

School of Engineering Brown University

1. In homework 4 Problem 1-3(iv), you used the Buckingham potential

 $V(d) = A \exp(-Bd) - \frac{C}{d^6}$ 

to get the stiffness k's of the six molecular bonds with the coefficients A, B and C as shown in Table 3.

Find the frequency  $\omega$ 's of bond stretching vibrations of the six molecular

Table 3	Selected	Values <sup>a</sup>	of the	e Buckingham	Potential
Paramete	ers A, B, a	and C.			

Interaction	10 <sup>-3</sup> A <sup>b</sup>	$B^{\mathfrak{b}}$	C <sup>b</sup>
C…C <sup>c</sup>	541.4	4.59	363.0
CC <sup>d</sup>	1820	4.59	556.7
N…N	393.2	4.59	547.3
00	135.8	4.59	217.2
S…S	906.3	3.90	3688
н…н	7.323	4.54	47.1

"Taken from Ref. 48.

<sup>b</sup>Units are such as to give energy in kcal mol<sup>-1</sup> for r in Å. <sup>c</sup>Aliphatic carbon atoms.

<sup>d</sup>Aromatic carbon atoms.

**EN40: Dynamics and Vibrations** 

Homework 5: Free Vibrations Due Friday March 22nd

bonds, and corresponding wavelengths of infrared (IR) light that excite the bondstretching vibrational mode. The wavelength  $\lambda$  of the light is given by  $\lambda = 2\pi c/\omega$ , and it is typically in the range of  $2.5 - 25 \mu m$ . In chemistry, the spectrum of the wavelength is traditionally denoted by the reciprocal  $1/\lambda \ cm^{-1}$ ; for example, experimental measurement of H – H bond IR spectrum is 4111  $cm^{-1}$ .

**Solution:** Use mupad as follows (Oxygen example)

```
\begin{bmatrix} reset \\ reset \\ R:=135.8*10^{3}*4.2 \\ 570360.0 \\ B:=4.59 \\ 4.59 \\ C:=217.2*4.2 \\ 912.24 \\ V:=A*exp(-B*d)-C/d^{6} \\ \frac{570360.0}{e^{4.59}d} - \frac{912.24}{d^{6}} \end{bmatrix}
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\begin{bmatrix} F:= -A*B*exp(-B*d)+6*C/d^{7} \\ \frac{5473.44}{d^{7}} - \frac{2617952.4}{e^{4.59\,d}} \\ eqsep := solve(F=0,d,Real)[2] \\ 3.039843952 \\ \end{bmatrix}
\begin{bmatrix} Fderiv:=A*B*B*exp(-B*d)-42*C/d^{8} \\ \frac{12016401.52}{e^{4.59\,d}} - \frac{38314.08}{d^{8}} \\ \end{bmatrix}
\begin{bmatrix} stif := float(subs(Fderiv,d=eqsep)) \\ 5.219333039 \\ \\ \\ S:=(%)*1000/6.02/10^{2}3/10^{6}(-20) \\ 0.8669988437 \end{bmatrix}
```

This is the stiffness of O-O bond in N/m. Now, we get the atomic mass (m) in kg as follows:

```
[m:=16/6.02/10^23/10^3
2.657807309 10<sup>-26</sup>
[omega:=sqrt(2*S/m)
8.077231146 10<sup>12</sup>
[lambda:=2*3.14*3*10^8*10^6/omega
233.2482463
```

This is the wavelength of IR light in  $\mu m$  for the O-O bond vibration.

If you repeat the calculation for the rest bonds, you will get the wavelength for each as,

C-C (aliphatic): 219.8  $\mu m$ C-C (aromatic): 231.1  $\mu m$ N-N : 145.8  $\mu m$ S-S : 156.5  $\mu m$ H-H : 64.99  $\mu m$ 

These numbers are about 25 times off the real IR wavelength – why? This may be because the Buckingham potential is not reliable for stiffness estimation, since it is primarily designed for potential well depth and equilibrium bond length estimation.

