Hydrogen Atom

In QM, often get important insight from classical problem. For a central force

$$E = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(r)$$

$$\vec{F} = -\nabla V = -\frac{dV}{dr}\hat{r}$$

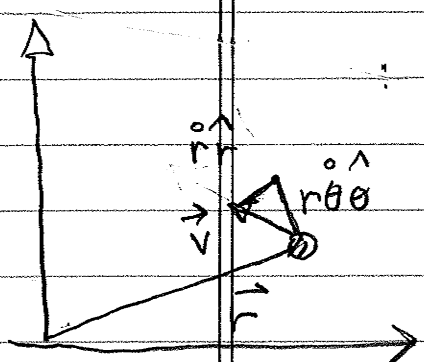
$$\vec{\tau} = \vec{r} \times \vec{F} = 0 \Rightarrow \vec{L} = \text{const}$$ } we will see clear QM analog!

Q: What does this tell us about trajectory

A: Motion lies in a plane!

Can then use polar coordinates r, θ for KE

$$E = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2) + V(r)$$



$$\vec{L} = \vec{r} \times m\vec{v} \qquad |\vec{L}| = r\,r\dot{\theta}\,m = mr^2\dot{\theta}$$

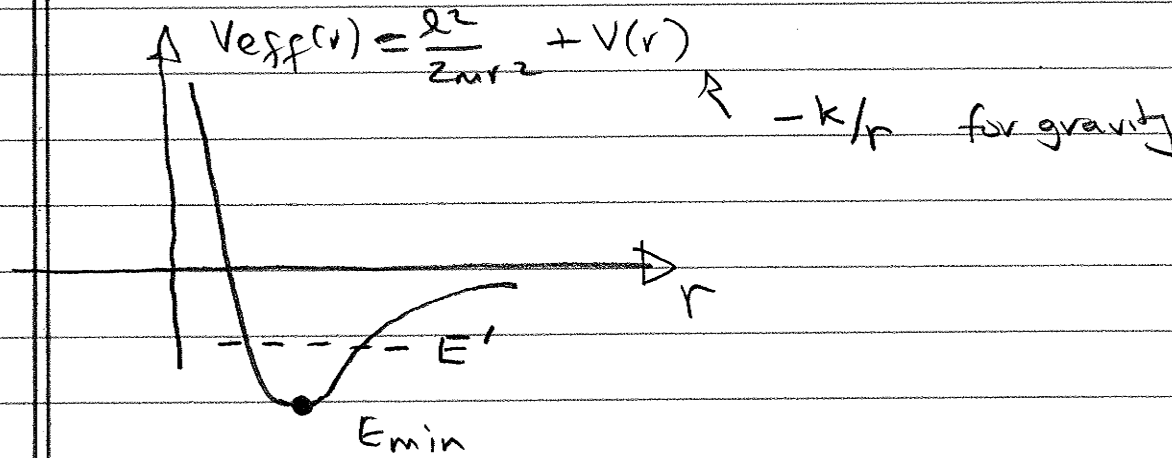
constant ℓ

$$\dot{\theta} = \ell / mr^2$$

$$E = \frac{1}{2}m\dot{r}^2 + \frac{\ell^2}{2mr^2} + V(r)$$

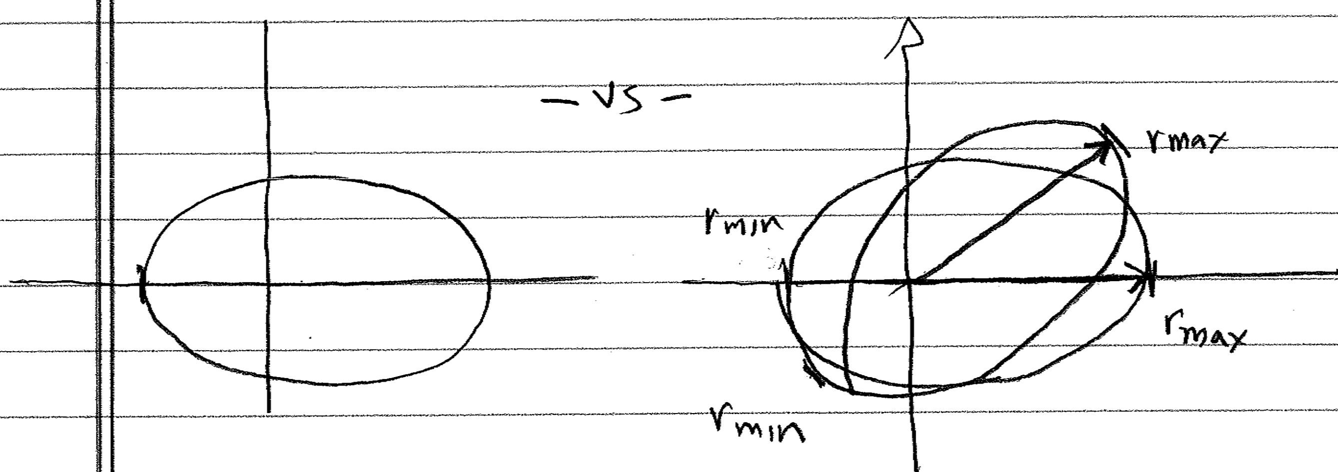
Q: What does this buy us?

