Solutions to Problem Set No. 1

1. Given $\frac{\partial f}{\partial t} - \frac{d}{dt}\left(f - \dot{x}\frac{\partial f}{\partial \dot{x}}\right) = 0$ ...(1)

Since $f = f(x, \dot{x}, t)$, $\frac{df}{dt} = \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial \dot{x}}\frac{d\dot{x}}{dt} + \frac{\partial f}{\partial t}$ ..(2)

Substituting (2) in (1):

$$\frac{\partial f}{\partial t} - \left(\frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial \dot{x}}\frac{d\dot{x}}{dt} + \frac{\partial f}{\partial t}\right) + \frac{d\dot{x}}{dt}\frac{\partial f}{\partial \dot{x}} + \dot{x}\frac{d}{dt}\frac{\partial f}{\partial \dot{x}} = 0$$

$\therefore \quad -\dot{x}\left(\frac{\partial f}{\partial x} - \frac{d}{dt}\frac{\partial f}{\partial \dot{x}}\right) = 0 \Rightarrow \frac{\partial f}{\partial x} - \frac{d}{dt}\frac{\partial f}{\partial \dot{x}} = 0$, which is the Euler equation.

2. Given the Lagrangian $\mathcal{L} = mc^2\left(1 - \sqrt{1 - \frac{v^2}{c^2}}\right) - V(r)$

The equations of motion are

$$\frac{\partial \mathcal{L}}{\partial r_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{r}_i} = 0, \quad i = 1, 2, 3 \qquad \text{...(1)}$$

$$\frac{\partial \mathcal{L}}{\partial r_i} = -\frac{\partial V(r)}{\partial r_i} = +F_i \qquad \text{...(2)}$$

$$\frac{\partial \mathcal{L}}{\partial v_i} = mc^2(-1)\frac{1}{2}\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}\left(-\frac{1}{c^2}\right)2v_i$$

$$= m\frac{v_i}{\sqrt{1 - v^2/c^2}} \qquad \text{...(3)}$$

Substituting (2) and (3) into (1)

$$\frac{d}{dt}\left(\frac{mv_i}{\sqrt{1 - v^2/c^2}}\right) = F_i$$

3. The given function ~~to~~ be extremized is $J = \int_{t_1}^{t_2} dt\, g(y, \dot{y}, t)$,

where $g = y(t)$

For an extremum, g must satisfy

$$\frac{\partial g}{\partial y} - \frac{d}{dt}\frac{\partial g}{\partial \dot{y}} = 0$$

But $\frac{\partial g}{\partial y} = 1$ and $\frac{\partial g}{\partial \dot{y}} = 0$, so the Euler equation reduces to $1=0$, implying there is no extreme value.

4. In the integral $I \equiv \int_{t_1}^{t_2} dt\, f(y,\dot{y},t)$, f is given by

$$f(y,\dot{y},t) = f_1(y,t) + \dot{y}\, f_2(y,t).$$

When I is extremized, $\frac{\partial f}{\partial y} - \frac{d}{dt}\frac{\partial f}{\partial \dot{y}} = 0$

$$\therefore \frac{\partial f}{\partial y} = \frac{\partial f_1}{\partial y} + \dot{y}\frac{\partial f_2}{\partial y} \quad \text{and} \quad \frac{\partial f}{\partial \dot{y}} = f_2$$

$$\therefore \frac{\partial f_1}{\partial y} + \dot{y}\frac{\partial f_2}{\partial y} - \frac{d}{dt} f_2 = 0$$

That is, $\frac{\partial f_1}{\partial y} + \dot{y}\frac{\partial f_2}{\partial y} - \frac{\partial f_2}{\partial y}\frac{dy}{dt} - \frac{\partial f_2}{\partial t} = 0$

$$\therefore \frac{\partial f_1}{\partial y} - \frac{\partial f_2}{\partial t} = 0$$

5. If H is time-independent, then

$$H = H(\{p\},\{q\})$$

$$\therefore dH = \sum_{i=1}^{N}\left(\frac{\partial H}{\partial p_i}\cdot dp_i + \frac{\partial H}{\partial q_i}\cdot dq_i\right)$$

$$\therefore \frac{dH}{dt} = \sum_{i=1}^{N}\left(\frac{\partial H}{\partial p_i}\cdot \dot{p}_i + \frac{\partial H}{\partial q_i}\cdot \dot{q}_i\right) = \sum_{i=1}^{N}\left(-\frac{\partial H}{\partial p_i}\cdot\frac{\partial H}{\partial q_i} + \frac{\partial H}{\partial q_i}\cdot\frac{\partial H}{\partial p_i}\right) = 0$$

which implies that H (ie, the total energy) is <u>conserved</u>.