2. Seiches is a phenomenon of harmonic oscillation of contained water in lakes, reservoirs, swimming pools, bays, harbors and seas when the motion is synchronously activated by atmospheric pressure variations or seismic waves. "The term was promoted by the Swiss hydrologist François-Alphonse Forel in 1890, who was the first to make scientific observations of the effect in Lake Geneva, Switzerland. The word originates in a Swiss French dialect word that means "to sway back and forth", which had apparently long been used in the region to describe oscillations in alpine lakes: [wiki]"

Consider an idealized model as follows. Water is contained in a pan of span of 2L and initially filled up to the depth of H. The level of the water surface is then dynamically tilted to have the elevation of the water level expressed as y(t) = xh(t)/L as shown in the figure below.

(1) Show that the center coordinate  $(x_c, y_c)$  of the mass of the water is located at  $x_c = \frac{1}{3} \left(\frac{L}{H}\right) h$ ,  $y_c = \frac{1}{6} \left(\frac{h}{H}\right) h - \frac{H}{2}$ .

$$x_{C} = \frac{1}{M} \int_{M} x_{(dM)} dM = \frac{1}{2\rho HL} \int_{-L}^{L} x\rho \left(H + \frac{h}{L}x\right) dx = \frac{1}{3} \left(\frac{L}{H}\right) h$$
$$y_{C} = \frac{1}{M} \int_{M} y_{(dM)} dM = \frac{1}{2\rho HL} \int_{-L}^{L} \frac{1}{2} (y - H) \rho \left(H + \frac{h}{L}x\right) dx = \frac{1}{6} \left(\frac{h}{H}\right) h - \frac{H}{2}$$

(2) With a crude approximation of treating the water motion as a rigid body motion of  $(x_c, y_c)$ , show that the water has the total energy as

$$E_T = \frac{M}{18} \left(\frac{L}{H}\right)^2 \dot{h}^2 + \frac{Mg}{6H} h^2 + C \quad \text{for } \frac{h}{L} \ll 1, \text{ where } C \text{ is a constant.}$$

Solution:

$$\begin{split} E_T &= \frac{1}{2}M\left(\dot{x}_C^2 + \dot{y}_C^2\right) + Mgy_C = \frac{M}{18} \left\{ \left(\frac{L}{H}\right)^2 + \left(\frac{h}{H}\right)^2 \right\} \dot{h}^2 + \frac{Mg}{6H}h^2 - \frac{MgH}{2} \\ &\approx \frac{M}{18} \left(\frac{L}{H}\right)^2 \dot{h}^2 + \frac{Mg}{6H}h^2 + C \quad \text{for } \frac{h}{L} \ll 1. \end{split}$$

(3) Set up the equation of motion for h(t) and show that the sloshing frequency is approximately given by  $\omega \approx \frac{H}{L} \sqrt{\frac{3g}{H}}$ . Solution:

$$\frac{dE_T}{dt} \approx \frac{M}{9} \left(\frac{L}{H}\right)^2 \dot{h}\ddot{h} + \frac{Mg}{3H}h\dot{h} \approx 0 \quad \Rightarrow \quad \ddot{h} + 3\left(\frac{H}{L}\right)^2 \frac{g}{H}h \approx 0$$
$$\ddot{h} + \omega^2 h = 0 \quad \Rightarrow \quad \omega \approx \frac{H}{L}\sqrt{\frac{3g}{H}}$$

(4) When we use a better model to take in to account of the fluid motion with  $v \approx -\frac{\dot{h}}{2HL} \left(x^2 - L^2\right)$ , we have the kinetic energy expression as  $\frac{M}{15} \left(\frac{L}{H}\right)^2 \dot{h}^2$  (you do not have to derive this result; just use it.). How much error of  $\omega$  is induced by

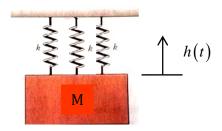
do not have to derive this result; just use it.). How much error of  $\omega$  is induced by the rigid body motion assumption compared to the prediction based on the fluid mechanics model?

