

Chem 2430 HW #5

The Morse potential is given by

$$V(x) = D_e \left(1 - e^{-a(x-x_e)} \right)^2$$

Consider the case for which $D_e = 0.1$, $x_e = 2$,
 $a = 0.1$ (in atomic units)

- Generate the harmonic approximation to the potential and using the $n=0$ HO wavefunction calculate the energy of the ground state of the Morse potential.
- Repeat the above calculation using the first two HO wavefunctions as the trial wave function in a variational calculation.
- In b) what are the coefficients of the two HO basis functions?