If $H = H(\{p\}, \{q\}, t)$, then

$$dH = \left(\sum_{i=1}^{N} \left(\frac{\partial H}{\partial p_i} \cdot dp_i + \frac{\partial H}{\partial q_i} \cdot dq_i \right) + \frac{\partial H}{\partial t} \right)$$

$\therefore$ $\frac{dH}{dt} = \frac{\partial H}{\partial t} \neq 0$ in general, which means total energy is <u>not</u> conserved.

6. In general, $\mathcal{L} = K - V$

where $K = \frac{m}{2}(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$ and $V = U(r)$

In spherical polar coordinates, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$ and $z = r\cos\theta$

$$\therefore \ \dot{x} = \dot{r}\sin\theta\cos\phi + r\dot{\theta}\cos\theta\cos\phi - r\dot{\phi}\sin\theta\sin\phi$$

$$\dot{y} = \dot{r}\sin\theta\sin\phi + r\dot{\theta}\cos\theta\sin\phi + r\dot{\phi}\sin\theta\cos\phi$$

$$\dot{z} = \dot{r}\cos\theta - r\dot{\theta}\sin\theta$$

$$\therefore \ \dot{x}^2 = \dot{r}^2\sin^2\theta\cos^2\phi + r^2\dot{\theta}^2\cos^2\theta\cos^2\phi + r^2\dot{\phi}^2\sin^2\theta\sin^2\phi + 2r\dot{r}\dot{\theta}\sin\theta\cos\theta\cos^2\phi - 2r\dot{r}\dot{\phi}\sin^2\theta\sin\phi\cos\phi - 2r^2\dot{\phi}\dot{\theta}\sin\theta\cos\theta\sin\phi\cos\phi$$

$$\dot{y}^2 = \dot{r}^2\sin^2\theta\sin^2\phi + r^2\dot{\theta}^2\cos^2\theta\sin^2\phi + r^2\dot{\phi}^2\sin^2\theta\cos^2\phi + 2r\dot{r}\dot{\theta}\sin\theta\cos\theta\sin^2\phi + 2r\dot{r}\dot{\phi}\sin^2\theta\sin\phi\cos\phi + 2r^2\dot{\phi}\dot{\theta}\sin\theta\cos\theta\sin\phi\cos\phi$$

$$\dot{z}^2 = \dot{r}^2\cos^2\theta + r^2\dot{\theta}^2\sin^2\theta - 2r\dot{r}\dot{\theta}\sin\theta\cos\theta$$

$$\therefore \ \dot{x}^2 + \dot{y}^2 + \dot{z}^2 = \dot{r}^2\sin^2\theta + r^2\dot{\theta}^2\cos^2\theta + r^2\dot{\phi}^2\sin^2\theta + \dot{r}^2\cos^2\theta + r^2\dot{\theta}^2\sin^2\theta$$

$$= \dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2\sin^2\theta$$

$\therefore$ the Lagrangian becomes

$$\mathcal{L} = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2\sin^2\theta\right) - U(r)$$

The conjugate momenta are $p_r = \frac{\partial \mathcal{L}}{\partial \dot{r}} = m\dot{r}$, $p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = mr^2\dot{\theta}$,

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and $p_\phi = \frac{\partial \mathcal{L}}{\partial \dot\phi} = mr^2 \dot\phi \sin^2\theta$

$\therefore$ the Hamiltonian H is

$$H = p_r \dot r + p_\theta \dot\theta + p_\phi \dot\phi - \mathcal{L}$$

$$= \frac{p_r^2}{m} + \frac{p_\theta^2}{mr^2} + \frac{p_\phi^2}{mr^2\sin^2\theta} - \frac{m}{2}\left(\frac{p_r^2}{m^2} + r^2\frac{p_\theta^2}{m^2r^4} + r^2\sin^2\theta \frac{p_\phi^2}{m^2r^4\sin^4\theta}\right)$$
$$+ U(r)$$

$$= \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2\sin^2\theta} + U(r)$$

$= K + V =$ total energy.

