Problem Set 1

1. This problem is very simple, as the N harmonic oscillators are non-interacting. So, if you know how to solve the equations of motion for one harmonic oscillator, then you have 'em all! [I.E. a many 1-body problem is easier than 1 many-body problem]. We can write the Lagrangian as:

$$L(\underset{\sim}{q}, \underset{\sim}{\dot{q}}, t) = \frac{1}{2}\sum_i m_i \dot{q}_i^2 - \frac{1}{2}\sum_i k_i q_i^2$$

We have the following N, Lagrange equations, 1 for each i:

$$\frac{\partial}{\partial q_i} L - \frac{d}{dt}\left(\frac{\partial}{\partial \dot{q}_i} L\right) = 0 \quad ; \forall i$$

Do the differentiation and we have:

$$-k_i q_i - m\ddot{q}_i = 0$$

or, $\ddot{q}_i + \omega_i^2 q_i = 0$, where $\omega_i^2 = \frac{k_i}{m_i}$

This is a standard differential equation, and we obtain:

$$q_i(t) = A_i \cos(\omega_i t) + B_i \sin(\omega_i t) \quad ; \forall_i = 1 \ldots N$$

We are also given initial conditions of:

$$q_i(0) = x_i = A_i$$
$$\dot{q}_i(0) = V_i = \omega_i B_i$$

$$q_i(t) = x_i \cos(\omega_i t) + \left(\frac{V_i}{\omega_i}\right) \sin(\omega_i t) \quad ; \forall_i = 1 \ldots N$$

The above is the equation of motion for the i^{th} oscillator and is the same for the other oscillators

2. The Lagrangian is:

$$L = a\dot{q}_1^{\,2} + b\frac{\dot{q}_2}{q_1} + c\dot{q}_1\dot{q}_2 + f q_1^2 \dot{q}_1 q_3 + g\dot{q}_2 - k\sqrt{q_1^2 + q_2^2}$$

We can get the momenta:

$$p_1 = \frac{\partial}{\partial \dot{q}_1} L = 2a\dot{q}_1 + c\dot{q}_2 + f q_1^2 q_3 \qquad (1)$$

$$p_2 = \frac{\partial}{\partial \dot{q}_2} L = \frac{b}{q_1} + c\dot{q}_1 + g \qquad (2)$$

$$p_3 = \frac{\partial}{\partial \dot{q}_3} L = 0$$

The Hamiltonian is given by:

$$\mathcal{H} = p_1\dot{q}_1 + p_2\dot{q}_2 - L$$

$$= 2a\dot{q}_1^{\,2} + c\dot{q}_1\dot{q}_2 + f q_1^2 \dot{q}_1 q_3 + \frac{b}{q_1}\dot{q}_2 + c\dot{q}_1\dot{q}_2 + g\dot{q}_2 - L$$

$$\mathcal{H} = a\dot{q}_1^{\,2} + c\dot{q}_1\dot{q}_2 + k\sqrt{q_1^2 + q_2^2}$$

Eliminating $\dot{q}_1$ and $\dot{q}_2$ from relations (1) and (2) above:

$$\boxed{\mathcal{H} = \frac{-a}{c^2}\left(p_2 - \frac{b}{q_1} - g\right)^2 + \left(p_2 - \frac{b}{q_1} - g\right)\left(p_1 - f q_1^2 q_3\right) + k\sqrt{q_1^2 + q_2^2}}$$

3. The 1-D oscillator (we've seen much of this in class):

a) $$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$$

$$H = \frac{1}{2m}\left(p^2 + m^2\omega^2 q^2\right)$$

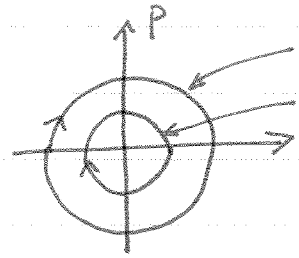
This describes an oval in p-q space, but if we scale our q coordinate:

$$q' = m\omega q$$

Then we have:

$$H = \frac{1}{2m}\left(p^2 + (q')^2\right)$$

← and this is a circle



energy is fixed on this circle

this circle is an oscillator with a different total energy E.

b) Hamilton's equations are $\dot{q}_i = \frac{\partial H}{\partial p_i}$ and $\dot{p}_i = -\frac{\partial H}{\partial q_i}$

