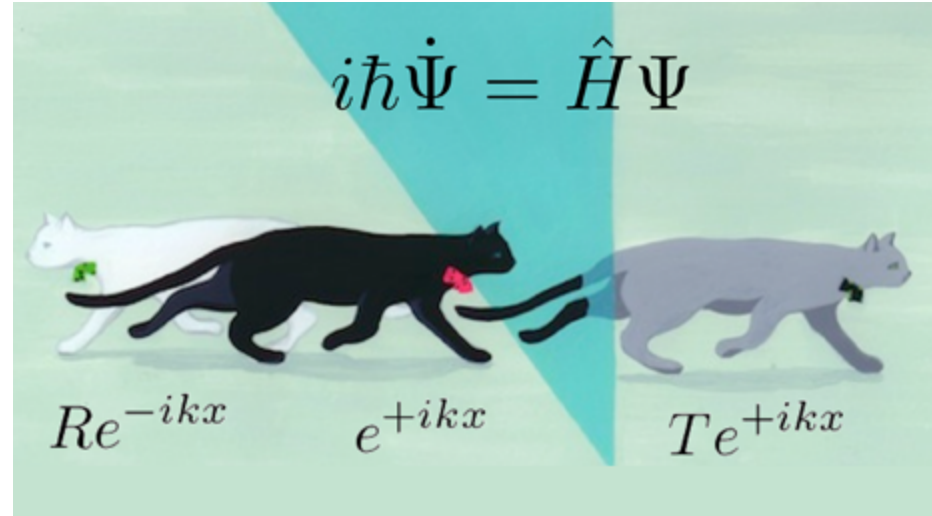


## Atomic Structure and Spectra

### Part IV. Still cracking the hydrogen code

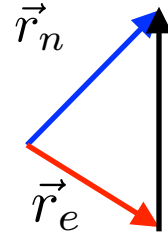


# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems

Nucleus: position, mass, electric charge  $\vec{r}_n; M; +Ze$

Electron: position, mass, electric charge  $\vec{r}_e; m; -e$



$$\vec{r} = \vec{r}_n - \vec{r}_e$$

$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

$$M\ddot{\vec{r}}_n = -Ze^2\vec{r}/r^3$$

$$m\ddot{\vec{r}}_e = +Ze^2\vec{r}/r^3$$

$$\ddot{\vec{r}} = -\left[\frac{1}{M} + \frac{1}{m}\right]Ze^2\vec{r}/r^3$$

$$\mu\ddot{\vec{r}} = -Ze^2\vec{r}/r^3$$

$$\frac{1}{\mu} = \left[\frac{1}{M} + \frac{1}{m}\right]$$

$$\vec{p} = \mu\dot{\vec{r}}$$

**First-order equations:**

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$

# Atomic Structure and Spectra

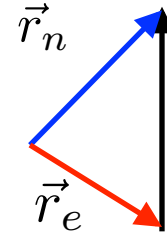
---

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$

Find constants of motion from products of  $\vec{p}$  and  $\vec{r}$  :



$$\vec{r} = \vec{r}_n - \vec{r}_e$$

$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

$$T = \frac{\vec{p} \cdot \vec{p}}{2\mu} = \frac{p^2}{2\mu}$$

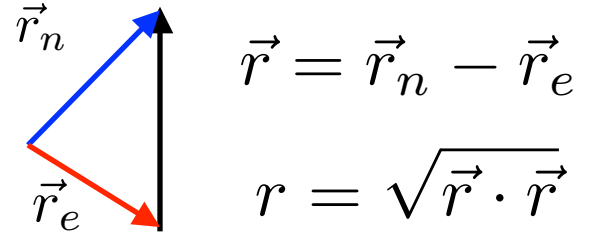
# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

$$\dot{\vec{p}} = -Ze^2 \vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu} \vec{p}$$

Find constants of motion from products of  $\vec{p}$  and  $\vec{r}$  :



$$T = \frac{\vec{p} \cdot \vec{p}}{2\mu} = \frac{p^2}{2\mu}$$

$$\dot{T} = \frac{\dot{\vec{p}} \cdot \vec{p}}{\mu} = -Ze^2 \dot{\vec{r}} \cdot \vec{r}/r^3 = -Ze^2 \dot{r}/r^3 = -\frac{\partial}{\partial t} \left( \frac{-Ze^2}{r} \right) = -\dot{V}(r)$$

