Ex 4.

repulsion attraction

$$(1.a)\quad V(X_1,X_2,x) = -\frac{K_1}{2}(X_1-X_2)^2 + \frac{K_2}{2}\left[(x-X_1)^2+(x-X_2)^2\right]$$

$$V_{X_1X_2}(x) = -\frac{K_1}{2}(X_1-X_2)^2 + K_2\left(\frac{X_1-X_2}{2}\right)^2 + \underline{K_2\left(x-\frac{X_1+X_2}{2}\right)^2}$$

$$H_{el} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{2K_2}{2}\left(x-\frac{X_1+X_2}{2}\right)^2 + V(X_1,X_2)$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(\Delta x)^2} + \frac{2K_2}{2}\Delta x^2 = \hbar\omega\left(a^+a+\frac{1}{2}\right)$$

where $\Delta x = x_0(a^+ + a)$

$x_0 = \sqrt{\frac{\hbar}{2m\omega}}$, $\omega = \sqrt{\frac{2K_2}{m}}$

$$V_{eff}(X_1,X_2) = \langle 0|V(X_1,X_2,x)|0\rangle = -\frac{K_1}{2}(X_1-X_2)^2 + K_2\left(\frac{X_1-X_2}{2}\right)^2 + K_2 x_0^2$$

independent of X_1, X_2

$$\begin{cases} M_1\omega^2 X_1 = \left(\frac{1}{2}K_2-K_1\right)X_1 - \left(\frac{1}{2}K_2-K_1\right)X_2 \\ M_2\omega^2 X_2 = -\left(\frac{1}{2}K_2-K_1\right)X_1 + \left(\frac{1}{2}K_2-K_1\right)X_2 \end{cases} \rightarrow \left(\frac{1}{2}K_2-K_1\right)\begin{vmatrix} \frac{1}{M_1}-\lambda & \frac{-1}{M_1} \\ -\frac{1}{M_2} & \frac{1}{M_2}-\lambda \end{vmatrix} = 0$$

where $\left(\frac{1}{2}K_2-K_1\right)\lambda = \omega^2$

$$\left(\frac{1}{2}K_2-K_1\right)\lambda\left[\lambda-\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\right] = 0 \rightarrow \begin{cases} \lambda = \omega^2 = 0 \rightarrow \text{translation} \\ \omega^2 = \left(\frac{1}{2}K_2-K_1\right)\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \end{cases}$$

Stable $\Rightarrow \omega^2 > 0 \Rightarrow \frac{1}{2}K_2 - K_1 > 0$

$$(1.b)\quad \omega = \sqrt{\left(\frac{1}{2}K_2-K_1\right)\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}$$

(1.c) let $\omega^2 = \lambda$

$$\begin{vmatrix} m\lambda-2K_2 & +K_2 & +K_2 \\ K_2 & M_1\lambda+K_1-K_2 & -K_1 \\ K_2 & -K_1 & M_2\lambda+K_1-K_2 \end{vmatrix} = 0$$

In case of $m=0$,

$$M_1\lambda\{K_2[M_2\lambda+(K_1-K_2)]+K_1K_2\} + M_2\lambda\{K_2[M_1\lambda+(K_1-K_2)]+K_1K_2\} = 0$$

$$\lambda K_2\{(M_1+M_2)(2K_1-K_2)+2M_1M_2\lambda\} = 0$$

$$\omega^2 = \lambda = \left(\frac{1}{M_1}+\frac{1}{M_2}\right)\left(\frac{1}{2}K_2-K_1\right)$$

In the case of $M_1=M_2=M$,

$$\begin{vmatrix} m\lambda-2k_2 & k_2 & k_2 \\ k_2 & M_1\lambda+k_1-k_2 & -k_1 \\ k_2 & -k_1 & M_2\lambda+k_1-k_2 \end{vmatrix} \overset{R_1=R_1+R_2+R_3}{=} \begin{vmatrix} m\lambda & M_1\lambda & M_2\lambda \\ k_2 & M_1\lambda+(k_1-k_2) & -k_1 \\ k_2 & -k_1 & M_2\lambda+(k_1-k_2) \end{vmatrix} \overset{M_1=M_2=M}{=}$$

$$\overset{\substack{R_2=R_2-R_3 \\ C_2=C_2+C_3}}{=} \begin{vmatrix} m\lambda & 2M\lambda & M\lambda \\ 0 & 0 & -M\lambda-(2k_1-k_2) \\ k_2 & M\lambda-k_2 & M\lambda+(k_1-k_2) \end{vmatrix} = 0$$

$$m\lambda\{(M\lambda-k_2)[M\lambda+(2k_1-k_2)]\}-2M\lambda k_2[M\lambda+(2k_1-k_2)]=0$$

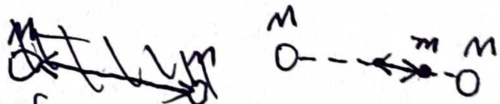
$$\lambda[M\lambda+(2k_1-k_2)]\{mM\lambda-mk_2-2Mk_2\}=0$$

$$\begin{cases} \lambda_0=0 \\ \lambda_1=\dfrac{\frac{1}{2}k_2-k_1}{M/2} \end{cases}$$

translation

nuc↔nuc.