For this system:

$$\frac{\partial H}{\partial p_i} = \frac{p}{m}$$

$$\frac{\partial H}{\partial q_i} = m\omega^2 q$$

Therefore:

$$\dot{q}_1 = \dot{q} = \frac{p}{m}$$

$$\dot{p}_i = -m\omega^2 q$$

$$\boxed{\dot{q} = \frac{p}{m} \qquad \dot{p} = -m\omega^2 q}$$

c) To do this part, we must solve:

$$\dot{q} = \frac{p}{m} \quad \underline{\text{and}} \quad \dot{p} = -m\omega^2 q$$

There's a couple of ways of doing this

1) since $\dot{q} = p/m$ take time derivative

$\ddot{q} = \dot{p}/m$ plug in $\dot{p}$ formula

$$\ddot{q} = -m\omega^2 q/m = -\omega^2 q$$

$$\ddot{q} + \omega^2 q = 0$$

solve by plugging in a known solution

$$q(t) = A\cos\omega t + B\sin\omega t$$
$$\dot{q}(t) = -\omega A\sin\omega t + B\omega\cos\omega t$$
$$\ddot{q}(t) = -\omega^2 A\cos\omega^2 - \omega^2 B\sin\omega t$$
$$= -\omega^2 q(t)$$

this solution works

Alternatively:

2) In matrix form:

$$\begin{pmatrix} dq/dt \\ dp/dt \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

or:

$$\dot{\underline{X}} = \underline{\underline{A}} \; \underline{X}$$

In general, we solve these matrix equations by diagonalizing

$$\underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1} = \underline{\underline{\Lambda}}$$

a diagonal matrix containing eigenvalues of A

$\underline{\underline{U}}$ is a <u>unitary</u> matrix where the column vectors are eigenvectors of $\underline{\underline{A}}$

In general; we want to define new variables

$$\underline{x}' = \underline{\underline{U}} \cdot \underline{x}$$

If we take our diff eq. expression and multiply by $\underline{\underline{U}}$, we get

$$\underline{\underline{U}} \cdot \underline{\dot{x}} = \underline{\underline{U}}\,\underline{\underline{A}} \cdot \underline{x}$$

$$\underline{\underline{\dot{x}}}' = \underline{\underline{U}}\,\underline{\underline{A}} \cdot \underline{x}$$

unitary matrices can be inserted here

$$\underline{\underline{\dot{x}}}' = \underbrace{\underline{\underline{U}}\,\underline{\underline{A}}\,\underline{\underline{U}}^{-1}}\,\underbrace{\underline{\underline{U}} \cdot \underline{x}}$$

$= 1$

$$\underline{\underline{\dot{x}}}' = \underline{\underline{\lambda}} \quad \underline{\underline{x}}'$$

this is now a <u>diagonal</u> matrix

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

which means we have <u>uncoupled</u> 1^{st} order equations

$$\dot{x}_a' = \lambda_a \, x_a'$$

$$\frac{dx_a}{dt} = \lambda_\alpha \, x_\alpha'$$

$$\frac{dx_a'}{x_a'} = \lambda_a \, dt$$

$$\Downarrow \text{ integrate}$$

$$\ln x_\alpha = \lambda_a t \implies x_\alpha' = e^{\lambda t} x_a'(0)$$

That's the most general way to solve coupled 1st order Diff Eq's.

Now, to our problem:

$$\underline{\underline{A}} = \begin{pmatrix} 0 & \frac{1}{m} \\ -m\omega^2 & 0 \end{pmatrix} \Bigg\} \qquad \underline{\underline{\lambda}} = \begin{pmatrix} -i\omega \\ +i\omega \end{pmatrix} \qquad \underline{\underline{U}} = \begin{pmatrix} i/m\omega & 1 \\ -i/m\omega & 1 \end{pmatrix}$$

time dependent solutions arising from eigenvalues $\underline{\lambda}$:

$$\underline{\underline{D}}(t) = \begin{pmatrix} e^{-i\omega t} & 0 \\ 0 & e^{i\omega t} \end{pmatrix}$$

$$X'_\alpha(t) = e^{-i\omega t} X'_\alpha(0)$$
$$X'_\beta(t) = e^{+i\omega t} X'_\beta(0)$$

These say the same thing!

