3.7: The Morse Oscillator

The Morse oscillator model is often used to go beyond the harmonic oscillator approximation. In this model, the potential $E_j(R)$ is expressed in terms of the bond dissociation energy D_e and a parameter a related to the second derivative k of $E_j(R)$ at $R_e k = \frac{d^2 E_j}{dR^2} = 2a^2 D_e$ as follows:

$$E_j(R) - E_j(R_e) = D_e \left[1 - e^{-a(R-R_e)}\right]^2.$$

The Morse oscillator energy levels are given by

$$E^0_{j,v} = E_j(R_e) + \hbar\frac{\sqrt{k}}{\mu}\left(v + \frac{1}{2}\right) - \frac{\hbar^2}{4}\left(\frac{k}{\mu D_e}\right)\left(v + \frac{1}{2}\right)^2$$

the corresponding eigenfunctions are also known analytically in terms of hypergeometric functions (see, for example, Handbook of Mathematical Functions , M. Abramowitz and I. A. Stegun, Dover, Inc. New York, N. Y. (1964)). Clearly, the Morse solutions display anharmonicity as reflected in the negative term proportional to $(v + \frac{1}{2})^2$.