

The potential energy then reduces to

$$V = \frac{k}{2}(\eta_2 - \eta_1)^2 + \frac{k}{2}(\eta_3 - \eta_2)^2,$$

or

$$V = \frac{k}{2}(\eta_1^2 + 2\eta_2^2 + \eta_3^2 - 2\eta_1\eta_2 - 2\eta_2\eta_3). \quad (6.49)$$

Hence, the **V** tensor has the form

$$\mathbf{V} = \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}. \quad (6.50)$$

The kinetic energy has an even simpler form:

$$T = \frac{m}{2}(\dot{\eta}_1^2 + \dot{\eta}_3^2) + \frac{M}{2}\dot{\eta}_2^2, \quad (6.51)$$

so that the **T** tensor is diagonal:

$$\mathbf{T} = \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix}. \quad (6.52)$$

Combining these two tensors, the secular equation appears as

$$|\mathbf{V} - \omega^2 \mathbf{T}| = \begin{vmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{vmatrix} = 0. \quad (6.53)$$

Direct evaluation of the determinant leads to the cubic equation in ω^2 :

$$\omega^2(k - \omega^2 m)(k(M + 2m) - \omega^2 Mm) = 0, \quad (6.54)$$

with the obvious solutions

$$\omega_1 = 0, \quad \omega_2 = \sqrt{\frac{k}{m}}, \quad \omega_3 = \sqrt{\frac{k}{m} \left(1 + \frac{2m}{M}\right)}. \quad (6.55)$$

The first eigenvalue, $\omega_1 = 0$, may appear somewhat surprising and even alarming at first sight. Such a solution does not correspond to an oscillatory motion at all, for the equation of motion for the corresponding normal coordinate is

$$\ddot{\xi}_1 = 0,$$

which produces a uniform translational motion. But this is precisely the key to the difficulty. The vanishing frequency arises from the fact that the molecule

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