We can back-solve to find $q(t)$ & $p(t)$

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \frac{-im\omega}{2} & \frac{im\omega}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} e^{-i\omega t} & 0 \\ 0 & e^{+i\omega t} \end{pmatrix} \begin{pmatrix} \frac{i}{m\omega} & 1 \\ \frac{-i}{m\omega} & 1 \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$$

$$\underline{X}(t) = \underline{\underline{U}}^{-1} \quad \underline{\underline{D}}(t) \quad \underline{\underline{U}} \quad \underline{X}(0)$$

solutions in eigenvalue space

transformation to $\begin{pmatrix} q \\ p \end{pmatrix}$ space

$$\therefore \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & \frac{+1}{m\omega}\sin\omega t \\ -m\omega \sin\omega t & \cos\omega t \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}$$

Therefore:

$$\boxed{\begin{aligned} q(t) &= q_0 \cos\omega t + \frac{p_0}{m\omega} \sin\omega t \\ p(t) &= -m\omega q_0 \sin\omega t + p_0 \cos\omega t \end{aligned}}$$

d) $$H(p_0, q_0) = \frac{p_0^2}{2m} + \frac{1}{2} m\omega^2 q_0^2$$

$$H(p(t), q(t)) = \frac{\left(-m\omega q_0 \sin\omega t + p_0 \cos\omega t\right)^2}{2m} + \frac{1}{2} m\omega^2 \left(q_0 \cos\omega t + \frac{p_0}{m\omega} \sin\omega t\right)$$

$$= \frac{1}{2m}\left[m^2\omega^2 q_0^2 \sin^2\omega t + p_0^2 \cos^2\omega t - 2m\omega q_0 p_0 \sin\omega t \cos\omega t\right]$$

$$+ \frac{m\omega^2}{2}\left[q_0^2 \cos^2\omega t + \frac{p_0^2}{m^2\omega^2} \sin^2\omega t + 2\frac{q_0 p_0}{m\omega} \cos\omega t \sin\omega t\right]$$

$$= \frac{p_0^2}{2m}\left[\cos^2\omega t + \sin^2\omega t\right] + \frac{1}{2} m\omega^2 q_0^2 \left[\sin^2\omega t + \cos^2\omega t\right]$$

$$+ q_0 p_0 \omega \left[\cos\omega t \sin\omega t - \sin\omega t \cos\omega t\right]$$

$$= \frac{p_0^2}{2m} + \frac{1}{2} m\omega^2 q_0^2$$

$$= H(p_0, q_0)$$

3 e.)

$$p = \sqrt{2m\omega J}\cos\theta \longrightarrow p^2 = 2m\omega J\cos^2\theta$$

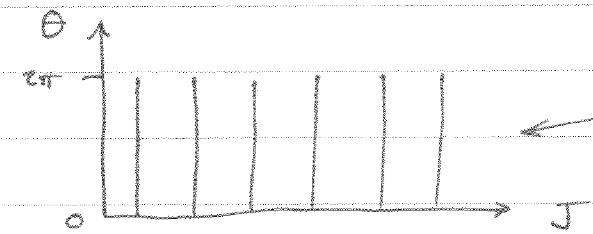
$$q = \sqrt{\frac{2J}{m\omega}}\sin\theta \qquad q^2 = \frac{2J}{m\omega}\sin^2\theta$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$$

$$= \omega J\cos^2\theta \quad \omega J\sin^2\theta \quad = \omega J\left[\cos^2\theta + \sin^2\theta\right]$$

$$\boxed{\mathcal{H} = \omega J}$$

f)



phase space is a series of <u>lines</u> depending on initial conditions.

g)

$$\frac{\partial \mathcal{H}}{\partial J} = \dot{\theta} \qquad \frac{\partial \mathcal{H}}{\partial \theta} = -\dot{J}$$

$$\therefore \dot{\theta} = \omega \qquad \dot{J} = 0$$

$$\therefore \boxed{\theta(t) = \theta(0) + \omega t \qquad J(t) = J(0)}$$

Each <u>ring</u> in the p-q phase space maps to a single line in the $J-\theta$ phase space.

4. a) $$\boxed{T = \frac{1}{2m}p_1^2 + \frac{1}{2m}p_2^2 + \frac{1}{2m}p_3^2}$$

(also $$T = \frac{1}{2}m\dot{x}_1^2 + \frac{1}{2}m\dot{x}_2^2 + \frac{1}{2}m\dot{x}_3^2$$)

b) $$\boxed{V(x_1, x_2, x_3) = \underbrace{\frac{1}{2}k\,(x_2 - x_1 - r_0)^2}_{\text{1-2 bond}} + \underbrace{\frac{1}{2}(x_3 - x_2 - r_0)^2}_{\text{2-3 bond}}}$$