Solution:

$$\frac{dE_T}{dt} \approx \frac{2M}{15} \left(\frac{L}{H}\right)^2 \dot{h}\ddot{h} + \frac{Mg}{3H} h\dot{h} \approx 0 \quad \Rightarrow \quad \ddot{h} + \frac{5}{2} \left(\frac{H}{L}\right)^2 \frac{g}{H} h \approx 0$$
$$\ddot{h} + \omega^2 h = 0 \quad \Rightarrow \quad \omega_f \approx \frac{H}{L} \sqrt{\frac{5g}{2H}} \Rightarrow \frac{\omega}{\omega_f} = \sqrt{\frac{6}{5}} \approx 1.1$$

"Lake seiches can occur very quickly: on July 13, 1995, a big seiche on Lake Superior caused the water level to fall and then rise again by three feet (one meter) within fifteen minutes, leaving some boats hanging from the docks on their mooring lines when the water retreated. The same storm system that caused the 1995 seiche on Lake Superior produced a similar effect in Lake Huron, in which the water level at Port Huron changed by six feet (1.8 m) over two hours. On Lake Michigan, eight fishermen were swept away and drowned when a 10-foot seiche hit the Chicago waterfront on June 26, 1954. [wiki]"

3. A mass M hung by three springs is vibrating as  $h(t) = h_0 \sin \omega t$  as shown in the figure. While it is vibrating the center spring is snapped as the mass was just passing the point  $h(t) = h_0/2$  with  $\dot{h}(t) < 0$ . Describe the motion of the mass after the spring is snapped.



### Solution:

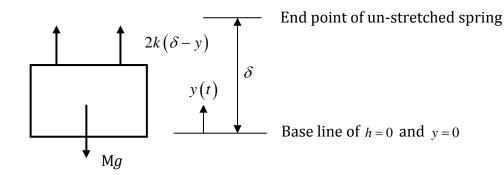
Before snapping it was vibrating as  $h(\tau) = h_0 \sin \hat{\omega} \tau$  with  $\hat{\omega} = \sqrt{3k/m}$  and the static deflection is

$$\delta = Mg/3k \,. \tag{1}$$

At the time of snapping we have

$$h = h_0/2$$
 and  $\dot{h} = -h_0 \hat{\omega} \sqrt{3}/2$ . (2)

Now we set these conditions as initial condition of the vibration after the snapping for which we describe the height location of the mass as y(t). Then, the free body diagram after the snapping shows as follows



 $\sum F_y = 2k(\delta - y) - Mg = M\ddot{y}$  this equation can be rearranged as

$$M\ddot{y} + 2ky = 2k\delta - Mg:$$
<sup>(3)</sup>

This is the standard form of shifted harmonic oscillation we studied in our class. Inserting (1) into (3) we have

$$\ddot{y} + \frac{2k}{M}y = -\frac{g}{3} \tag{4}$$

This differential equation has the general solution of

$$y(t) = C\sin\left(\sqrt{\frac{2k}{M}}t + \phi\right) - \frac{Mg}{6k}.$$
(5)

Now we use the initial conditions in (2) to determine C and  $\phi$  as

$$y(0) = C\sin\phi - \frac{Mg}{6k} = \frac{h_0}{2} \text{ or } C\sin\phi = \frac{h_0}{2} + \frac{Mg}{6k}$$
 (6)

$$\dot{y}(0) = C\sqrt{\frac{2k}{M}}\cos\phi = -\frac{\sqrt{3}h_0}{2}\hat{\omega} = -\frac{\sqrt{3}h_0}{2}\sqrt{\frac{3k}{M}} \text{ or } C\cos\phi = -\frac{3h_0}{2\sqrt{2}}$$
 (7)

Dividing (6) by (7), we have

$$\tan\phi = -\frac{\sqrt{2}}{3} - \frac{\sqrt{2}Mg}{9kh_0} \tag{8a}$$

and  $(6)^{2+(7)}$  will lead to

$$C = \sqrt{\left(\frac{h_0}{2} + \frac{Mg}{6k}\right)^2 + \frac{9h_0^2}{8}}$$
(8b)

4. An old pendulum clock is sitting on a table spinning with angular speed of  $\Omega$  with respect to y axis as shown in the figure; the (x, y) plane spins with respect to y axis. The pendulum in the clock is attached at the origin of the (x, y) coordinate and oscillates only in the spinning (x, y) plane. The pendulum length is denoted by l and the swing angle in the (x, y) plane by  $\theta$ .

