PHYS 452 Quantum Mechanics II (Fall 2017)
Homework #1, due Thursday Sept 14 in class

The variational method

1. Consider a particle of mass m moving in a 1D finite square well:

$$V(x) = \begin{cases} 0, & -l/2 \le x \le l/2 \\ \frac{b\hbar^2}{ml^2}, & |x| > l/2 \end{cases},$$

where b is a positive constant and l is the width of the well. Using the trial wave function in the form

$$\phi(x) = \begin{cases} A(x-c)(x+c), & -c \le x \le c \\ 0, & |x| > c \end{cases},$$

where c is an adjustable parameter and A is the normalization constant, find the expression for the ground state energy as a function of c. Solve this equation numerically using any relevant software tool of your choice (e.g. Mathematica, Maple, Matlab, Python, etc.) and obtain the best estimate of the ground state energy with the above trial function.

2. Consider a 1D system with a potential that depends on the fourth power of x:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + bx^4. \tag{1}$$

First, introduce the dimensionless distance $y = \frac{x}{a}$ and get rid of $\hbar$, m, and b in the Hamiltonian (in other words, introduce natural units in which $\hbar = m = b = 1$). Then approximate the ground state wave function with the following gaussians expansion:

$$\psi(y) = \sum_{i=1}^{N} c_i e^{-\alpha_i y^2}, \tag{2}$$

where $N = 3$, $\alpha_1 = 0.5$, $\alpha_2 = 1$, and $\alpha_3 = 1.5$, while c_i's are unknown expansion coefficients (linear variational parameters). Find the corresponding energy. Is it possible to meaningfully approximate the wave function of an excited state with this expansion? If so, which excited state (i.e. corresponding to which quantum number)? To answer that question it is helpful to think about the symmetry of the trial wave function (2) as well as the symmetry of the exact eigenstates of the Hamiltonian (1). Compute the corresponding approximate energy of the excited state.

In this problem you will need to find the solutions of a generalized eigenvalue problem with $N \times N$ matrices. To do so, write out those matrices explicitly and solve the generalized eigenvalue problem numerically using a package of your choice. For example, in Mathematica there is a command `Eigensystem[{H,S}]` that finds generalized eigenvalues and eigenvectors, while in Python you can use a `scipy` library function called `scipy.linalg.eigh`

Bonus task: Using the two approximate wave functions (for the ground and excited states) compute $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$. When doing this, make sure that the generalized eigenvectors you obtain obey the property $c^T S c = 1$, where S is the overlap matrix and $c = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$. This property ensures correct normalization of the wave function (convince yourself in that). The computer algebra packages listed above by default may or may not return eigenvectors that are normalized this way.