Ph-507. Homework 7 (due: Wednesday, April 9).

PROBLEM 7-1 (4 pts)

Find the normal modes and their frequencies for a triangular molecule made of three identical atoms of mass m. All the bonds are identical, having spring constant k.

PROBLEM 7-2 (3 pts)

An oxygen atom in a linear CO_2 molecule adsorbs a momentum p from an X-ray photon. This momentum is directed along the main axis of the molecule (i.e. along the O=C=O direction). How much energy has been adsorbed by the lowest-frequency longitudinal oscillatory mode? Masses of O and C atoms are m and M, respectively. Assume that energy is high enough to neglect the effects of quantization.

PROBLEM 7-3 (3 pts.)

A cylindric hole of radius $r/2$ is drilled in a uniform cylinder of radius r, parallel to its symmetry axis. The central axis of the hole is at distance $r/4$ from that of the cylinder. Find the period of small oscillation of this object on a flat surface. The gravitational acceleration is g, and the cylinder rocks without sliding.

PROBLEM 7-4 (2 pts)
a) Starting with the followiing Hamiltonian, obtain the Lagrangian of the system:

$$H = p^4 + \frac{kq^2}{2}$$

b) Starting with the Lagrangian of a heavy spinning top, obtain its Hamiltonian and Hamilton equations of motion.

PROBLEM 7-5 (3 pts)

Let q and p be canonical variables. Which of the following transformations are canonical?

$$P = p^2 + q^2; \qquad Q = p^2 - q^2$$

$$P = p^2 + q^2; \qquad Q = \frac{1}{2} \arctan p/q$$

$$P = p^2 + q^2; \qquad Q = pq$$

For a harmonic oscillator with the following Hamiltonian

$$H = \frac{\varpi_0^2}{2} \left(p^2 + q^2\right),$$

write the equations of motion in the form $\dot{P} = f\,(P, Q)$ and $\dot{Q} = g\,(P, Q)$. You may choose any pair of P, Q from the above list.

Solution to Problem 7-1

If $\mathbf{r}_1 = (x_1, y_1)$ and $\mathbf{r}_2 = (x_2, y_2)$ are displacements of two atoms, 1 and 2, the displacement of the third one is, $\mathbf{r}_3 = -(\mathbf{r}_1 + \mathbf{r}_2)$, in the reference frame of Center of Mass. The total kinetic energy is given by:

$$T = \frac{m}{2}\left[(\dot{\mathbf{r}}_1 + \dot{\mathbf{r}}_2)^2 + \dot{\mathbf{r}}_1^2 + \dot{\mathbf{r}}_2^2\right]$$

We choose coordinate system such that $\hat{\mathbf{x}}$ is directed from particle 1 to 2. The unit vectors along the sides of the triangle are, $\hat{\mathbf{n}}_{12} = \hat{\mathbf{x}}$, $\hat{\mathbf{n}}_{23} = \left(-\hat{\mathbf{x}} + \sqrt{3}\hat{\mathbf{y}}\right)/2$, $\hat{\mathbf{n}}_{31} = \left(-\hat{\mathbf{x}} - \sqrt{3}\hat{\mathbf{y}}\right)/2$. The corresponding deformations of the springs, are

$$\delta l_{12} = \hat{\mathbf{n}}_{12} \cdot (\mathbf{r}_2 - \mathbf{r}_1) = x_2 - x_1,$$

$$\delta l_{23} = \hat{\mathbf{n}}_{23} \cdot (\mathbf{r}_3 - \mathbf{r}_2) = \left(\frac{x_1}{2} + x_2\right) - \sqrt{3}\left(\frac{y_1}{2} + y_2\right),$$

$$\delta l_{31} = \hat{\mathbf{n}}_{31} \cdot (\mathbf{r}_1 - \mathbf{r}_3) = -\left(x_1 + \frac{x_2}{2}\right) - \sqrt{3}\left(y_1 + \frac{y_2}{2}\right),$$

We can use the mirror symmetry of the problem with respect to the axis lying halfway between atoms 1 and 2. All the normal modes must be either symmetric or antisymmetric with respect to this mirror reflection transformation.

