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CLASSICAL MECHANICS I (PHY 401A) 2020-21 ODD SEMESTER

Tutorial sheet 9 solutions

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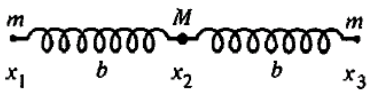
1. **Linear triatomic molecule**

   A simple model of a triatomic molecule consists of three atoms of which two are of mass m and the third one is of mass M. They are arranged according to the figure below. The attractive force between them can be modelled by two springs, each of stiffness k. The position of the three atoms are denoted by x_1, x_2 and x_3 as shown in the figure. In the equilibrium configuration (x_{01}, x_{02}, x_{03}), the distance between two adjacent atoms are given by b. Find the normal modes and normal coordinates for the system.



Solution: In position coordinates, the potential energy can be written as

$$V = \frac{k}{2}(x_2 - x_1 - b)^2 + \frac{k}{2}(x_3 - x_2 - b)^2 \tag{1}$$

we now introduce coordinates relative to equilibrium position:

$$\eta_l = x_l - x_{0l}, \tag{2}$$

where

$$x_{02} - x_{01} = b = x_{03} - x_{01}. \tag{3}$$

the potential energy reduces to

$$V = \frac{k}{2}(\eta_2 - \eta_1)^2 + \frac{k}{2}(\eta_3 - \eta_2)^2, \tag{4}$$

or

$$V = \frac{k}{2}(\eta_1^2 + 2\eta_2^2 + \eta_3^2 - 2\eta_1\eta_2 - 2\eta_2\eta_3) \tag{5}$$

hence the **V** tensor has the form

$$\begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix} \tag{6}$$

the kinetic energy has the following form

$$T = \frac{m}{2}(\dot{\eta}_1^2 + \dot{\eta}_3^2) + \frac{M}{2}\dot{\eta}_2^2 \tag{7}$$

so the **T** tensor is diagonal

$$\begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix} \tag{8}$$

combining these two tensors, the secular equation will be

$$|V - \omega^2 T| = \begin{vmatrix} k - \omega^2 m & -k & 0 \\ -k & 2k - \omega^2 M & -k \\ 0 & -k & k - \omega^2 m \end{vmatrix} \tag{9}$$

the determinant leads to the cubic equation in ω^2: with the obvious solution

$$\omega_1 = 0, \quad \omega_2 = \sqrt{\frac{k}{m}}, \quad \omega_3 = \sqrt{\frac{k}{m}(1 + \frac{2m}{M})} \tag{10}$$

along with the normalization condition (i.e. the center of mass remains stationary at the origin)

$$m(a_{1j}^2 + a_{3j}^2) + M a_{2j}^2 = 0 \tag{11}$$

for ω_1, we have

$$a_{11} = a_{21} = a_{31} \tag{12}$$

using the normalization condition, the values of a_{1j}

$$a_{11} = \frac{1}{\sqrt{(2m + M)}}, \quad a_{12} = \frac{1}{\sqrt{(2m + M)}}, \quad a_{13} = \frac{1}{\sqrt{(2m + M)}}, \tag{13}$$

for the second mode ω_2

$$a_{22} = 0, \quad a_{12} = -a_{32} \tag{14}$$

using normalization condition

$$a_{12} = \frac{1}{\sqrt{2m}}, \quad a_{22} = 0, \quad a_{32} = \frac{1}{\sqrt{2m}} \tag{15}$$

in this mode, the center atom is at rest and the other two vibrate exactly out of phase. for ω_3, a_{13} and a_{33} must be equal. the values are following

$$a_{13} = \frac{1}{\sqrt{2m(1 + \frac{2m}{M})}}, \quad a_{23} = \frac{-2}{\sqrt{2M(1 + \frac{M}{m})}}, \quad a_{33} = \frac{1}{\sqrt{2m(1 + \frac{2m}{M})}} \tag{16}$$

