PHYS 452: Quantum Mechanics II (Spring 2015)
Homework #1, due Thursday January 22, in class

1. Use the Gaussian trial wave function, $\psi(r) = A\exp(-\beta r^2)$, to find the variational upper bound to the ground state energy of the hydrogen atom.

2. Consider the halved harmonic oscillator potential:

$$V(x) = \begin{cases} \infty, & x < 0 \\ \frac{m\omega^2 x^2}{2}, & x > 0 \end{cases}$$

Using the trial function in the form

$$\psi(x) = \begin{cases} 0, & x < 0 \\ Ax\exp(-\lambda x), & x > 0 \end{cases}$$

Estimate the ground state energy and compare your result to the exact solution (the halved harmonic oscillator problem appeared in Homework #4 in PHYS451 last Fall)

3. Consider a Hamiltonian that in some units has the following form:

$$H = -\frac{1}{2}\frac{d^2}{dx^2} - \sqrt{\pi}\delta(x).$$

Make an estimate of the ground state energy using the trial function in the form of a linear combination,

$$\psi(x) = c_1 e^{-x^2/2} + c_2 e^{-2x^2}.$$

Here c_1 and c_2 are variational parameters. In this problem you will need to solve a generalized eigenvalue problem with 2×2 matrices. Write out those matrices explicitly and solve the generalized eigenvalue problem numerically using any computer algebra package (e.g. MATHEMATICA, MAPLE, MATHCAD, MATLAB, OCTAVE, etc.). Make sure that the generalized eigenvectors you obtain obey the property $c^T S c = 1$, where S is the overlap matrix and $c = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$. Plot in a single figure the trial wavefunction with optimal c_1 and c_2 against the exact solution (see chapter 2.5.2 in Griffiths) and each of the Gaussians (normalized) used in the above linear combination. You should see that the linear combination fits the exact wave function considerably better than any of the Gaussians taken separately.