QM Helium&Scatter Feb13

Helium Atom Cleanup

Hamiltonian:

$$H = H_1 + H_2 + H_{12}$$

We have our trial wave function

$$\Psi(\vec{r}_1\sigma_1, \vec{r}_2\sigma_2) = \Phi(\vec{r}_1\vec{r}_2)\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

We said a natural choice for $\Phi(r_1, r_2) = \psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2) = \frac{Z'^3}{\pi a_0^3}e^{-Z(r_1+r_2)/a_0}$
Where Z' is a variational parameter.

check $\langle\Psi|\Psi\rangle = 1$

$$\begin{aligned}\epsilon &= \langle\Phi|(H_1 + H_2 + H_{12})|\Phi\rangle \\ &= \int\int \Phi^*(\vec{r}_1, \vec{r}_2)\left[\left(\frac{\hbar^2}{2m}(\nabla_1^2 - \nabla_2^2)\right) + \left(-\frac{2e^2}{r_1} - \frac{2e^2}{r_2}\right) + \left(\frac{e^2}{r_{12}}\right)\right]\Phi(\vec{r}_1, \vec{r}_2)\, dr_1\, dr_2\end{aligned}$$

How to do this integral?
See Sakurai section 7.4

It turns our the first two terms in the brackets are easy, while the last term is difficult. This is because for the first two terms, the two variables are completely separable.

For the third term, we will need to use

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1r_2\cos\gamma}} = \sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}P_l(\cos\gamma)$$

Just do the integral, and we should have the answer

$$\epsilon = \left(\frac{e^2}{a_0}\right)\left[2\cdot\frac{Z'^2}{2} - 2\cdot 2Z' + \frac{5}{8}Z'\right]$$

Optimal value of Z'^* is given by

$$\frac{\partial\epsilon}{\partial Z'^*} = 0 \implies Z'^* = 2 - \frac{5}{16}$$

Note that our optimal $Z' < 2$. This is physical because one of the electron "shields" the other electron from the nucleus.

Best variational estimate of the ground state energy of the helium atom

$$\epsilon(Z'^{*}) \approx -77.5\mathrm{eV}$$

The experimental value (double ionization)

$$E_0 = -78.6\mathrm{eV}$$

Note that $\epsilon(Z') \geq E_0$. This is a constraints for variational method.

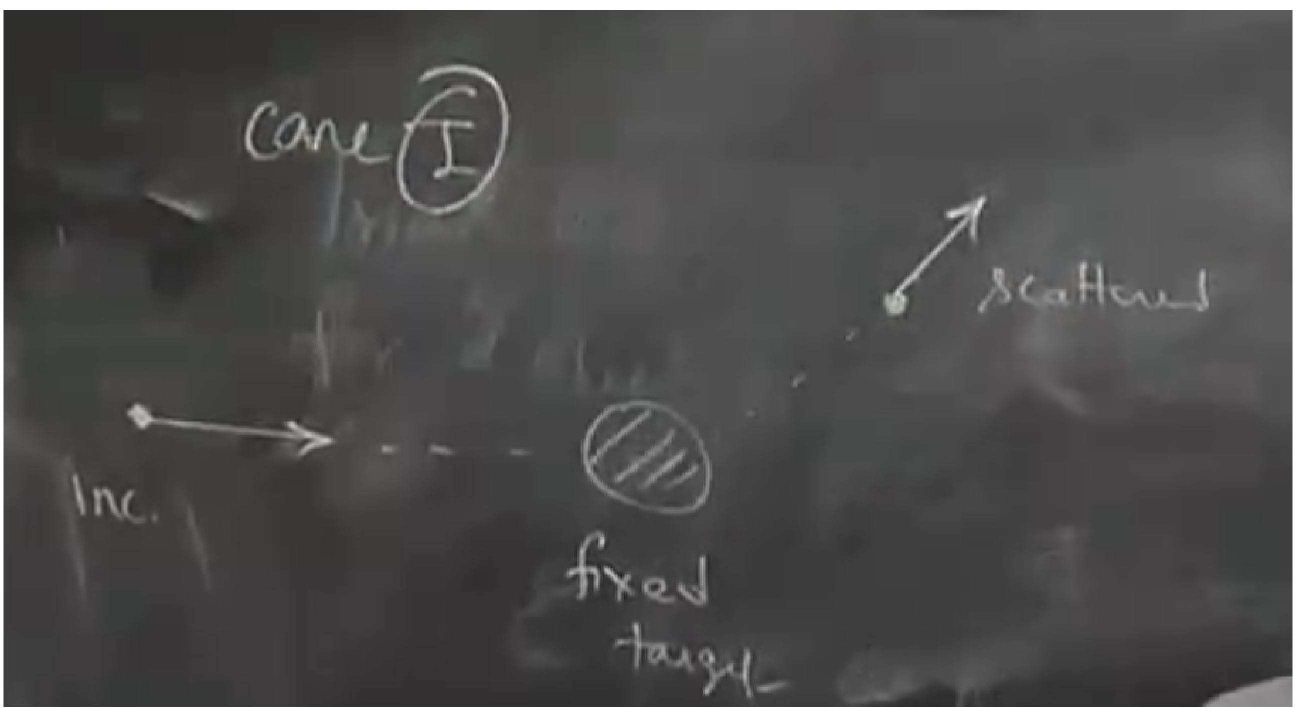
Scattering

Assumptions:

