Physics 491 - Quantum Mechanics I

Lecture 9a: The two-body problem (Hydrogen)

So far we have consider only single particles moving in an external potential. We now generalize to consider two particles interacting with one another. The Hamiltonian is of the form

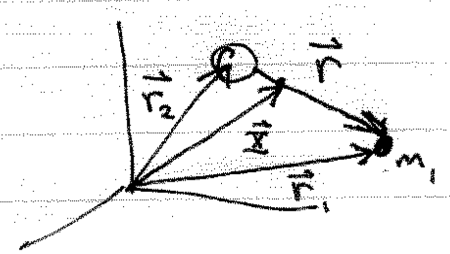
$$\hat{H} = \frac{\hat{P}_1^2}{2m_1} + \frac{\hat{P}_2^2}{2m_2} + V(\hat{\vec{r}}_1 - \hat{\vec{r}}_2)$$

We have assumed a potential that depends on $\vec{r} = \vec{r}_1 - \vec{r}_2$, the relative coordinate

Note, Unless $V(\hat{\vec{r}}_1 - \hat{\vec{r}}_2) = V_1(\hat{\vec{r}}_1) + V_2(\hat{\vec{r}}_2)$ the Hamiltonian is <u>not separable</u> in $\vec{r}_1$ and $\vec{r}_2$.

However, we can change coördinates to consider <u>relative motion</u> and <u>center of mass</u>.

Classical Mechanics.



<u>Center-of-mass</u>

$$\vec{X} \equiv \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{M}$$

$$M = m_1 + m_2$$

<u>Relative coördinate</u>

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

$$\Rightarrow \vec{r}_1 = \vec{X} + \frac{m_2}{M}\vec{r}, \qquad \vec{r}_2 = \vec{X} - \frac{m_1}{M}\vec{r}$$

Center of Mass frame $\vec{V}_{CM} = \dot{\vec{X}}$, $\vec{P}_{CM} = M\vec{V}_{CM}$

In that frame $\dot{\vec{r}}_1{}' = \frac{m_2}{M}\dot{\vec{r}}$, $\dot{\vec{r}}_2{}' = -\frac{m_1}{M}\dot{\vec{r}}$

$$\Rightarrow \vec{p}_1{}' = \frac{m_1 m_2}{M}\dot{\vec{r}} \qquad \vec{p}_2{}' = +m_2\dot{\vec{r}}_2 = -\frac{m_2 m_1}{M}\dot{\vec{r}}$$

$$\Rightarrow \underbrace{\vec{p}_1{}' = -\vec{p}_2{}'}_{\text{Newton's Law}} \equiv \vec{p}_{rel} = \mu\dot{\vec{r}}, \quad \mu = \frac{m_1 m_2}{M}$$

(reduced mass)

In lab frame, $\vec{p}_1 = m_1\dot{\vec{r}}_1 = m_1\dot{\vec{X}} + \vec{p}_{rel}$

$$\vec{p}_2 = m_2\dot{\vec{r}}_2 = m_2\dot{\vec{X}} - \vec{p}_{rel}$$

$$\Rightarrow \vec{P}_{total} = \vec{p}_1 + \vec{p}_2 = M\dot{\vec{X}} = \vec{P}_{cm}$$

Kinetic Energy

$$T = \tfrac{1}{2}m_1\dot{\vec{r}}_1^{\,2} + \tfrac{1}{2}m_2\dot{\vec{r}}_2^{\,2}$$

$$= \tfrac{1}{2}m_1\left(\dot{\vec{X}}^2 + 2\frac{m_2}{M}\dot{\vec{r}}\cdot\dot{\vec{X}} + \left(\frac{m_2}{M}\right)^2\dot{\vec{r}}^{\,2}\right)$$

$$+ \tfrac{1}{2}m_2\left(\dot{\vec{X}}^2 - 2\frac{m_1}{M}\dot{\vec{r}}\cdot\dot{\vec{X}} + \left(\frac{m_1}{M}\right)^2\dot{\vec{r}}^{\,2}\right)$$

$$= \tfrac{1}{2}M\dot{\vec{X}}^2 + \tfrac{1}{2}\mu\dot{\vec{r}}^{\,2}$$

$$\Rightarrow \boxed{T = \frac{\vec{P}_{CM}^2}{2M} + \frac{\vec{p}_{rel}^{\,2}}{2\mu}}$$

The kinetic energy is separable in CM and relative coördinates.

Thus, in the absence of any other external forces the Hamiltonian separates in relative and center-of-mass

$$H = \underbrace{\frac{\vec{P}_{cm}^{\,2}}{2M}}_{H_{CM}} + \underbrace{\frac{\vec{P}_{rel}^{\,2}}{2\mu} + V(\vec{r})}_{H_{rel}}$$

The CM is a free particle, while the relative motion dynamics are dictated by the interaction potential $V(\vec{r})$

<u>Quantum Problem:</u>

We now have quantum operators

$$\hat{\vec{X}}_{cm} \qquad \hat{\vec{P}}_{cm} \doteq \frac{\hbar}{i}\vec{\nabla}_{\vec{X}}$$

$$\hat{\vec{r}}, \qquad \hat{\vec{P}}_{rel} = \frac{\hbar}{i}\vec{\nabla}_{\vec{r}}$$

$$\hat{H} = \underbrace{\frac{\hat{\vec{P}}_{cm}^{\,2}}{2M}}_{\hat{H}_{CM}} + \underbrace{\left(\frac{\hat{\vec{P}}_{rel}^{\,2}}{2\mu} + V(\hat{\vec{r}})\right)}_{\hat{H}_{rel}}$$

Because the Hamiltonian is separable in these coords $\exists$ stationary state $|\Psi\rangle = |\psi_{cm}\rangle \otimes |\psi_{rel}\rangle$

with $\hat{H}_{CM}|\psi_{cm}\rangle = E_{cm}\,|\psi_{cm}\rangle$ $\qquad E = E_{cm} + E_{rel}$

$$\hat{H}_{rel}\,|\psi_{rel}\rangle = E_{rel}\,|\psi_{rel}\rangle$$

The CM problem is a free particle (assuming no external potential).