A: An effectively 1-d problem: just r



Q If $E = E_{min}$ what type of orbit? Circular
If $E = E'$ " " " " Elliptical
Can see perihelion and apihelion (r_{min}, r_{max})

Q For elliptical orbit, how do you know it is closed?



A fancy answer: Runge-Lenz Vector:

H3

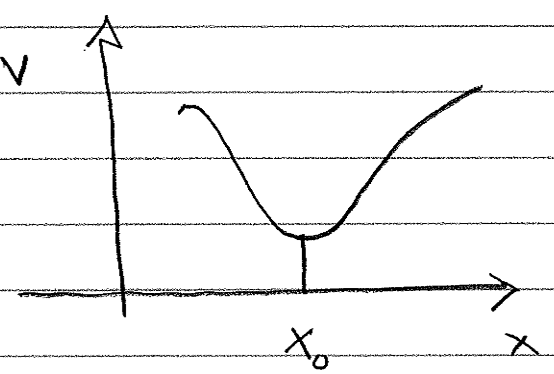
Let's do a prelim exam problem

Suppose there is a perturbation $V(r) = -\frac{k}{r} + \lambda r^2$

Show elliptical orbits precess.

Q: Did you do this in 200A?

Recall small oscillations problems (why physicists are obsessed with mass on spring). For any $V(x)$



① Find x_0 for which

$$F(x_0) = -\frac{dV}{dx}\bigg|_{x_0} = 0$$

② Expand

$$V(x) = V(x_0) + \cancel{V'(x_0)}^{\,0}(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2$$

looks like harmonic oscillator with $m\omega^2 = V''(x_0)$

H4

Consider our kepler problem with $\lambda = 0$

$$V_{eff}(r) = \frac{\ell^2}{2mr^2} - \frac{k}{r}$$

$$V'_{eff}(r) = -\frac{\ell^2}{mr^3} + \frac{k}{r^2} = 0$$

This tells us $\quad \ell^2 = mkr = m^2 r^4 \omega_0^2 \quad \leftarrow$ Sloppy? $\dot{\theta} = \omega_0$ not really constant. but perturb about circular

$$m\omega_0^2 = k/r^3$$

$$V''_{eff}(r) = \frac{3\ell^2}{mr^4} - \frac{2k}{r^3} = m\omega^2$$

$\uparrow$ oscillation freq about minimum (circular orbit)

$$\frac{3k}{r^3} - \frac{2k}{r^3} = m\omega^2$$

$$\omega^2 = k/r^3$$

$\ast$ Frequency ω of small oscillations about circular precisely equals frequency to go around circle (ellipse)

$\Rightarrow$ closed orbits

H5

Now add perturbation

$$V_{eff}(r) = \frac{\ell^2}{2mr^2} - \frac{k}{r} + \lambda r^2$$

$$V'_{eff}(r) = \frac{-\ell^2}{mr^3} + \frac{k}{r^2} + 2\lambda r = 0$$

$$\ell^2 = mkr + 2\lambda m r^4$$

$$\ell = m\omega_0 r^2$$

$$\ell^2 = m^2\omega_0^2 r^4 = mkr + 2\lambda m r^4$$

$$m\omega_0^2 = \frac{k}{r^3} + 2\lambda$$

frequency increased as is reasonable (bigger central force)

$$V''_{eff}(r) = \frac{3\ell^2}{mr^4} - \frac{2k}{r^3} + 2\lambda \Leftarrow m\omega^2$$

$$m\omega^2 = \frac{3}{mr^4}\left[mkr + 2\lambda m r^4\right] - \frac{2k}{r^3} + 2\lambda$$

$$\left.\begin{aligned} m\omega^2 &= \frac{k}{r^3} + 8\lambda \\ \text{but}\quad m\omega_0^2 &= \frac{k}{r^3} + 2\lambda \end{aligned}\right\} \text{no match} \Rightarrow \text{precession}$$

H6

Turn now to QM. Operators! But many similarities.