c) If
$$u = x_2 - x_1 - r_0 \Rightarrow \dot{u} = \dot{x}_2 - \dot{x}_1$$
$$v = x_3 - x_2 - r_0 \Rightarrow \dot{v} = \dot{x}_3 - \dot{x}_2$$
$$w = \frac{1}{3}(x_1 + x_2 + x_3) \Rightarrow \dot{w} = \frac{1}{3}(\dot{x}_1 + \dot{x}_2 + \dot{x}_3)$$

$$V(u, v, w) = \frac{1}{2}k\,u^2 + \frac{1}{2}v^2 = \frac{1}{2}k\,(u^2 + v^2)$$

T is harder:
$$\left.\begin{aligned} \dot{u}^2 &= \dot{x}_2^2 + \dot{x}_1^2 - 2\dot{x}_1\dot{x}_2 \\ \dot{v}^2 &= \dot{x}_3^2 + \dot{x}_2^2 - 2\dot{x}_3\dot{x}_2 \end{aligned}\right\}$$ adding these won't give you T!

Write it as a matrix equation.
$$\begin{pmatrix} \dot{u} \\ \dot{v} \\ \dot{w} \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix}$$

To solve for $\dot{x}_1\ \dot{x}_2\ \dot{x}_3$ in terms of $\dot{u}, \dot{v}, \dot{w}$:
$$\vec{y} = \underline{A} \cdot \vec{x}$$
$$\underline{A}^{-1}\vec{y} = \underline{A}^{-1}\underline{A} \cdot \vec{x}$$
$$A^{-1}\vec{y} = \vec{x}$$

This gives us:

$$\dot{x}_1 = \dot{w} - \frac{2}{3}\dot{u} - \frac{1}{3}\dot{v}$$

$$\dot{x}_2 = \dot{w} + \frac{1}{3}\dot{u} - \frac{1}{3}\dot{v}$$

$$\dot{x}_3 = \dot{w} + \frac{1}{3}\dot{u} + \frac{2}{3}\dot{v}$$

Multiplying $\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2$ out we get:

$$\boxed{T(\dot{u}, \dot{v}, \dot{w}) = \frac{1}{6m}\left(2\dot{u}^2 + 2\dot{u}\dot{v} + 2\dot{v}^2 + 9\dot{w}^2\right)}$$

$$\boxed{V(u, v, w) = \frac{1}{2}k\left(u^2 + v^2\right)}$$

$$\boxed{\mathcal{H} = \frac{1}{6m}\left(2\dot{u}^2 + 2\dot{u}\dot{v} + 2\dot{v}^2 + 9\dot{w}^2\right) + \frac{1}{2}k\left(u^2 + v^2\right)}$$

(Note that there is <u>no</u> w in the potential, so $\dot{w}$ is a conserved coordinate, and w is linearly growing in time.)

There's still the pesky $\dot{u}\dot{v}$ coupling term in the kinetic energy.

This is a <u>local mode</u> picture of molecular vibrations.

We can also use normal modes:

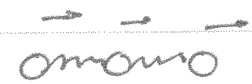
4d)

To obtain the normal coordinates, one uses the rows of the Eigenvector matrix $\underline{\underline{u}}$:

zero frequency: <u>not vibration</u>

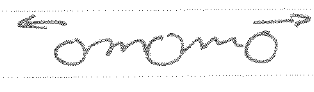
translation: $\omega_1 = 0$

$\vec{u}_1 = x_1 + x_2 + x_3$



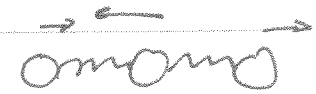
symmetric stretch: $\omega_2 = \omega$

$\vec{u}_2 = -x_1 + x_3$



asymmetric stretch: $\omega_3 = \sqrt{3}\,\omega$

$\vec{u}_3 = x_1 - 2x_2 + x_3$



We can also <u>reverse</u> this to obtain the cartesian coords in terms of the normal modes

$$x_1 = \frac{1}{6}\left(2u_1 - 3u_2 + u_3\right)$$

$$x_2 = \frac{1}{3}\left(u_1 - u_3\right)$$

$$x_3 = \frac{1}{6}\left(2u_1 + 3u_2 + u_3\right)$$

$$V = \frac{1}{2}k\left(x_2 - x_1 - r_0\right)^2 + \frac{1}{2}k\left(x_3 - x_2 - r_0\right)^2$$

$$\boxed{V = \frac{k}{4}\left(4r_0^2 - 4r_0 u_2 + u_2^2 + u_3^2\right)}$$ ← uncoupled in V

$$\boxed{T = \frac{m}{12}\left(2\dot{u}_1^2 + 3\dot{u}_2^2 + \dot{u}_3^2\right)}$$ ← uncoupled in T