7. By definition

$$\langle B(t)\rangle = \int dp\,dq\, f\, e^{it\mathcal{L}} B$$

$$= \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \int dp\,dq\, f\,(i\mathcal{L})(i\mathcal{L})^{n-1} B$$

We know that $i\mathcal{L} = \dot q \frac{\partial}{\partial q} + \dot p \frac{\partial}{\partial p}$

$$\therefore \langle B(t)\rangle = \sum_{n=0}^{\infty} \frac{t^n}{n!} \int dp\,dq\, f\left(\dot q\frac{\partial}{\partial q} + \dot p \frac{\partial}{\partial p}\right)(i\mathcal{L})^{n-1} B$$

$$= \sum_{n=0}^{\infty} \frac{t^n}{n!}\left[\int dp\left\{f \dot q (i\mathcal{L})^{n-1} B\Big|_{-\infty}^{\infty} - \int dq\left((i\mathcal{L})^{n-1}B\right)\frac{\partial}{\partial q} f\dot q\right\}\right.$$
$$\left. + \int dq \left\{ f\dot p (i\mathcal{L})^{n-1} B\Big|_{-\infty}^{\infty} - \int dp \left((i\mathcal{L})^{n-1}B\right)\frac{\partial}{\partial p} f \dot p\right\}\right]$$

$$= -\sum_{n=0}^{\infty} \frac{t^n}{n!} \int dp\,dq\left((i\mathcal{L})^{n-1}B\right)\left\{f\left(\frac{\partial}{\partial q}\dot q + \frac{\partial}{\partial p}\dot p\right) + \dot q \frac{\partial f}{\partial q} + \dot p\frac{\partial f}{\partial p}\right\}$$

Now $\frac{\partial}{\partial q}\dot q + \frac{\partial}{\partial p}\dot p = \frac{\partial}{\partial q}\frac{\partial H}{\partial p} + \frac{\partial}{\partial p}\left(-\frac{\partial H}{\partial q}\right) = 0$

$$\therefore \langle B(t)\rangle = -\sum_{n=0}^{\infty} \frac{t^n}{n!} \int dp\, dq \left(\left(\dot{q}\frac{\partial}{\partial q} + \dot{p}\frac{\partial}{\partial p}\right) f\right) (i\mathcal{L})^{n-1} B$$

$$= -\sum_{n=0}^{\infty} \frac{t^n}{n!} \int dp\, dq\, (i\mathcal{L} f)\; i\mathcal{L}\, (i\mathcal{L})^{n-2} B$$

$$= +\sum_{n=0}^{\infty} \frac{t^n}{n!} \int dp\, dq \left((i\mathcal{L})^2 f\right) (i\mathcal{L})^{n-2} B$$

After repeating these operations, eventually

$$\langle B(t)\rangle = \sum_{n=0}^{\infty} \frac{(-t)^n}{n!} \int dp\, dq\, \left((i\mathcal{L})^n f\right) B$$

$$= \int dp\, dq \left(e^{-it\mathcal{L}} f\right) B$$

$$= \int dp\, dq\, f(\Gamma, t)\, B(\Gamma)$$

8. (a) By definition, $i\mathcal{L} = \sum_{i=1}^{N} \left(\frac{\partial H}{\partial p_i} \cdot \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \cdot \frac{\partial}{\partial p_i}\right)$

So when $\{p_i\} \to \{-p_i\}$, $i\mathcal{L} \to -i\mathcal{L}$

Since

$$\frac{\partial B}{\partial t} = i\mathcal{L} B \quad \text{and} \quad B(t) = e^{i\mathcal{L}t} B, \text{ then } e^{-i\mathcal{L}t} B \to B(-t),$$

which is why $\{p_i\} \to \{-p_i\}$ corresponds to time reversal

(b) Under the transformation $\{q_i, p_i\} \to \{q_i, -p_i\}$,

$$H \to H$$
$$f_0(\Gamma) \to f_0(\Gamma) \quad (\text{because } f_0 \propto e^{-\beta H})$$
$$i\mathcal{L} \to -i\mathcal{L}$$
$$A \to \gamma_A A \quad \text{and so } A^* \to \gamma_A A^*$$
$$B \to \gamma_B B \quad \text{and so } B^* \to \gamma_B B^*$$

and $d\Gamma \to d\Gamma$ (because for each momentum component we have $\int_{-\infty}^{\infty} dp_{i\alpha} \xrightarrow{p_{i\alpha} \to -p_{i\alpha}} -\int_{\infty}^{-\infty} dp_{i\alpha} = +\int_{-\infty}^{\infty} dp_{i\alpha}$)