The remain problem is relative coordinate. Understanding that, we will drop the "rel" ~~label~~ label

$$\hat{H}_{rel} |\psi_{rel}\rangle = E_{rel} |\psi_{rel}\rangle$$

$$\hookrightarrow \hat{H} |\psi\rangle = E |\psi\rangle$$

where $\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} + V(\vec{r})$, $\vec{p} \doteq \frac{\hbar}{i} \vec{\nabla}_{\vec{r}}$

<u>Central potential:</u> If $V(|\vec{r}|)$ (i.e., only depends on the distantance between particles) we again have a spherical symmetric potential, now in the relative coordinate.

$$\Rightarrow \hat{H} = \frac{\hat{P}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + V(r)$$

where $\vec{p}_r$ and $\vec{L}$ are radial/ang mom for relative motion

Solutions to T.I.S.E. $\psi(r,\theta,\phi) = R_\ell(r)\, Y_\ell^m(\theta,\phi)$

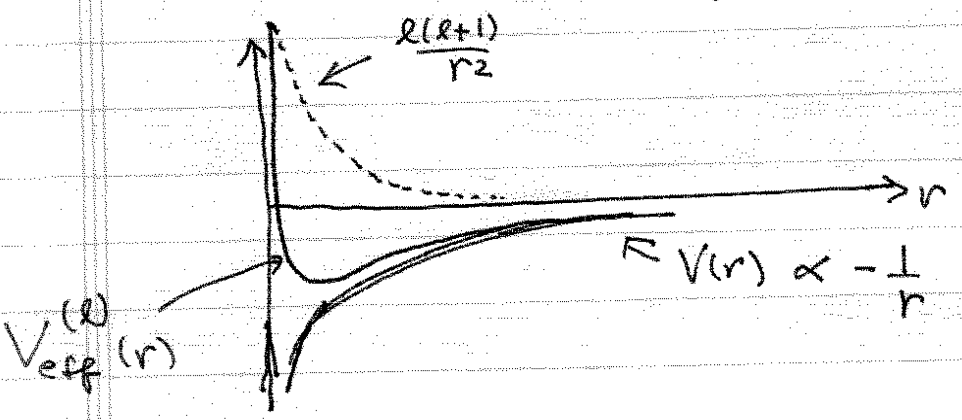
where $\hat{L}^2 Y_\ell^m = \hbar^2 \ell(\ell+1)\, Y_\ell^m$

$$\left(\frac{\hat{P}_r^2}{2m} + V_{eff}^{(\ell)}(r)\right) R_\ell(r) = E\, R_\ell(r)$$

$$V_{eff}^{(\ell)} = V(r) + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2}$$

Coulomb Interaction: $V(r) = \frac{q_1 q_2}{r}$ $\left(\begin{array}{c} \text{cgs units} \\ \frac{1}{4\pi\epsilon_0} \to 1 \end{array} \right)$
(two charges q_1, q_2)

Suppose opposite charges $q_1 q_2 < 0$



The combination of the attractive Coulomb potential and centripetal barrier creates an attractive well.

For $E<0 \Rightarrow$ bound states

$E>0 \Rightarrow$ unbound states

Hydrogen atom

Hydrogen: bound state of an electron and proton

$$q_e = -e \qquad q_p = +e$$

$$m_e \cong 0.5 \frac{\text{MeV}}{c^2} \qquad M_p \cong 1 \frac{\text{GeV}}{c^2} = 2000\, m_e$$

$$\Rightarrow \text{reduced mass } \mu = \frac{m_e M_p}{m_e + M_p} \approx \frac{m_e M_p}{M_p} = m_e$$

Center of mass essentially at proton

Relative coordinate Hamiltonian ≈ Electron Hamiltonian with proton fixed at the origin

$$\hat{H} \cong \frac{\hat{P}_r^2}{2m_e} + \frac{\hat{L}^2}{2m_e \hat{r}^2} - \frac{e^2}{\hat{r}}$$

Bound state $\quad \hat{H}|\psi\rangle = -E_b |\psi\rangle$

binding energy

$$\psi(r,\theta,\phi) = R_\ell(r)\, Y_\ell^m(\theta,\phi)$$

Radial equation for reduced radial wave function

$$u_\ell(r) \equiv r R_\ell(r)$$

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m_e}\frac{d^2 u_\ell}{dr^2} + \left(\frac{\hbar^2 \ell(\ell+1)}{2m_e r^2} - \frac{e^2}{r}\right) u_\ell = -E_b u_\ell}$$

The solutions to this equation yield the spectrum of Hydrogen, one the first great successes of the Schrödinger equation. We will study its solutions in the next lecture