(1) By aligning the spinning coordinate axes (x, y, z) and the inertial frame coordinate axes (X, Y, Z) at time at t = 0, the inertial coordinate position of the pendulum mass m is given by  $X = l \sin \theta \cos \Omega t$ ,  $Y = -l \cos \theta$  and  $Z = -l \sin \theta \sin \Omega t$ . Using the law,  $\sum F_X = -T \sin \theta \cos \Omega t - N \sin \Omega t = m\ddot{X}$ ,



 $\sum F_{Y} = -mg + T\cos\theta = m\ddot{Y}$  and  $\sum F_{Z} = T\sin\theta\sin\Omega t - N\cos\Omega t = m\ddot{Z}$ , show that the equation of motion is reduced to  $\ddot{\theta} + (g/l)\sin\theta - \Omega^{2}\cos\theta\sin\theta = 0$ . Here *T* is the tension and *N* the force normal to (x, y) plane, transmitted through the pendulum bar.

#### Solution:

$$X = l\sin\theta\cos\Omega t$$
  

$$\dot{X} = l\dot{\theta}\cos\theta\cos\Omega t - l\Omega\sin\theta\sin\Omega t$$
  

$$\ddot{X} = l\ddot{\theta}\cos\theta\cos\Omega t - l\dot{\theta}^{2}\sin\theta\cos\Omega t - 2l\dot{\theta}\Omega\cos\theta\sin\Omega t - l\Omega^{2}\sin\theta\cos\Omega t$$
  

$$Y = -l\cos\theta$$
  

$$\dot{Y} = l\dot{\theta}\sin\theta$$
  

$$\ddot{Y} = l\ddot{\theta}\sin\theta + l\dot{\theta}^{2}\cos\theta$$

 $Z = -l\sin\theta\sin\Omega t$  $\dot{Z} = -l\dot{\theta}\cos\theta\sin\Omega t - l\Omega\sin\theta\cos\Omega t$  $\ddot{Z} = -l\ddot{\theta}\cos\theta\sin\Omega t + l\dot{\theta}^{2}\sin\theta\sin\Omega t - 2l\dot{\theta}\Omega\cos\theta\cos\Omega t + l\Omega^{2}\sin\theta\sin\Omega t$ 

Once we plug into the given equations of motion, you get

$$\ddot{\theta} + (g/l)\sin\theta - \Omega^2\cos\theta\sin\theta = 0$$

(2) Linearize the equation of motion and find the pendulum swing period in terms of l,  $\Omega$  and the gravitational acceleration g.

# Solution:

Put  $\sin\theta \approx \theta$  and  $\cos\theta \approx 1$  for  $\theta \ll 1$  to have  $\ddot{\theta} + (g/l - \Omega^2)\theta = 0$ 

(3) At what spin speed  $\Omega$  does the clock stop?

### Solution:

$$\Omega = \sqrt{\frac{g}{l}}$$

(4) Compare the linearized solution of  $\theta(t)$  with the solution of the full nonlinear equation in (1) numerically solved by MATLAB for  $0 \le \theta(t) \le \frac{\pi}{6}$ , for  $\Omega = \frac{1}{2}\sqrt{\frac{g}{l}}$ .

# Solution:

Linearized solution:  $\theta = \frac{\pi}{6} \sin \frac{1}{2} \sqrt{\frac{3g}{l}t}$ 

Full nonlinear solution: MATLAB

5. Consider two pendulums, a and b, with the same string length l, but with different bob masses  $m_a$  and  $m_b$ . They are coupled by a spring of spring constant k which is attached to the bobs.

