CHE 477 November 14, 2016

Schrödinger Equation Project

Project 2

1 Problem Statement

Your goal is to solve Schrdöinger's Equation using multiple basis sets. This will require you to be able to represent functions on grids and find elements in a function points which are stationary for a given operator.

2 Mathematics

The Schrödinger Equation is

$$\hat{H}\Psi(x) = E\Psi(x)$$

where $\hat{H}$ is an operator that maps from L_2 of complex functions to L_2. Note that the inner-product on complex L_2 is

$$\langle f(x) \mid g(x) \rangle = \int dx f(x)\overline{g(x)}$$

where $^{-}$ denotes complex conjugate. It so happens that $\hat{H}$ is a linear operator, similar to our example in class. $\Psi(x)$ is a complex valued function, so that its range is a complex number and its domain is a real vector. The Schrödinger equation states that the wavefunciton which satisfies that equation is the one that describes a system. For the first phase of your project, your goal is to be able to evaluate the Hamiltonian operator on a given wavefunction.

The definition of $\hat{H}\Psi(x)$ is

$$-c\nabla^2\Psi(x) + V_0\Psi(x)$$

where V_0 is a constant potential energy, c is a constant, and ∇^2 is the Laplacian.

3 Project

You will write code in any language of your choice that can take as input (1) the potential energy V_0, (2) c the constant, (3) the size of the basis set, (4) the choice of basis set function, and (5) a domain (if needed). You should output a wavefunction corresponding to the lowest-energy state of the Hamiltonian. Recall that the energy itself is $\langle \Psi(x) | \hat{H} | \Psi(x) \rangle$. Your result can will basis set coefficients. Please see the supplemental hand-out in your reading to see how finding the eigenvalue-eigenvectors coresponds to solving this problem.

Your program should allow the following basis set functions: Fourier and Legendre Polynomials. The potential energy is the same format as in the Langevin project.