$\therefore \langle A|B\rangle = \int d\Gamma\, f_0(\Gamma) A^*(\Gamma) B(\Gamma) \xrightarrow[\text{reversal}]{\text{time}} \int d\Gamma\, f_0(\Gamma)\, \gamma_A A^*(\Gamma)\, \gamma_B B(\Gamma)$

$= \gamma_A \gamma_B \langle A|B\rangle$

$\therefore$ if $\gamma_A \neq \gamma_B$, $\gamma_A\gamma_B = -1$, $\Rightarrow \langle A|B\rangle = -\langle A|B\rangle$, which can be true only if $\langle A|B\rangle = 0$

(c) By definition

$$C_{AB}(t) = \int d\Gamma\, f_0(\Gamma) A^*(\Gamma)\, e^{i\mathcal{L}t} B(\Gamma) \qquad \ldots(1)$$

$$\xrightarrow[\text{reversal}]{\text{time}} \int d\Gamma\, f_0(\Gamma)\, \gamma_A A^*(\Gamma)\, e^{-it\mathcal{L}}\, \gamma_B B(\Gamma) \qquad \ldots(2)$$

$$= \gamma_A\gamma_B \int d\Gamma\, f_0(\Gamma)\, B(\Gamma)\, e^{+it\mathcal{L}} A^*(\Gamma)$$

$$= \gamma_A\gamma_B \left(\int d\Gamma\, f_0(\Gamma)\, B^*(\Gamma)\, e^{it\mathcal{L}} A(\Gamma)\right)^*$$

$$= \gamma_A\gamma_B \langle B|A(t)\rangle^* = \gamma_A\gamma_B\, C^*_{BA}(t)$$

$$= \gamma_A\gamma_B \langle A|B(-t)\rangle \quad (\text{from } (2)) = \gamma_A\gamma_B\, C_{AB}(-t)$$

9. (a) Under the transformation $\Gamma \to -\Gamma$ (inversion)

$H \to H$ (because system has a centre of inversion and the moment appear quadratically)

$i\mathcal{L} \to i\mathcal{L}$

$f_0(\Gamma) \to f_0(\Gamma)$

$d\Gamma \to d\Gamma$

Consider

$$C_{AB}(t) = \langle A|B(t)\rangle = \int d\Gamma\, f_0(\Gamma) A^*(\Gamma)\, e^{it\mathcal{L}} B(\Gamma)$$

$\therefore \quad C_{AB}(t) \xrightarrow{\Gamma \to -\Gamma} \gamma_A \gamma_B \int d\Gamma\, f_0(\Gamma) A^*(\Gamma)\, e^{it\mathcal{L}} B(\Gamma)$

$= \gamma_A \gamma_B C_{AB}(t)$

So if $\gamma_A \neq \gamma_B$, $\gamma_A \gamma_B = -1$, and $C_{AB}(t) = 0$

(b) Under reflection

$\{x_i, y_i, z_i, p_{ix}, p_{iy}, p_{iz}\} \to \{x_i, -y_i, z_i, p_{ix}, -p_{iy}, p_{iz}\}, \ \forall i,$

we have

$H \to H$

$i\mathcal{L} \to i\mathcal{L}$ (because the Liouvillian has terms like $\frac{\partial H}{\partial y_i}\frac{\partial}{\partial p_{iy}} - \frac{\partial H}{\partial p_{iy}}\frac{\partial}{\partial y_i}$)

$f_0(\Gamma) \to f_0(\Gamma)$ (because $f_0 \propto e^{-\beta H}$)

$d\Gamma \to d\Gamma$

Consider

$C_{AB}(t) = \langle A | B(t) \rangle = \int d\Gamma\, f_0(\Gamma) A^*(\Gamma)\, e^{i\mathcal{L}t} B(\Gamma)$

$\therefore C_{AB}(t) \xrightarrow{\text{reflection}} \alpha_A \alpha_B \int d\Gamma\, f_0(\Gamma) A^*(\Gamma)\, e^{i\mathcal{L}t} B(\Gamma)$

$= \alpha_A \alpha_B C_{AB}(t)$

$\therefore$ if $\alpha_A \neq \alpha_B$, $\alpha_A \alpha_B = -1$, and $C_{AB}(t) = 0$