(1) Show that the equations motion (for small oscillations) are

$$m_{a} \frac{d^{2} \theta_{a}}{dt^{2}} = -m_{a} \frac{g}{l} \theta_{a} + k \left(\theta_{b} - \theta_{a}\right)$$
$$m_{b} \frac{d^{2} \theta_{b}}{dt^{2}} = -m_{b} \frac{g}{l} \theta_{b} - k \left(\theta_{b} - \theta_{a}\right).$$

# Solution:

Draw the free body diagrams of two bobs and use the law of motion as

$$\sum F_x^a = -m_a g \theta_a + kl (\theta_b - \theta_a) = m_a \frac{d^2 l \theta_a}{dt^2}$$
$$\sum F_x^a = -m_b g \theta_b - kl (\theta_b - \theta_a) = m_b \frac{d^2 l \theta_b}{dt^2}$$
$$\Rightarrow \begin{cases} m_a \frac{d^2 \theta_a}{dt^2} = -m_a \frac{g}{l} \theta_a + k (\theta_b - \theta_a) \\ m_b \frac{d^2 \theta_b}{dt^2} = -m_b \frac{g}{l} \theta_b - k (\theta_b - \theta_a) \end{cases}$$

(2) Solve these two equations for the two normal modes, showing that  $\theta_1 \equiv (m_a \theta_a + m_b \theta_b) / (m_a + m_b)$  and  $\theta_2 \equiv \theta_a - \theta_b$  are normal coordinates.

## Solution:

$$m_{a} \frac{d^{2} \theta_{a}}{dt^{2}} = -m_{a} \frac{g}{l} \theta_{a} + k \left(\theta_{b} - \theta_{a}\right)$$
(1)  
$$m_{b} \frac{d^{2} \theta_{b}}{dt^{2}} = -m_{b} \frac{g}{l} \theta_{b} - k \left(\theta_{b} - \theta_{a}\right)$$
(2)

Add (1) and (2) to have

$$m_{a}\frac{d^{2}\theta_{a}}{dt^{2}} + \frac{d^{2}}{dt^{2}} = -m_{a}\frac{g}{l}\theta_{a} - m_{b}\frac{g}{l}\theta_{b}$$
$$\Rightarrow \frac{d^{2}(m_{a}\theta_{a} + m_{b}\theta_{b})}{dt^{2}} = -\frac{g}{l}(m_{a}\theta_{a} + m_{b}\theta_{b})$$

Devide it with  $m_a + m_b$  to have

$$\frac{d^2}{dt^2} \left\{ \frac{\left( m_a \theta_a + m_b \theta_b \right)}{m_a + m_b} \right\} = -\frac{g}{l} \left\{ \frac{\left( m_a \theta_a + m_b \theta_b \right)}{m_a + m_b} \right\}$$

Subtract  $m_b \times (2)$  from  $m_a \times (1)$  to have

$$m_{b}m_{a}\frac{d^{2}\theta_{a}}{dt^{2}} = -m_{a}m_{b}\frac{g}{l}\theta_{a} + km_{b}\left(\theta_{b} - \theta_{a}\right) \qquad :m_{b}\times(1)$$

$$m_{a}m_{b}\frac{d^{2}\theta_{b}}{dt^{2}} = -m_{a}m_{b}\frac{g}{l}\theta_{b} - km_{a}\left(\theta_{b} - \theta_{a}\right) \qquad :m_{a}\times(2)$$

$$\Rightarrow m_{b}m_{a}\frac{d^{2}\left(\theta_{a} - \theta_{b}\right)}{dt^{2}} = -\left\{m_{a}m_{b}\frac{g}{l} + k\left(m_{a} + m_{b}\right)\right\}\left(\theta_{a} - \theta_{b}\right)$$

(3) Find the frequencies and configurations of the modes. What is the physical significances of  $\theta_1$ ? Of  $\theta_2$ ?

#### Solution:

$$\omega_1^2 = \frac{g}{l} \text{ for } \theta_1 = \frac{\left(m_a \theta_a + m_b \theta_b\right)}{m_a + m_b} \text{: moving together mode}$$
$$\omega_2^2 = \frac{g}{l} + k \left(\frac{1}{m_a} + \frac{1}{m_b}\right) \text{ for } \theta_1 = \left(\theta_a - \theta_b\right) \text{: separation mode}$$

(4) Find a superposition of the two modes which corresponds to the initial conditions at time t = 0 that both pendulums have zero velocity, that bob *a* have amplitude *A*, and that bob *b* amplitude zero.

