SET – 15

(Classical) Hydrogen atom

1. $\vec{r}_1$ – position of nucleus.
   $\vec{r}_2$ – position of electron.

$$\vec{p}_i = m_i \dot{\vec{r}}_i$$

$$V = -\frac{Ze^2}{|\vec{r}_1 - \vec{r}_2|}$$

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\vec{r}_1, \vec{r}_2)$$

$$= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\vec{r}_1 - \vec{r}_2)$$

$$L = \vec{p}_1 \cdot \frac{d\vec{r}_1}{dt} + \vec{p}_2 \cdot \frac{d\vec{r}_2}{dt} - H$$

2. Define :

$$(m_1 + m_2)\vec{R} = m_1 \vec{r}_1 + m_2 \vec{r}_2$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{P} = \vec{p}_1 + \vec{p}_2$$

$$(m_1 + m_2)\vec{p} = m_2 \vec{p}_1 - m_1 \vec{p}_2$$

$\vec{R}$ – center of mass position
$\vec{r}$ – relative position
$\vec{P}$ – total momentum
$\vec{p}$ – relative momentum.

3. Note that, in the Lagrangian.

$$\delta \vec{p}_1 : \quad \frac{d\vec{r}_1}{dt} - \frac{\vec{p}_1}{m_1} = 0 \quad \Rightarrow \quad \vec{p}_1 = m_1 \frac{d\vec{r}_1}{dt}$$

$$\delta \vec{p}_2 : \quad \frac{d\vec{r}_2}{dt} - \frac{\vec{p}_2}{m_2} = 0 \quad \Rightarrow \quad \vec{p}_2 = m_2 \frac{d\vec{r}_2}{dt}.$$

$$\tilde{m}_i = \frac{m_i}{m_1+m_2}.$$

$$\tilde{m}_1 + \tilde{m}_2 = 1$$

(4)
$$\vec{R} = \tilde{m}_1 \vec{r}_1 + \tilde{m}_2 \vec{r}_2$$
$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{r}_1 = \vec{R} + \tilde{m}_2 \vec{r}$$
$$\vec{r}_2 = \vec{R} - \tilde{m}_1 \vec{r}$$

$$\frac{d\vec{r}_1}{dt} = \frac{d\vec{R}}{dt} + \tilde{m}_2 \frac{d\vec{r}}{dt}$$
$$\frac{d\vec{r}_2}{dt} = \frac{d\vec{R}}{dt} - \tilde{m}_1 \frac{d\vec{r}}{dt}.$$

(5)
$$\vec{P} = \vec{p}_1 + \vec{p}_2$$
$$\vec{p} = \tilde{m}_2 \vec{p}_1 - \tilde{m}_1 \vec{p}_2$$
$$\vec{p}_1 = \vec{p} + \tilde{m}_1 \vec{P}$$
$$\vec{p}_2 = -\vec{p} + \tilde{m}_2 \vec{P}$$

(6)
$$\vec{p}_1 \cdot \frac{d\vec{r}_1}{dt} + \vec{p}_2 \cdot \frac{d\vec{r}_2}{dt} = \left(\vec{p} + \tilde{m}_1 \vec{P}\right)\cdot\left(\frac{d\vec{R}}{dt} + \tilde{m}_2 \frac{d\vec{r}}{dt}\right) + \left(-\vec{p} + \tilde{m}_2 \vec{P}\right)\cdot\left(\frac{d\vec{R}}{dt} - \tilde{m}_1 \frac{d\vec{r}}{dt}\right)$$
$$= \vec{p}\cdot\frac{d\vec{r}}{dt} + \vec{P}\cdot\frac{d\vec{R}}{dt}$$

(7)
$$\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = \frac{1}{2m_1}\left(\vec{p} + \tilde{m}_1 \vec{P}\right)^2 + \frac{1}{2m_2}\left(-\vec{p} + \tilde{m}_2 \vec{P}\right)^2$$
$$= \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\frac{p^2}{2} + \left(\frac{\tilde{m}_1^2}{2m_1} + \frac{\tilde{m}_2^2}{2m_2}\right) P^2$$
$$= \frac{p^2}{2\mu} + \frac{P^2}{2M}$$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$M = m_1 + m_2$$

(8) Thus, we have.

$$H = \frac{p^2}{2\mu} + \frac{P^2}{2M} + V(\vec{r})$$

$$L = \vec{p} \cdot \frac{d\vec{r}}{dt} + \vec{P} \cdot \frac{d\vec{R}}{dt} - H$$

(9) Variations define:

$$\delta\vec{p} : \quad \frac{d\vec{r}}{dt} - \frac{\vec{p}}{\mu} = 0 \quad \Rightarrow \quad \vec{p} = \mu \frac{d\vec{r}}{dt}.$$

$$\delta\vec{P} : \quad \frac{d\vec{R}}{dt} - \frac{\vec{P}}{M} = 0 \quad \Rightarrow \quad \vec{P} = M \frac{d\vec{R}}{dt}.$$

