PHSX 615/815, CHEM 914: Homework 5 DRAFT

Due date TBD

Numerical Solution of the 1-d Time Independent Schrödinger Equation

Introduction

There are a number of numerical techniques available for problems like the 1-d TISE for potential wells which can be classified as a two-point boundary value type problem. In this assignment we will explore both the matching method and the matrix-based approach. The matching method is described in some detail in Giordano 10.2 and in the class hand-out from An Introduction to Computational Physics by Pang. The matrix-based approach is sketched in Giordano 10.3. We have discussed both in class.

The matching method could be characterized as fickle, and requiring some considerable care in implementing robust methods for bracketing eigenvalues, and in numerically specifying the continuity conditions. It is a method rather amenable to finding particular solutions with high precision given a reasonable starting point for iteration. The high precision is particularly true when implemented with a high quality ODE evolver (like 4th order Runge-Kutta or Numerov).

The matrix-based approach, consisting of discretizing the problem to N points on the line, is a really powerful sledge-hammer approach which yields approximate eigenvalues and eigenvectors rather easily given access to a high quality eigensystem solver. But is ultimately limited in precision by the necessity of solving for N eigenvalues, which can be very expensive given very small step sizes where one deals with N x N matrices. Particular attention to selecting appropriate eigensystem solver routines can be important for efficiency, eg. you may only be interested in calculating a few of the eigenvectors. Including some CPU time monitoring code can serve as useful input data for developing effective strategies.

Perhaps, the best way of viewing this, is to consider the matrix approach as an excellent way to characterize the overall problem, and the matching method as a potentially laborious but arguably satisfying way of really pinning down each solution with high precision.

Problem 1.
Calibration on problem with known "analytic" solution

Use the matrix method to find the eigen-energies of the bound states (negative energy) for the following 1-dimensional potential well, with $\alpha = 2$, $\lambda = 7.5$:

$$V(x) = -\frac{\hbar^2}{2m}\alpha^2\lambda(\lambda - 1)/\cosh^2(\alpha x)$$

For all the bound-states, plot the properly normalized wave-functions. You will probably find it easier to set $\hbar = 1$, $m = \frac{1}{2}$.

This is called the modified Pöschl-Teller potential. The analytic solution is given in Problem 39 in S. Flügge, Practical Quantum Mechanics, Volume 1 (Library number: QC174.1.F5713). However you will probably realize that having the analytic solution at hand is not exactly a great help!

The eigen-energies of the bound states are:

$$E_n = -\frac{\hbar^2}{2m}\alpha^2(\lambda - 1 - n)^2$$

for $n = 0,1,2, \dots \text{int}(\lambda-1)$, and you should be able to use the deviation of your found solution from the analytic solution to gauge the numerical errors in your program, and further reduce them. Also for one or two eigen-values, see how dependent your results are on the range used for the x-axis, and also the step-size.

For the least well bound state (the highest value of n with a bound state), use the matching method, to determine a refined value for the eigen-energy and the normalized wavefunction, and compare with that found from the matrix method. You may want to use the matrix method solution as a starting point for the matching method.

Problem 2. We'll modify the potential of problem 1, by multiplying the potential by a Breit-Wigner distribution, f(x) (aka in math land as a Cauchy distribution) centered at the origin.

$$f(x; c, x_0, \Gamma) = (c/2\pi)\Gamma/[(x - x_0)^2 + (\Gamma/2)^2]$$

With c=1, this would be a properly normalized probability density function for a Breit-Wigner. We'll choose, $c = \pi\Gamma/2$, $x_0 = 0$, $\Gamma = 1.0$, so a Breit-Wigner function with width, Γ, of 1.0 and mean of 0.0, and designed to have a probability density of 1.0 at $x = 0.0$.

Now for this modified potential, $V'(x) = V(x)f(x)$, find the eigen-energies and wavefunctions of any bound states. Plots of the wavefunctions would be appreciated. (Note that this normalization ensures the same well depth). Use whichever method you prefer.