_1)$ is the wave number inside the well and $r=\mathrm{sqrt}(V_2-E)$ is the imaginary wave number (decay constant) outside the well. The first even solution must be between $k=0$ and $k=\pi/2$ (where f has its first singularity), the second must be between $k=\pi/2$ and $k=3\pi/2$, etc., until we reach $E=V_2$.

(1) The code Quantum.py, included with this assignment, finds the ground state energy of the well using the bisection method. Run this code to obtain the ground state energy, and then modify it appropriately to find the next even eigenvalue (i.e., the second lowest).

(2) As discussed in class, the wave function is given by $\psi(x) = A\cos(kx)$ for $|x|<1$ and $\psi(x) = B\exp(-r|x|)$ for $|x|>1$, where A and B are obtained using wave function continuity: $A\cos(k)=B\exp(-r)$, and the usual normalization condition $\int dx\, |\psi(x)|^2 = 1$. Find A and B for the *second lowest* even solution, and plot the wave function. Does your wave function have the correct number of nodes?

(3) Modify the program to use Newton's method instead of the bisection method to find the second lowest even solution. Start with $E_0=25.0$, and then use $E_{n+1} = E_n - f(E_n)/f'(E_n)$. $f'(E)$ may be evaluated analytically or numerically. How many steps do you need for Newton's method to converge to machine precision? Is the rate of convergence of Newton's method consistent with what we predicted in class?

[Required for 6170 students only, extra credit for 3170 students] Find the range of starting points E_0 for which the answer converges to the second lowest even eigenvalue. What happens if you start with E_0 outside of this range?

(4) Use Newton's method to find the second lowest even eigenvalue as a function of well height V_2, as V_2 is increased from $V_2=70$ to $V_2=10000$ with some suitable step size. Note: you may first find the eigenvalue for $V_2=70$, as in the previous problem, then use that energy as the initial guess for the eigenvalue at $V_2=80$, etc. Plot the eigenvalue as a function of V_2, and compare with the asymptotic answer, $E=V_1+(3\pi/2)^2$, for $V_2=\infty$.

(5) [Required for 6170 students only, extra credit for 3170 students] When V_2 is very large, we know the second solution is given by $k=(3\pi/2) - \varepsilon$, and $r=\mathrm{sqrt}(V_2-V_1-(3\pi/2)^2) + O(\varepsilon)$. Then our equation $f(E)=0$ becomes $(3\pi/2 - \varepsilon)\tan((3\pi/2) - \varepsilon) - \mathrm{sqrt}(V_2-V_1-(3\pi/2)^2)$

$+O(\varepsilon) = 0$. Expand $\tan((3\pi/2) - \varepsilon)$ for small ε, write out our equation dropping all terms of $O(\varepsilon)$, and solve for ε. Plug back in to $E=V_1+k^2=V_1+(3\pi/2 - \varepsilon)^2$ to obtain an analytic expression for E when V_2 is very large, but not infinite. Compare with your numerical results in Problem 4.