Recall some 215A stuff. In <u>position</u> <u>basis</u>

$$L_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \qquad L_x = \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$L_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad \Longleftrightarrow \quad L_y = \frac{\hbar}{i}\left(-\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \qquad L_z = \hbar/i\,\partial/\partial\phi$$

$$L^2 = \ldots$$

Q: What are eigenfunctions and eigenvalues?

$$L^2\, Y_{\ell m}(\theta,\phi) = \ell(\ell+1)\hbar^2\, Y_{\ell m}(\theta,\phi)$$

$$L_z\, Y_{\ell m}(\theta,\phi) = m\hbar\, Y_{\ell m}(\theta,\phi)$$

$$Y_{00} = 1/\sqrt{4\pi}$$

$$Y_{11} = -\sqrt{3/8\pi}\,\sin\theta\, e^{i\phi}$$

$$Y_{10} = \sqrt{3/4\pi}\,\cos\theta$$

$$Y_{1-1} = \sqrt{3/8\pi}\,\sin\theta\, e^{-i\phi}$$

H7.

for $\vec{F} \sim \hat{r}$

a) Analog of $\vec{\tau} = \vec{r} \times \vec{F} = 0 \Rightarrow \frac{d\vec{L}}{dt} = 0$

is what?

A: $[\hat{H}, \hat{L}^2] = \phi$

$[\hat{H}, \hat{L}_z] = \phi$ if $V = V(r)$ only

In fact $[\hat{H}, \hat{L}_x] = \phi$

$[\hat{H}, L_y] = \phi$ as well,

How do we know this? Explicit computation!

For example (do not need to work specifically in position basis)

$$\left[\frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}, \hat{x}\hat{p}_y - \hat{y}\hat{p}_x\right]$$

$$= \frac{1}{2m}\left(\left[\hat{p}_x^2, \hat{x}\hat{p}_y\right] - \left[\hat{p}_y^2, \hat{y}\hat{p}_x\right]\right) = 0$$ (See page H7A)

So $\hat{L}_z$ commutes with KE

Examining form of L_x, L_y, L_z it is clear

they commute with $V(r)$ since they only involve $\frac{\partial}{\partial\theta}$ and $\frac{\partial}{\partial\phi}$!

H7A

$$[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}\hat{B}\hat{C}\hat{D} - \hat{C}\hat{D}\hat{A}\hat{B}$$

$$= \hat{A}\hat{B}\hat{C}\hat{D} - \hat{A}\hat{C}\hat{B}\hat{D} + \hat{A}\hat{C}\hat{B}\hat{D} - \hat{C}\hat{D}\hat{A}\hat{B}$$

$$= \hat{A}[\hat{B}, \hat{C}]\hat{D} + \hat{A}\hat{C}\hat{B}\hat{D} - \hat{A}\hat{C}\hat{D}\hat{B} + \hat{A}\hat{C}\hat{D}\hat{B} - \hat{C}\hat{D}\hat{A}\hat{B}$$

$$= \hat{A}[\hat{B}, \hat{C}]\hat{D} + \hat{A}\hat{C}[\hat{B}, \hat{D}] + \hat{A}\hat{C}\hat{D}\hat{B} - \hat{C}\hat{A}\hat{D}\hat{B}$$

$$+ \hat{C}\hat{A}\hat{D}\hat{B} - \hat{C}\hat{D}\hat{A}\hat{B}$$

$$= \hat{A}[\hat{B}, \hat{C}]\hat{D} + \hat{A}\hat{C}[\hat{B}, \hat{D}] + [\hat{A}, \hat{C}]\hat{D}\hat{B} - \hat{C}[\hat{A}, \hat{D}]\hat{B}$$

So $$[\hat{p}_x^2, \hat{x}\hat{p}_y] = [\underset{A}{\hat{p}_x}\, \underset{B}{\hat{p}_x}, \underset{C}{\hat{x}}, \underset{D}{\hat{p}_y}]$$

$$= \hat{p}_x \hat{p}_y \frac{\hbar}{i} + \frac{\hbar}{i} \hat{p}_y \hat{p}_x$$

$$[\hat{p}_y^2, \hat{y}\hat{p}_x] = [\underset{A}{\hat{p}_y}\, \underset{B}{\hat{p}_y}, \underset{C}{\hat{y}}\, \underset{D}{\hat{p}_x}]$$

$$= \hat{p}_y \hat{p}_x \frac{\hbar}{i} + \frac{\hbar}{i} \hat{p}_x \hat{p}_y$$

$\Rightarrow$ * on H7 is zero!

So to solve any central force problem in QM

We can search for sol'ns $\psi(r,\theta,\phi)$

amongst $R(r)\,Y_{\ell m}(\theta,\phi)$!

Just as in classical case we needed to examine

effective 1d problem

$$\frac{1}{2m}\,\dot{r}^2 + V_{eff}(r) \leftarrow \frac{\ell^2}{2mr^2} + V(r))$$

Here we need to solve effective 1d proble

$$\Big[\underbrace{-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}\,r + \frac{\ell(\ell+1)\hbar^2}{2mr^2}} + V(r)\Big]R(r) = E\,R(r)$$

KE can be written as $-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}\,r + \frac{L^2}{2mr^2}$