- Symmetric solution: $\mathbf{r}_1 = (x, y)$, $\mathbf{r}_2 = (-x, y)$.

$$U = \frac{k}{2}\left(\delta l_{12}^2 + \delta l_{23}^2 + \delta l_{31}^2\right) = \frac{k}{2}\left(4x^2 + \frac{2}{4}\left(x + 3\sqrt{3}y\right)^2\right)$$

$$\hat{V} - \varpi^2\hat{\mu} = \frac{1}{2}\begin{pmatrix} 9k - 4m\varpi^2 & 3\sqrt{3}k \\ 3\sqrt{3}k & 3\left(9k - 4m\varpi^2\right) \end{pmatrix}$$

Characteristic equation gives:

$$9k - 4m\varpi^2 = \pm 3k$$

Normal modes ($\mathbf{q}_n = [(x_1, y_1); (x_2, y_2); (x_3, y_3)]$):

$$\varpi_1 = \pm\sqrt{\frac{3k}{m}} \qquad \mathbf{q}_1 = \left[\frac{1}{2}\left(\sqrt{3}, 1\right); \frac{1}{2}\left(-\sqrt{3}, 1\right); (0, -1)\right]$$

$$\varpi_2 = \pm\sqrt{\frac{3k}{2m}} \qquad \mathbf{q}_2 = \left[\frac{1}{2}\left(\sqrt{3}, -1\right); \frac{1}{2}\left(-\sqrt{3}, -1\right); (0, 1)\right]$$

- Symmetric solution: $\mathbf{r}_1 = (x, y)$, $\mathbf{r}_2 = -(-x, y) = (x, -y)$.

$$U = \frac{k}{2}\left(\frac{1}{4}\left(3x + \sqrt{3}y\right)^2 + \left(-3x - \sqrt{3}y\right)^2\right) = \frac{3k}{2}\left(3x^2 + 2\sqrt{3}y + y^2\right)$$

$$\hat{V} - \varpi^2\hat{\mu} = \frac{1}{2}\begin{pmatrix} 3\left(3k - 4m\varpi^2\right) & 3\sqrt{3}k \\ 3\sqrt{3}k & 3k - 4m\varpi^2 \end{pmatrix}$$

Characteristic equation gives:

$$3k - 4m\varpi^2 = \pm 3k$$

Normal modes:

$$\varpi_3 = \pm\sqrt{\frac{3k}{2m}} = \varpi_2 \qquad \mathbf{q}_3 = \left[\frac{1}{2}\left(1, \sqrt{3}\right); \frac{1}{2}\left(1, -\sqrt{3}\right); (-1, 0)\right]$$

$$\varpi_4 = 0 \qquad \mathbf{q}_4 = \left[\frac{1}{2}\left(1, -\sqrt{3}\right); \frac{1}{2}\left(1, \sqrt{3}\right); (-1, 0)\right]$$

$\mathbf{q}_4$ corresponds to rotation ("zero mode").

Solution to Problem 7-2

At $t = 0$ velocities of the three atoms are $(p/m, 0, 0)$ and the velocity of the center of mass is $p/(2m + M)$. Therefore, in CM reference frame velocities are

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} p/m \\ 0 \\ 0 \end{pmatrix} - \frac{p}{2m+M} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{p}{2m+M} \begin{pmatrix} 1 + M/m \\ -1 \\ -1 \end{pmatrix}$$

There are two oscillatory longitudinal modes: symmetric and antisymmetric.

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = C_1 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \sin \varpi_1 t + C_2 \begin{pmatrix} 1 \\ -2m/M \\ 1 \end{pmatrix} \sin \varpi_2 t$$

Here we have taken into account that $x_1 = x_2 = x_3 = 0$ at $t = 0$. This determines the phases of the both modes.