#### Solution:

$$\theta_a = A \left( \frac{m_a}{m} \cos \omega_1 t + \frac{m_b}{m} \cos \omega_2 t \right)$$
$$\theta_a = A \frac{m_a}{m} \left( \cos \omega_1 t - \cos \omega_2 t \right)$$

where  $m = m_a + m_b$ .

(5) Let  $E_a(t) \approx m_a g l \Theta_a^2/2$  and  $E_b(t) \approx m_b g l \Theta_b^2/2$  be the total energy of the pendulum *a* and *b* respectively, ignoring the spring energy for weak coupling. Here  $\Theta_a$  and  $\Theta_b$  denote the envelope function of the beat oscillation. Find an expression for  $E_a(t)$  and for  $E_b(t)$ . Does the energy of bob *a* transfer completely to bob *b* during a beat? Is it perhaps the case that if the pendulum which initially has all the energy is the heavy one, the energy is not completely transferred, but if it is the light one, the energy is completely transferred?

# Solution:

After defining the modulation  $\omega_{\text{mod}} = (\omega_2 - \omega_1)/2$  and the average frequency  $\omega_{av} = (\omega_2 + \omega_1)/2$ , one finds

$$\theta_{a} = \left(A\cos\omega_{\text{mod}}t\right)\cos\omega_{av}t + \left(A\frac{m_{a}-m_{b}}{m}\sin\omega_{\text{mod}}t\right)\sin\omega_{av}t$$
$$\theta_{b} = \left(2A\frac{m_{a}}{m}\sin\omega_{\text{mod}}t\right)\sin\omega_{av}t$$

As  $\omega_{\rm mod} \ll \omega_{\rm av}$  we have the slow varying envelope function gives the energy variation as

$$\begin{split} E_{a} &= \left(A\cos\omega_{\mathrm{mod}}t\right)^{2} + \left(A\frac{m_{a}-m_{b}}{m}\sin\omega_{\mathrm{mod}}t\right)^{2} \\ &= A^{2}\left\{\frac{1+\cos 2\omega_{\mathrm{mod}}t}{2} + \left(\frac{m_{a}-m_{b}}{m}\right)^{2}\frac{1-\cos 2\omega_{\mathrm{mod}}t}{2}\right\} \\ &= \frac{A^{2}}{2}\left\{1 + \left(\frac{m_{a}-m_{b}}{m}\right)^{2} + \left(1 - \left(\frac{m_{a}-m_{b}}{m}\right)^{2}\right)\cos 2\omega_{\mathrm{mod}}t\right\} \\ &= A^{2}\left\{\frac{m_{a}^{2}+m_{b}^{2}}{m^{2}} + \frac{2m_{a}m_{b}}{m^{2}}\cos(\omega_{2}-\omega_{1})t\right\} \\ E_{b} &= \left(2A\frac{m_{a}}{m}\sin\omega_{\mathrm{mod}}t\right)^{2} \\ &= 4A^{2}\left(\frac{m_{a}}{m}\right)^{2}\sin^{2}\omega_{\mathrm{mod}}t \\ &= 2A^{2}\left(\frac{m_{a}}{m}\right)^{2}\left\{1 - \cos(\omega_{2}-\omega_{1})t\right\} \quad \text{with } m_{a} \approx m_{b} \text{ for } \omega_{\mathrm{mod}} \ll \omega_{av} \end{split}$$

Thus we see that

$$E_a = A^2 \left(\frac{m_a^2 + m_b^2}{m^2}\right) + 2A^2 \frac{m_a m_b}{m^2} \cos\left(\omega_2 - \omega_1\right) t$$
$$E_b \approx 2A^2 \frac{m_a m_b}{m^2} - 2A^2 \frac{m_a m_b}{m^2} \cos\left(\omega_2 - \omega_1\right) t$$

The total energy is  $E_a + E_b = A^2$ .