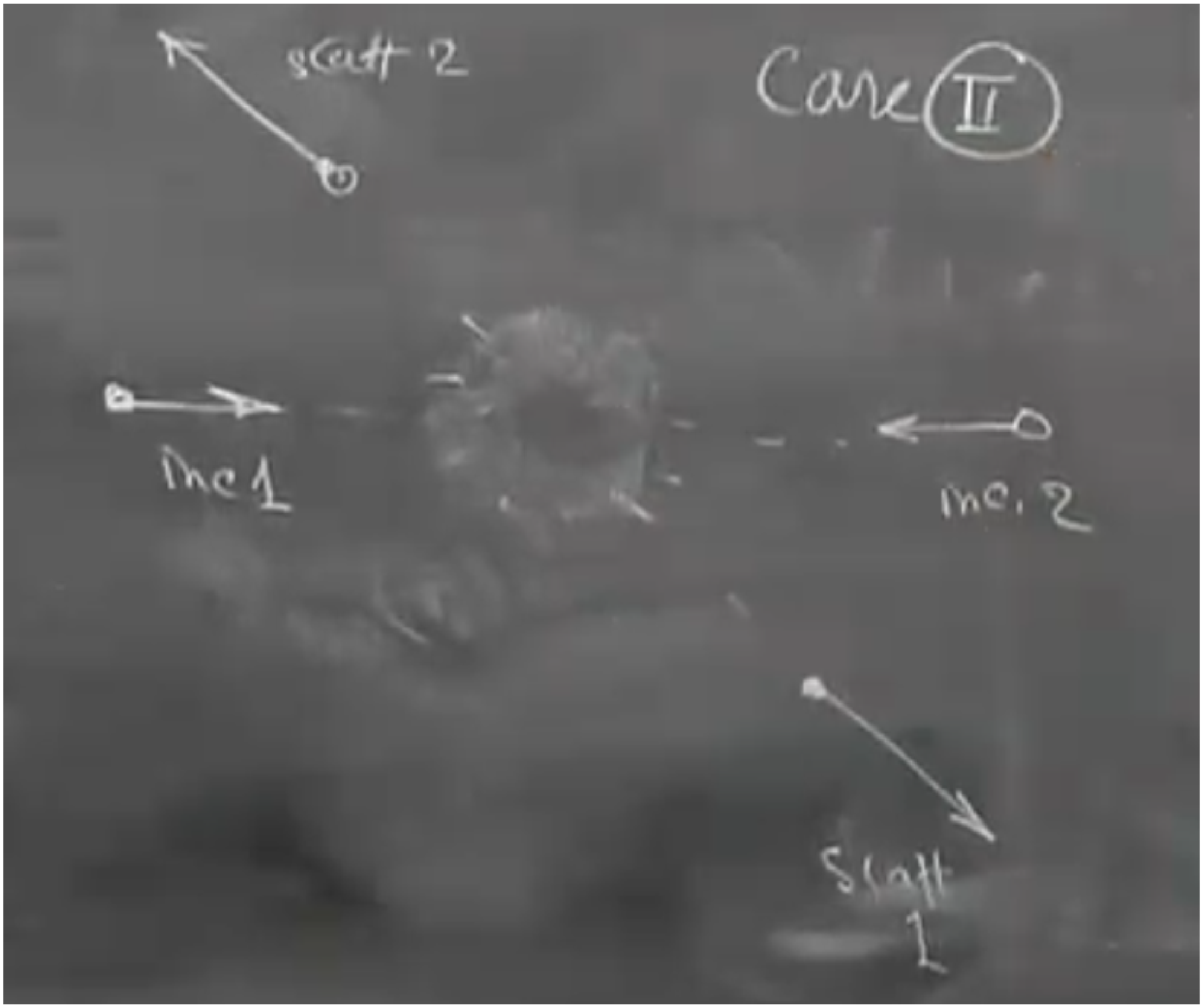
1. We assumes collisions are none-relativistic
2. Elastic Scattering
3. No new particle created

The geometry of the scattering:

- Cast I



- Case 2



With the assumptions above, case 2 can be reduced to case 1.