(10) Thus, the Lagrangian splits into external and internal

$$L = L_{ext} + L_{int}$$

$$L_{ext} = \vec{P} \cdot \frac{d\vec{R}}{dt} - H_{ext} \qquad H_{ext} = \frac{P^2}{2M}$$

$$L_{int} = \vec{p} \cdot \frac{d\vec{r}}{dt} - H_{int} \qquad H_{int} = \frac{p^2}{2\mu} + V(\vec{r})$$

(11) Equations of motion:

$$\frac{d\vec{r}}{dt} = \frac{\partial H}{\partial \vec{p}}$$

$$\frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{r}}$$

(12) $$H_{int} = \frac{p^2}{2\mu} + V(\vec{r})$$
$$= \frac{p^2}{2\mu} - \frac{Ze^2}{r}$$

(13) $$\frac{d\vec{r}}{dt} = \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p}}{\mu}$$

(14) $$\frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{r}} = \vec{\nabla}\left(\frac{Ze^2}{r}\right)$$
$$= -\frac{Ze^2\,\vec{r}}{r^3}$$

(15) $$\vec{L} = \vec{r} \times \vec{p}$$
$$\frac{d\vec{L}}{dt} = \left(\frac{d\vec{r}}{dt}\right) \times \vec{p} + \vec{r} \times \left(\frac{d\vec{p}}{dt}\right)$$
$$= \frac{\vec{p}}{\mu} \times \vec{p} - \vec{r} \times Ze^2 \frac{\vec{r}}{r^3}$$
$$= 0.$$

Thus, angular momentum is a constant of motion.

(16) What else is conserved?

(17) Consider

$$
\begin{aligned}
\frac{d}{dt}\left(\frac{\vec{r}}{r}\right) &= \frac{d\vec{r}}{dt}\,\frac{1}{r} + \vec{r}\,\frac{d}{dt}\frac{1}{r} \\
&= \frac{\vec{p}}{\mu}\,\frac{1}{r} + \vec{r}\,\frac{d\vec{r}}{dt}\cdot\nabla\frac{1}{r} \\
&= \frac{\vec{p}}{\mu}\,\frac{1}{r} - \vec{r}\,\frac{\vec{p}}{\mu}\cdot\frac{\vec{r}}{r^3} \\
&= \frac{1}{\mu}\,\frac{1}{r^3}\left[\vec{p}\,(\vec{r}\cdot\vec{r}) - \vec{r}\,(\vec{p}\cdot\vec{r})\right] \\
&= -\frac{1}{\mu}\,\frac{1}{r^3}\,\vec{r}\times(\vec{r}\times\vec{p}) \\
&= +\frac{1}{\mu Z e^2}\left(\frac{d\vec{p}}{dt}\right)\times(\vec{r}\times\vec{p}) \\
&= \frac{1}{\mu Z e^2}\left(\frac{d\vec{p}}{dt}\right)\times\vec{L} \\
&= \frac{1}{\mu Z e^2}\,\frac{d}{dt}\,(\vec{p}\times\vec{L}) \qquad \because\ \frac{d\vec{L}}{dt} = 0.
\end{aligned}
$$

$$\Rightarrow \quad \frac{d\vec{A}}{dt} = 0$$

where $\vec{A} = \dfrac{\vec{r}}{r} - \dfrac{1}{\mu Z e^2}\,\vec{p}\times\vec{L}$

Laplace-Runge-Lenz vector.

(18) Let us investigate the magnitude and direction of $\vec{A}$.

$$\vec{A} \cdot \vec{L} = \left(\frac{\vec{r}}{r} - \frac{1}{\mu Z e^2} \vec{p} \times \vec{L} \right) \cdot \vec{L}$$

$$= \frac{\vec{r}}{r} \cdot (\vec{r} \times \vec{p}) - \frac{1}{\mu Z e^2} (\vec{p} \times \vec{L}) \cdot \vec{L}$$

$$= 0 .$$

(19)
$$\vec{A} \cdot \vec{r} = \left(\frac{\vec{r}}{r} - \frac{1}{\mu Z e^2} \vec{p} \times \vec{L} \right) \cdot \vec{r}$$

$$= r - \frac{1}{\mu Z e^2} \vec{r} \cdot (\vec{p} \times \vec{L})$$

$$= r - \frac{1}{\mu Z e^2} (\vec{r} \times \vec{p}) \cdot \vec{L}$$

$$= r - \frac{L^2}{\mu Z e^2}$$

(20)
$$r A \cos\theta = r - \frac{L^2}{\mu Z e^2}$$

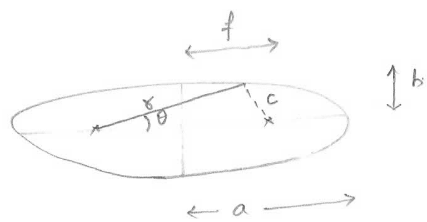
$$r (1 - A \cos\theta) = \frac{L^2}{\mu Z e^2} .$$

$$r = \frac{\left(\frac{L^2}{\mu Z e^2} \right)}{(1 - A \cos\theta)} .$$

21 Equation of ellipse with origin at the center is

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1.$$

22 Let the origin be at the foci.



For an ellipse,
$r + c =$ constant.
which for $\theta = 0$ reads.
$(a+f) + (a-f) =$ constant.
$\Rightarrow \quad r + c = 2a.$
$c = 2a - r$

Using law of Cosines,

$$2(2f)\, r \cos\theta = (2f)^2 + r^2 - c^2$$

$$4 f r \cos\theta = 4f^2 + r^2 - (2a-r)^2.$$
$$= 4f^2 - 4a^2 + 4ar$$

$$ar - f r \cos\theta = a^2 - f^2.$$

$$r\left(1 - \frac{f}{a}\cos\theta\right) = a\left(1 - \frac{f^2}{a^2}\right)$$

$e = \frac{f}{a} \rightarrow$ eccentricity

for an ellipse $e < 1$.

