

HW #5 Answers.

Morse potential with $D_e = 0.1$, $x_e = 2$, $a = 0.1$

The series expansion gives

$$0.001(x-2)^2 - 0.0001(x-2)^3 + 5.833 \times 10^{-6}(x-2)^4$$

$$k = 0.002 \Rightarrow \omega = 0.0447, \text{ assuming } \mu = 1$$

H_{11} and H_{22} will have contributions from the quadratic term. H_{12} involves only the cubic term when using the harmonic oscillator basis set.

$$H_{11} = \frac{0.0447}{2} + 0.00219$$

$$H_{22} = \frac{3}{2}(0.0447) + 0.0110$$

$$H_{12} = 0.0112$$

$$\underline{H} = \begin{pmatrix} 0.0252 & 0.0112 \\ 0.0112 & 0.0780 \end{pmatrix}$$

Eigenvalues $\rightarrow 0.0228, 0.0804$