Chem. 540
Instructor: Nancy Makri

Variational Principle - Problem 1

A bound system in one dimension is described by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) .$$

In this homework with are interested in two potential forms,

(a) $V(x) = \frac{1}{2} m\omega^2 x^2$ (harmonic potential) and

(b) $V(x) = bx^4$ (quartic potential).

Consider the one-parameter, un-normalized, trial wavefunction

$$\Psi_\lambda(x) = e^{-\lambda x^2} .$$

Evaluate the expectation value of the Hamiltonian for each of the two cases by calculating the normalization integral, the kinetic energy integral, and the two potential integrals. Then minimize it with respect to the parameter λ to obtain the variational approximation to the ground state energy in each of the two cases. In the case of the harmonic potential, compare your results (ground state energy estimate and approximation to the eigenfunction) to the known expression. In the case of the quartic potential, state your conclusion about the true ground state energy of the system. You may look up the integrals, but do show all other work.