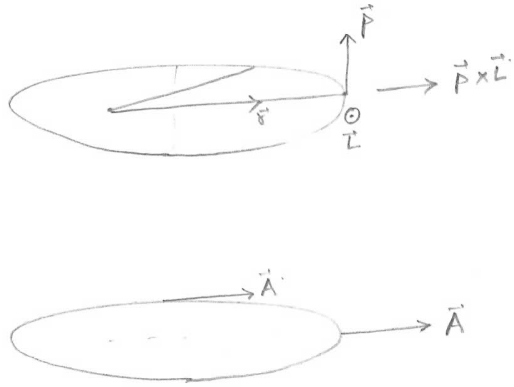
$$r = \frac{a(1-e^2)}{1 - e\cos\theta}$$

23 Comparing 20 and 22 we learn that $|\vec{A}|$ is the eccentricity of the ellipse.

$$e = A$$

$$a = \frac{1}{\mu Z e^2} \frac{L^2}{(1-A^2)}$$

(23) To determine the direction of $\vec{A}$, consider $\theta = 0$



→ $\vec{A}$ is not a pseudo vector. It is called axial vector probably because it points in the direct of axis of ellipse.

(24)
$$\vec{A} = \frac{\vec{r}}{r} - \frac{1}{\mu Z e^2} \vec{p} \times \vec{L}$$

$$A^2 = 1 + \frac{1}{\mu^2 Z^2 e^4} (\vec{p} \times \vec{L}) \cdot (\vec{p} \times \vec{L}) - \frac{2}{\mu Z e^2} \frac{1}{r} \vec{r} \cdot \vec{p} \times \vec{L}$$

(25)
$$\begin{aligned}
(\vec{p} \times \vec{L}) \cdot (\vec{p} \times \vec{L}) &= \epsilon_{ijk} p_j L_k \, \epsilon_{imn} p_m L_n \\
&= (\delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km}) p_j p_m L_k L_n \\
&= p_j p_j L_k L_k - p_j p_k L_k L_j \\
&= p^2 L^2 - \underbrace{(\vec{p} \cdot \vec{L})^2}_{= 0} \\
&= p^2 L^2
\end{aligned}$$

(26)
$$A^2 = 1 + \frac{p^2 L^2}{\mu^2 Z^2 e^4} - \frac{2 L^2}{\mu Z e^2} \frac{1}{r}$$

$$= 1 + \frac{p^2 L^2}{\mu^2 Z^2 e^4} - \frac{2 L^2}{\mu Z^2 e^4} \frac{Z e^2}{r}$$

27 $$A^2 = 1 + \frac{2L^2}{\mu Z^2 e^4}\left(\frac{p^2}{2\mu} - \frac{Ze^2}{r}\right)$$

$$= 1 + \frac{2L^2}{\mu Z^2 e^4} H$$

$$H = -\frac{\mu Z^2 e^4}{2} \frac{(1-A^2)}{L^2}.$$

28 Bohr model: $L = n\hbar$ (let $A=0$)

$$H = -\frac{\mu Z^2 e^4}{2\hbar^2} \cdot \frac{1}{n^2}$$

$L = n\hbar$ allows $n=0$.

But, $n=0$ is not allowed in hydrogen atom.

29 Summary:

$$H = \frac{p^2}{2\mu} - \frac{Ze^2}{r}$$

$$\frac{d\vec{r}}{dt} = \frac{\partial H}{\partial \vec{p}} = \frac{\vec{p}}{\mu}$$

$$\frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{r}} = -\frac{Ze^2\,\vec{r}}{r^3}$$

$$\frac{d\vec{L}}{dt} = 0 \qquad \vec{L} = \vec{r}\times\vec{p}.$$

$$\vec{A} = \frac{\vec{r}}{r} - \frac{1}{\mu Z e^2}\vec{p}\times\vec{L}.$$

$$\frac{d\vec{A}}{dt} = 0$$

$$\vec{A}\cdot\vec{L} = 0$$

$e = A$ — eccentricity. $e = \frac{f}{a}$.

$a(1-e^2) = \frac{L^2}{\mu Z e^2}$ a — major axis.

$$r = \frac{\left(\frac{L^2}{\mu Z e^2}\right)}{(1 - A\cos\theta)}$$

$$H = -\frac{\mu Z^2 e^4}{2\hbar^2}\frac{(1-A^2)}{L^2}.$$