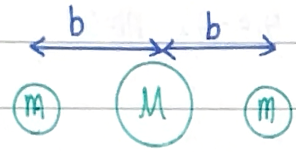
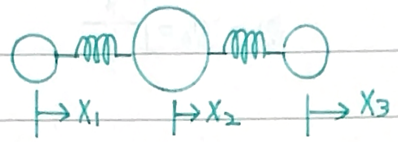
Molecular Vibrations

cosider here only the vibrations occuring in a plane

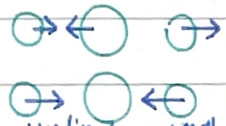
eliminate the translational and rotational degree of freedom

for motion in a plane, there are 2n degrees of freedom $\left[\begin{array}{l}\text{two are translational} \\ \text{one is rotational}\end{array}\right.$

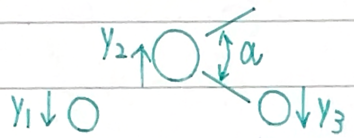




longitudinal description



longitudinal normal nodes



transverse normal mode

$$m(x_1+x_3)+Mx_2=0 \; , \; x_2=-\frac{m}{M}(x_1+x_2)$$

$$T=\frac{1}{2}m\left(\frac{dx_1}{dt}\right)^2+\frac{1}{2}m\left(\frac{dx_3}{dt}\right)^2+\frac{1}{2}M\left(\frac{dx_2}{dt}\right)^2$$

dynamic coupling

$$=\frac{1}{2}m\left(\frac{dx_1}{dt}\right)^2+\frac{1}{2}m\left(\frac{dx_3}{dt}\right)^2+\frac{1}{2}\frac{m^2}{M}\left[\left(\frac{dx_3}{dt}\right)^2+\left(\frac{dx_1}{dt}\right)^2+2\overbrace{\frac{dx_3}{dt}\frac{dx_1}{dt}}\right]$$

let $q_1=x_3+x_1$, $q_2=x_3-x_1$ $\rightarrow$ $x_3=\frac{1}{2}(q_1+q_2)$, $x_1=\frac{1}{2}(q_1-q_2)$ $\quad x_2=-\frac{m}{M}q_1$

$$T=\frac{m}{4}\left(\frac{dq_2}{dt}\right)^2+\frac{mM+2m^2}{4M}\left(\frac{dq_1}{dt}\right)^2 \qquad U=\frac{1}{2}k_1(x_2-x_1)^2+\frac{1}{2}k_1(x_3-x_2)^2$$

$$=\left(\frac{2m+M}{2M}\right)^2k_1q_1^2+\frac{1}{4}k_1q_2^2$$

$$\begin{vmatrix} \frac{1}{2}\left(\frac{2m+M}{M}\right)^2k_1-\omega^2\frac{mM+2m^2}{2M} & 0 \\ 0 & \frac{k_1}{2}-\omega^2\frac{m}{2} \end{vmatrix}=0$$

Per-Duet

NO:

DATE: / /

$\omega_1^2 = \frac{2m+M}{mM} k_1 \qquad \omega_2^2 = \frac{k_1}{m}$

$q_1 = a_{11}\eta_1 + a_{12}\eta_2$ but $a_{12}=0$ $a_{21}=0$ $q_1 = a_{11}\eta_1$

$q_2 = a_{21}\eta_1 + a_{22}\eta_2$ $q_2 = a_{22}\eta_2$

mode	eigenfrequencies	variable	motion
1	$\sqrt{\frac{2m+M}{mM} k_1}$	$q_1 = X_1 + X_3$	$X_3 = X_1$, $q_2 = 0$ $X_2 = -\frac{2m}{M} X_1$
2	$\sqrt{\frac{k_1}{m}}$	$q_2 = X_3 - X_1$	$X_3 = -X_1$ $q_1 = 0$ $X_2 = 0$

$m(y_1+y_3) + My_2 = 0$, $y_2 = -\frac{m}{M}(y_1+y_3)$ $\quad a = \frac{(y_1-y_2)+(y_3-y_2)}{b}$

$T = \frac{1}{2} m\left[\left(\frac{dy_1}{dt}\right)^2 + \left(\frac{dy_3}{dt}\right)^2\right] + \frac{1}{2} M\left(\frac{dy_2}{dt}\right)^2$ because $y_1 = y_3$

$a = \frac{2y_1}{bM}(2m+M)$

$T = \frac{m}{M}(M+2m)\left(\frac{dy_1}{dt}\right)^2 = \frac{mMb^2}{4(2m+M)}\left(\frac{da}{dt}\right)^2$ assume $F \propto \frac{d\,ba}{dt}$

$U = \frac{1}{2} k_2 (ba)^2$

$\omega_3^2 = \frac{2(M+2m)}{mM} k_2 \qquad y_1 = y_3 \qquad y_2 = -\frac{m}{M}(y_1+y_3)$