The lowest frequency mode is always symmetric, therefore, we need to find amplitude C_1. Use the orthogonality of normal modes:

$$(1, 0, -1) \cdot \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix}_{t=0} = \varpi_1 C_1 \left[(1, 0, -1) \cdot \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \right] = 2\varpi_1 C_1$$

Therefore,

$$C_1 = \frac{1}{2\varpi_1} (1, 0, -1) \cdot \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \frac{p}{2m\varpi_1}$$

At the initial moment all the energy of the mode is in kinetic form:

$$E_1 = \frac{C_1^2 \varpi_1^2}{2} (1, 0, -1) \cdot \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & m \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \frac{p^2}{4m}$$

Solution to Problem 7-3

The kinetic energy of the object can be found as the sum of the contributions from translation and rotation of (a) complete uniform cylinder of mass m, and (2) smaller cylinder of negative mass $m' = -m/4$:

$$T = \frac{\dot{\theta}^2}{2} \left(m \left[r^2 + \frac{r^2}{2} \right] - \frac{m}{4} \left[\left(\frac{5r}{4} \right)^2 + \frac{1}{2} \left(\frac{r}{2} \right)^2 \right] \right) = \frac{69}{64} \frac{mr^2\dot{\theta}^2}{2}$$

Hence, the complete Lagrangian can be written as

$$L = \frac{69}{64} \frac{mr^2\dot{\theta}^2}{2} + \frac{mg}{4} \frac{r}{4} \cos\theta \approx \frac{m}{32} \left(\frac{69}{4} r^2 \dot{\theta}^2 - gr\theta^2 \right) + const$$

The oscillation period is:

$$T = \pi \sqrt{\frac{69r}{g}}.$$

Solution to Problem 7-4

a)

$$H = p^4 + \frac{kq^2}{2}$$

$$\dot{q} = \frac{\partial H}{\partial p} = 4p^3; \quad \text{hence } p\left(q, \dot{q}\right) = \left(\dot{q}/4\right)^{1/3}$$

$$L\left(\dot{q}, q\right) = p\dot{q} - H\left(p, q\right) = 3p^4 - \frac{kq^2}{2} = 3\left(\frac{\dot{q}}{4}\right)^{4/3} - \frac{kq^2}{2}$$

b)

$$L = \frac{I_{\perp}}{2}\left(\dot{\theta}^2 + \dot{\phi}^2 \sin^2\theta\right) + \frac{I_{\parallel}}{2}\left(\dot{\psi} + \dot{\phi}\cos\theta\right)^2 - mgl\cos\theta$$

$$p_{\theta} = \frac{\partial L}{\partial \dot{\theta}} = I_{\perp}\dot{\theta}$$

$$p_{\psi} = \frac{\partial L}{\partial \dot{\psi}} = I_{\parallel}\left(\dot{\psi} + \dot{\phi}\cos\theta\right)$$

$$p_{\phi} = \frac{\partial L}{\partial \dot{\phi}} = I_{\parallel}\left(\dot{\psi} + \dot{\phi}\cos\theta\right)\cos\theta + I_{\perp}\dot{\phi}\sin^2\theta = p_{\psi}\cos\theta + I_{\perp}\dot{\phi}\sin^2\theta$$

Since the Lagrangian is bi-linear in velocity, we can obtain the Hamiltonian by simply revbersing the sign of potential energy, and changing the variables from velocities to momenta:

$$H\left(p_{\theta}, p_{\psi}, p_{\phi}, \theta, \psi, \phi\right) = \frac{p_{\theta}^2}{2I_{\perp}} + \frac{\left(p_{\phi} - p_{\psi}\cos\theta\right)^2}{2I_{\perp}\sin^2\theta} + \frac{p_{\psi}^2}{2I_{\parallel}} + mgl\cos\theta$$

Solution to Problem 7-5

The simplest way to check if the variables are canonical is to calculate their Poisson brackets. In our case, the only canonical pair is number 2:

$$\{P, Q\} = \frac{1}{2}\frac{\partial\left(p^2 + q^2\right)}{\partial p}\frac{\partial \arctan p/q}{\partial q} - \frac{1}{2}\frac{\partial\left(p^2 + q^2\right)}{\partial q}\frac{\partial \arctan p/q}{\partial p} = -1$$

It should be noted that the result is -1, not 1, therefore P and Q should be interchanged: P is canonical variable, and Q is its canonically conjugated momentum.

Now, Hamiltonian can be rewritten in terms of P and Q:

$$H\left(Q, P\right) = \frac{\varpi_0^2}{2}P$$

The Hamilton equations of motion for this pair of variables have a very simple form:

$$\dot{P} = \frac{\partial H\left(Q, P\right)}{\partial Q} = 0$$

$$\dot{Q} = -\frac{\partial H\left(Q, P\right)}{\partial P} = -\frac{\varpi_0^2}{2}$$