Case 2:

$$H = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\vec{r}_1 - \vec{r}_2) \qquad \text{(Lab Frame)}$$

We can change this to center of mass coordiate

$$\vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}$$
$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$M = m_1 + m_2$$
$$m = \frac{m_1 m_2}{m_1 + m_2}$$

This gives

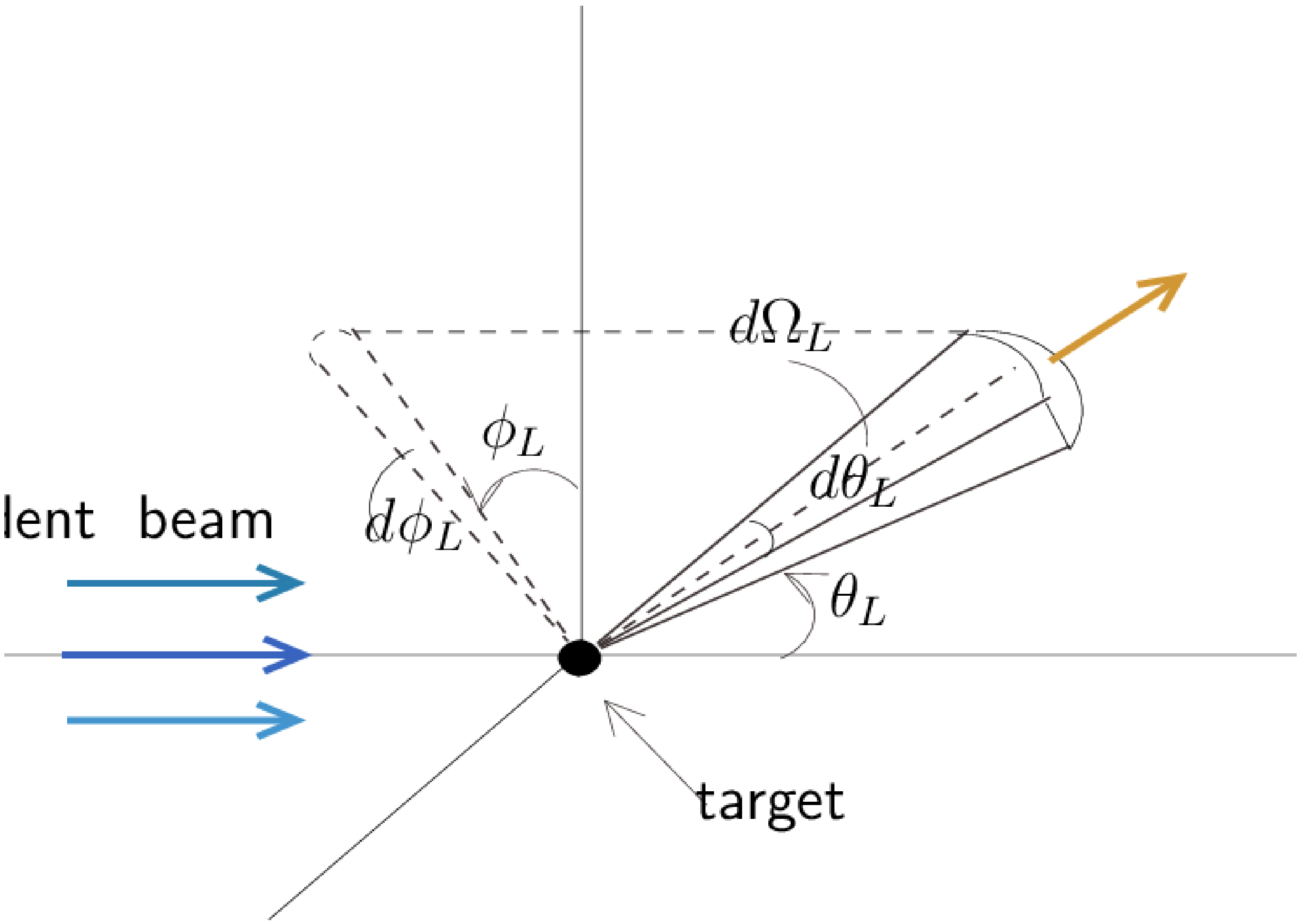
$$H = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2m}\nabla_r^2 + V(\vec{r}) \qquad \text{(CoM frame)}$$

where

$$\Psi(\vec{r}_1, \vec{r}_2) = \Phi_{cm}(\vec{R})\psi(\vec{r})$$

Because we can always use this transformation, we can focus on case one.

Scattering crosssestion



The incident Flux $\vec{J}_{inc} = J_{inc}\hat{z}$, $J = \text{number of particle per unit area per unit time}$
The dector distance r away measures # of particles scattered into the detector per unit time
measurement $= J_{inc}\sigma(\theta,\phi)d\Omega$ where $\sigma(\theta,\phi)$ is the definition of the scattering cross section.
Note: some book call $\sigma(\theta,\phi) \leftrightarrow \frac{d\sigma(\theta,\phi)}{d\Omega}$. It is crucial to realize $[\sigma(\theta,\phi)] = L^2$

Scattering flux into detector $J_{scatt} = \frac{\#\text{of particle per unit time}}{\text{Area of detector}} = \frac{J_{inc}\sigma(\theta,\phi)}{r^2 d\Omega}$
$\implies \sigma(\sigma,\phi) = \frac{r^2 J_{scatt}}{J_{inc}}$