# Mechanics Fall 2007, Solutions 9

1. **A Hamiltonian system**

(i) In general, a Legendre transformation looks as follows:

$$H = \frac{\partial L}{\partial \dot{q}} \dot{q} - L$$

We know that

$$\left.\frac{\partial H}{\partial p}\right|_q = \dot{q}\,, \qquad \left.\frac{\partial H}{\partial q}\right|_p = -\dot{p} = -\frac{\partial L}{\partial q}\,.$$

and we can therefore express the above formula with

$$H = p\frac{\partial H}{\partial p} - L$$

Thus

$$L = p\frac{\partial H}{\partial p} - H\,.$$

We can see here that the inverse of a Legendre transformation is again a Legendre transformation. $L$ should depend on $q$ and $\dot{q}$.

(ii)

$$L(x, \dot{x}) = p\dot{x} - c\sqrt{(mc)^2 + p^2} - e\mathbf{E}\cdot\mathbf{x} \tag{1}$$

Here, L$(x, \dot{x})$ still contains $p$, on which it shouldn't depend. Therefore, we need to express $p$ as a function of $x$ and/or $\dot{x}$ . Using

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{cp}{\sqrt{m^2c^2 + p^2}} \tag{2}$$

we find

$$p = m\dot{x}c\frac{1}{\sqrt{c^2 - \dot{x}^2}} \tag{3}$$

Now we can substitute $p$ in $L$

$$L = m\dot{x}^2 c\frac{1}{\sqrt{c^2 - \dot{x}^2}} - c\sqrt{m^2c^2 + \frac{m^2c^2\dot{x}^2}{c^2 - \dot{x}^2}} - e\mathbf{E}\cdot\mathbf{x} \tag{4}$$

and find by rearranging the terms above slightly

$$L(x, \dot{x}) = -cm\sqrt{c^2 - \dot{x}^2} - e\mathbf{E} \cdot \mathbf{x} \tag{5}$$

Using

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \tag{6}$$

we obtain

$$\frac{d}{dt}\left(\frac{\dot{\mathbf{x}}}{\sqrt{1 - \frac{\dot{\mathbf{x}}^2}{c^2}}}\right) = -\frac{e}{m}\mathbf{E} \tag{7}$$

Compare this to the non-relativistic equation:

$$\frac{d}{dt}\dot{\mathbf{x}} = -\frac{e}{m}\mathbf{E} \tag{8}$$

The second equation of motion is here trivially

$$\frac{d}{dt}\mathbf{x} = \dot{\mathbf{x}} \tag{9}$$

Note: It is not possible to solve equation (7) for $\ddot{x}$ , since it is inside a scalar product. However, $\ddot{x}$ is not a useful quantity in the relativistic case anyway, as you will learn in your EM lecture.

2. **Lennard-Jones Potential between two molecules**

(a) The center of mass of the system is given by $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) = (x, y, z)$, the reduced mass is $\mu = \frac{m^2}{m+m} = \frac{m}{2}$, and the total mass is $M = 2m$. Let $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. Then the kinetic energy of the system is

$$\begin{aligned} T &= \frac{1}{2}M\dot{\mathbf{R}}^2 + \frac{1}{2}\mu\dot{\mathbf{r}} \\ &= \frac{1}{2}M\dot{\mathbf{R}}^2 + \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\varphi}^2\sin^2\theta) \end{aligned}$$

and the Lagrangian is

$$\begin{aligned} L &= T - V \\ &= \frac{1}{2}M(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\varphi}^2\sin^2\theta) + \frac{2A}{r^6} - \frac{B}{r^{12}}\ , \end{aligned}$$

where $r, \theta, \phi$ are the spherical coordinates of a frame fixed at the center of mass. The generalized momenta are

$$\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{x}} = M\dot{x}, \qquad p_y = \frac{\partial L}{\partial \dot{y}} = M\dot{y}, \qquad p_z = \frac{\partial L}{\partial \dot{z}} = M\dot{z}, \\ p_r &= \frac{\partial L}{\partial \dot{r}} = \mu\dot{r}, \qquad p_\theta = \frac{\partial L}{\partial \dot{\theta}} = \mu r^2\dot{\theta}, \qquad p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = \mu r^2\dot{\varphi}\sin^2\theta\ . \end{aligned}$$

The Hamiltonian is

$$\begin{aligned} H &= \sum_i p_i \dot{q}_i - L \\ &= \frac{1}{2M}(p_x^2 + p_y^2 + p_z^2) + \frac{1}{2\mu}\left(p_r^2 + \frac{1}{r^2}p_\theta^2 + \frac{1}{r^2 \sin^2\theta}p_\varphi^2\right) - \frac{2A}{r^6} + \frac{B}{r^{12}} \ . \end{aligned}$$

(b) The lowest energy state corresponds to $p_x = p_y = p_z = p_r = p_\theta = p_\varphi = 0$ and an $r_0$ which minimizes

$$-\frac{2A}{r^6} + \frac{B}{r^{12}} \ .$$

Letting

$$\frac{d}{dt}\left(-\frac{2A}{r^6} + \frac{B}{r^{12}}\right) = 0 \ ,$$

we obtain $r_0 = (B/A)^{1/6}$ as the distance between the two atoms for the lowest energy classical state. For this state the energy of the system is

$$H = \frac{-A^2}{B} \ .$$

(c) If the energy is only slightly higher than the lowest and the degrees of freedom corresponding to $x, y, z, \theta, \varphi$ are not excited yet ($p_x = p_y = p_z = p_\theta = p_\varphi = 0$), we have

$$H = \frac{p_r^2}{2\mu} - \frac{2A}{r^6} + \frac{B}{r^{12}} \ .$$

As

$$\left(\frac{d^2V}{dr^2}\right)_{r_0} = 72A\left(\frac{A}{B}\right)^{\frac{4}{3}} \ ,$$

the Lagrangian is

$$L = T - V = \frac{1}{2}\mu\dot{r}^2 - 36A\left(\frac{A}{B}\right)^{\frac{4}{3}}(r - r_0)^2 = \frac{1}{2}\mu\dot{\rho}^2 - 36A\left(\frac{A}{B}\right)^{\frac{4}{3}}\rho^2 \ ,$$

where $\rho = r - r_0 \ll r_0$. Lagrange's equations gives

$$\mu\ddot{\rho} + 72A\left(\frac{A}{B}\right)^{\frac{4}{3}}\rho = 0 \ .$$

Hence

$$\omega = \sqrt{\frac{72A}{\mu}\left(\frac{A}{B}\right)^{\frac{4}{3}}} = 12\left(\frac{A}{m}\right)^{\frac{1}{2}}\left(\frac{A}{B}\right)^{\frac{2}{3}} \ .$$