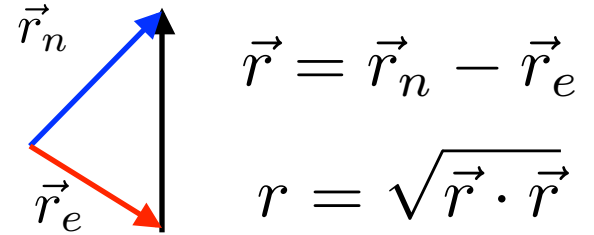
$$V(r) = -Ze^2/r$$

# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$



Find constants of motion from products of  $\vec{p}$  and  $\vec{r}$  :

$$T = \frac{\vec{p} \cdot \vec{p}}{2\mu} = \frac{p^2}{2\mu}$$

$$\dot{T} = \frac{\vec{p} \cdot \dot{\vec{p}}}{\mu} = -Ze^2\dot{\vec{r}} \cdot \vec{r}/r^3 = -Ze^2\dot{r}/r^3 = -\frac{\partial}{\partial t} \left( \frac{-Ze^2}{r} \right) = -\dot{V}(r)$$

$$V(r) = -Ze^2/r$$

We have found a constant of motion:

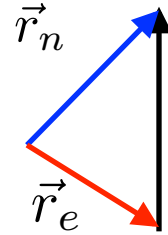
$$E = T + V(r)$$

# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$



$$\vec{r} = \vec{r}_n - \vec{r}_e$$

$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

Find constants of motion from products of  $\vec{p}$  and  $\vec{r}$  :

$$T = \frac{\vec{p} \cdot \vec{p}}{2\mu} = \frac{p^2}{2\mu} \quad || \quad V(r) = -Ze^2/r \quad || \quad \boxed{E = T + V(r)}$$

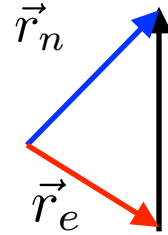
What about a constant of motion involving  $\vec{r} \cdot \vec{r}$  or  $\vec{r} \cdot \vec{p}$  ?

# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$



$$\vec{r} = \vec{r}_n - \vec{r}_e$$

$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

Find constants of motion from products of  $\vec{p}$  and  $\vec{r}$  :

$$T = \frac{\vec{p} \cdot \vec{p}}{2\mu} = \frac{p^2}{2\mu} \quad || \quad V(r) = -Ze^2/r \quad || \quad \boxed{E = T + V(r)}$$

What about a constant of motion involving  $\vec{r} \cdot \vec{r}$  or  $\vec{r} \cdot \vec{p}$  ?

How about  $\vec{L} = \vec{r} \times \vec{p}$  ?

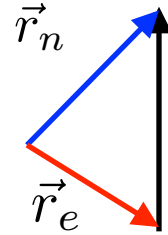
$$\dot{\vec{L}} = \dot{\vec{r}} \times \vec{p} + \vec{r} \times \dot{\vec{p}}$$

# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$



$$\vec{r} = \vec{r}_n - \vec{r}_e$$

$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

Find constants of motion from products of  $\vec{p}$  and  $\vec{r}$  :

$$T = \frac{\vec{p} \cdot \vec{p}}{2\mu} = \frac{p^2}{2\mu} \quad \parallel \quad V(r) = -Ze^2/r \quad \parallel \quad \boxed{E = T + V(r)}$$

What about a constant of motion involving  $\vec{r} \cdot \vec{r}$  or  $\vec{r} \cdot \vec{p}$  ?

How about  $\vec{L} = \vec{r} \times \vec{p}$  ?

We have found a constant of motion:

$$\dot{\vec{L}} = \dot{\vec{r}} \times \vec{p} + \vec{r} \times \dot{\vec{p}}$$

$$\vec{L} = \vec{r} \times \vec{p}$$



# Atomic Structure and Spectra

## Classical equations of motion for hydrogen-like systems : Hamiltonian form

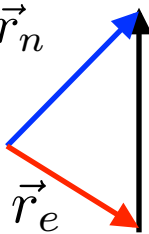
$$\dot{\vec{p}} = -Ze^2\vec{r}/r^3$$

$$\dot{\vec{r}} = \frac{1}{\mu}\vec{p}$$

$$E = T + V(r) = \frac{p^2}{2\mu} - \frac{Ze^2}{r}$$

$$\vec{L} = \vec{r} \times \vec{p}$$

Note that  $\vec{r}$  and  $\vec{p}$  define a plane that is perpendicular to  $\vec{L}$


$$\vec{r} = \vec{r}_n - \vec{r}_e$$
$$r = \sqrt{\vec{r} \cdot \vec{r}}$$