4d) Normal Modes: (i.e. symmetric stretch & asymmetric stretch)

To find these we must find a set of coordinates in which the force constant matrix is diagonal:

$$\underline{\underline{\omega}}^2 = \underline{\underline{U}}^{*} \underline{\underline{K}}\, \underline{\underline{U}}^{-1}$$

diagonal matrix of frequencies

$$\underline{\underline{K}} = \begin{pmatrix} \frac{\partial^2 V}{\partial x_1^2} \cdot \frac{1}{m_1} & \frac{\partial^2 V}{\partial x_1 \partial x_2} \frac{1}{\sqrt{m_1 m_2}} \\ \frac{\partial^2 V}{\partial x_2 \partial x_1} \frac{1}{\sqrt{m_2 m_1}} & \frac{\partial^2 V}{\partial x^2} \frac{1}{m_2} & \cdots \end{pmatrix}$$

$\underline{\underline{K}}$ is called a Hessian matrix or a mass-weighted force constant matrix.

For our system:

$$\underline{\underline{K}} = \frac{1}{m} \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}$$

$$= \frac{k}{m} \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} = \omega^2 \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

So we need the eigenvalues ($\underline{\underline{\omega}}^2$) and eigenvectors ($\underline{\underline{U}}^{*}$) of this matrix

$$\underline{\underline{\omega}}^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \omega^2 & 0 \\ 0 & 0 & 3\omega^2 \end{pmatrix} \qquad \underline{\underline{U}} = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & -2 & 1 \end{pmatrix}$$

5. This is a famous unsolved problem. I just wanted to see who could tackle it and take it the farthest:

$$\mathcal{H} = \frac{1}{2}\left(p_1^2 + p_2^2 + q_1^2 + q_2^2\right) + q_1 q_2^2 - \frac{1}{3} q_1^3$$

$$p_1 = f_1(J_1)\cos\theta_1 \qquad p_2 = f_2(J_2)\cos\theta_2$$

$$q_1 = f_1(J_1)\sin\theta_1 \qquad q_2 = f_2(J_2)\sin\theta_2$$

$$\mathcal{H} = \frac{1}{2}\left(f_1(J_1)^2 + f_2(J_2)^2 \right] + f_1(J_1) f_2(J_2)^2 \sin\theta_1 \sin^2\theta_2 - \frac{1}{3} f_1(J_1)^3 \sin^3\theta_1$$

$$p_i = q_i \cot\theta_i = \frac{\partial G_i}{\partial q_i}$$

$$G_i = \frac{1}{2} q_i^2 \cot\theta_i$$

$$J_i = -\frac{\partial G_i}{\partial \theta_i} = \frac{q_i^2}{2\sin^2\theta_i}$$

Thus:

$$q_i = \sqrt{2J_i}\,\sin\theta_i$$

So:

$$f_i(J_i) = \sqrt{2J_i}$$

Hence:

$$\mathcal{H} = \frac{1}{2}\left(2J_1 + 2J_2\right) + 2\sqrt{2J_1}\,J_2 \sin\theta_1 \sin^2\theta_2 - \frac{1}{3}\sqrt[3]{2J_1}\,\sin^3\theta_1$$

$$= J_1 + J_2 + 2\sqrt{2}\,J_1^{1/2} J_2 \sin\theta_1 \sin^2\theta_2 - \frac{2\sqrt{2}}{3} J_1^{3/2} \sin^3\theta_1$$

$$\mathcal{H}_0 = J_1 + J_2$$

$$V = 2\sqrt{2}\,J_1^{1/2} J_2 \sin\theta_1 \sin^2\theta_2 - \frac{2\sqrt{2}}{\ } J^{3/2} \sin^3\theta$$

With no perturbation, there would be two frequencies ω_1 and ω_2 such that

$$\omega_1 = \frac{\partial \mathcal{H}_0}{\partial J_1} \qquad \omega_2 = \frac{\partial \mathcal{H}_0}{\partial J_2}$$

Since V is periodic in θ_1 and θ_2 we can rewrite gV as a Fourier series:

$$gV = \sum_{n_1 n_2} g V_{n_1 n_2}(J_1 J_2)\, e^{i(n_1\theta_1 + n_2\theta_2)}$$

Moser's 1974 paper [Moser, J in The Stability of the Solar System (ed. Y. Kozai) pp. 1-9, International Astronomical Union] has a long discussion about perturbation theories and where to go next. . . .