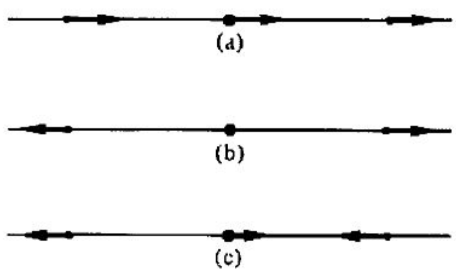


Abbildung 1: longitudinal normal modes of linear symmetric triatomic molecule

here the two outer atoms vibrate with the same amplitude, while the inner one oscillates out of phase with them with different amplitude.

the transformation from the η_i to a new set of generalized coordinates that are all simple periodic function of time, known as normal coordinates.

$$\eta_i = a_{ij}\zeta_j \tag{17}$$

so the normal coordinates can be written as following

$$\zeta_1 = \frac{1}{\sqrt{(2m+M)}}(\sqrt{m}\eta_1 + \sqrt{M}\eta_2 + \sqrt{m}\eta_3) \tag{18}$$

$$\zeta_2 = \frac{1}{\sqrt{2}}(\eta_1 - \eta_3) \tag{19}$$

$$\zeta_3 = \frac{1}{\sqrt{(2m+M)}}[\sqrt{\frac{M}{2}}(\eta_1 + \eta_3) - \sqrt{2m}\eta_2] \tag{20}$$

2. **System of two interacting oscillators**

Determine the normal oscillations of a system of two oscillators whose combined Lagrangian is given by

$$L = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) + \frac{\omega_0^2}{2}\left(x^2 + y^2\right) + \alpha xy,$$

where α is a nonzero constant.

Solution: From Euler-Lagrange equation-

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\partial L}{\partial x} \Longrightarrow \ddot{x} + \omega_0^2 x = \alpha y \tag{21}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) = \frac{\partial L}{\partial y} \Longrightarrow \ddot{y} + \omega_0^2 y = \alpha x \tag{22}$$

Assuming solution of the form -

$$x = A_x e^{i\omega t} \tag{23}$$

$$y = A_y e^{i\omega t} \tag{24}$$

Substituting above in equations (21, 22), we get -

$$A_x(\omega^2 - \omega_0^2) = A_y \alpha \tag{25}$$

$$A_y(\omega^2 - \omega_0^2) = A_x \alpha \tag{26}$$

For having non-zero solution of above system, the determinant of coefficient must vanish.

$$(\omega^2 - \omega_0^2)^2 = \alpha^2 \tag{27}$$

Above equations give following normal frequencies -

$$\omega_{1,2}^2 = \omega_0^2 \pm \alpha \tag{28}$$

So normal mode X_1' corresponding to ω_1 will be -

$$\begin{pmatrix} \alpha & -\alpha \\ -\alpha & \alpha \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Longrightarrow A_x = A_y \tag{29}$$

$$X_1' \equiv \begin{pmatrix} x \\ y \end{pmatrix} = \pm \frac{e^{i\omega_1 t}}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{30}$$

Similarly normal mode corresponding to ω_2 can be obtained -

$$-\begin{pmatrix} \alpha & \alpha \\ \alpha & \alpha \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Longrightarrow A_x = -A_y \tag{31}$$

$$X_2' \equiv \begin{pmatrix} x \\ y \end{pmatrix} = \pm \frac{e^{i\omega_2 t}}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{32}$$

If U_1, U_2 are the corresponding normal co-ordinates such that-

$$\ddot{U}_{1,2} = -\omega_{1,2}^2 U_{1,2} \tag{33}$$

and if, $X' = PU$, then -

$$P = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{34}$$

So,

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \end{pmatrix} \tag{35}$$

And $U = P^{-1}X'$,

$$P^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{36}$$

So,

$$\begin{pmatrix} U_1 \\ U_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{37}$$

$$U_1 = \frac{1}{\sqrt{2}}(x + y) \tag{38}$$

$$U_2 = \frac{1}{\sqrt{2}}(x - y) \tag{39}$$