$$\lambda_2=\left(\frac{1}{2M}+\frac{1}{m}\right)2k_2$$

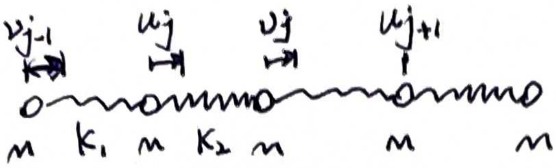


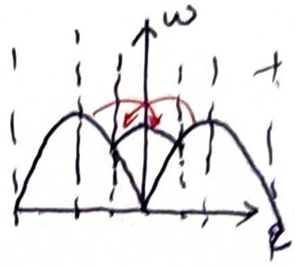
el ↔ geometric center

COM of

In reference frame of M_1, M_2, its geometric center will move with nuc-nuc vib

but for $M_1=M_2=M$, geometric center coincide with COM, thus at relatively rest.

(2.a) 



$+\ \omega(q) = 2\sqrt{\frac{K}{M}}\left|\sin\left(\frac{qa}{2}\right)\right|$

$$V = \sum_j \frac{1}{2}K_1(v_{j-1}-u_j)^2 + \frac{1}{2}K_2(u_j - v_j)^2$$

or $-M\ddot{u}_j$ $\quad M\omega^2 u_j = \{(K_1+K_2)u_j - K_1 v_{j-1} - K_2 v_j\}$. $\quad u_q = \sum_j e^{-i\vec{q}\cdot\vec{R}_j} u_j = \sum_n e^{-iq(2na)} \cdot u_n$

$-M\ddot{v}_j$ $\quad M\omega^2 v_j = \{(K_1+K_2)v_j - K_1 u_{j+1} - K_2 u_j\}$ $\quad v_q = \quad = \sum_n e^{-iq(2n+1)a} v_j$

Subsoitute u_q, v_q

$$-M\ddot{u}_q = -M\sum_n e^{-iq\cdot 2an}\ddot{u}_n = \sum_n e^{-iq\cdot 2an}\{(K_1+K_2)\underset{u_q}{u_n} - K_1 \underset{e^{-iqa}v_q}{v_{n-1}} - K_2 \underset{e^{+iqa}v_q}{v_n}\}.$$

$$= (K_1+K_2)u_q - K_1 e^{-iqa} v_q - K_2 e^{+iqa} v_q$$

$$-M\ddot{v}_q = (K_1+K_2)v_q - K_1 e^{+iqa}u_q - K_2 e^{-iqa} u_q$$

Solving 2x2 system of each q-sector

$$\begin{pmatrix} K_1+K_2 & -K_1 e^{+iqa} - K_2 e^{-iqa} \\ -K_1 e^{-iqa} - K_2 e^{+iqa} K_2 & K_1+K_2 \end{pmatrix}\begin{pmatrix} C_u \\ C_v \end{pmatrix} = \underbrace{M\omega^2}_{\lambda}\begin{pmatrix} C_u \\ C_v \end{pmatrix}.$$

$$\{(K_1+K_2)-\lambda\}^2 - (K_1 e^{+iqa} + K_2 e^{-iqa})(K_1 e^{-iqa} + K_2 e^{+iqa}) = 0$$

$$\lambda^2 - 2(K_1+K_2)\lambda + 4K_1K_2\sin^2(qa) = 0$$

$$M\omega_\pm^2 = \lambda_\pm = (K_1+K_2) \pm \sqrt{(K_1+K_2)^2 - 4K_1K_2\sin^2(qa)}, \text{ Let } \alpha = \frac{K_1}{K_2}$$

$$= K_2\{(1+\alpha) \pm \sqrt{(1+\alpha)^2 - 4\alpha\sin^2(qa)}$$

In the case of $\alpha = 1$

$$M\omega_\pm^2 = K_2\{2 \pm 2\cos(qa)\}.$$

$$= 2K_2\{1 \pm \cos(qa)\}$$

$$\omega_- = 2\sqrt{\frac{K}{M}}\left|\sin\left(\frac{qa}{2}\right)\right|$$

$$\omega_+ = 2\sqrt{\frac{K}{M}}\left|\cos\left(\frac{qa}{2}\right)\right|$$

In the case of $\alpha \ll 1$, $\sqrt{1+2x} \approx 1+x$

$$M\omega_\pm^2 = K_2\{(1+\alpha) \pm [1+\alpha(1-2\sin^2(qa))]$$

$$M\omega_-^2 = 2K_2\alpha\sin^2(qa) = 2K_1\sin^2(qa)$$

$$\omega_- = \sqrt{\frac{2K_1}{M}}|\sin(qa)|$$

$\alpha \ll 1$, $M\omega_+^2 = 2K_2$, $\omega_+ = \sqrt{\frac{2K_2}{M}}$