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

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

\frac{1}{r{12}}=\frac{1}{\sqrt{ r{1}^2 +r{2}^2 - 2r{1}r{2}\cos \gamma}}=
\sum{l=0}^\infty \frac{r{<}^l}{r{>}^{l+1}}P_{l}(\cos \gamma)

$$Justdotheintegral, andweshouldhavetheanswer$$

\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 th electron "sheilds" the other electron from nucleus.

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

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

The experimental value (double ionization)

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

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

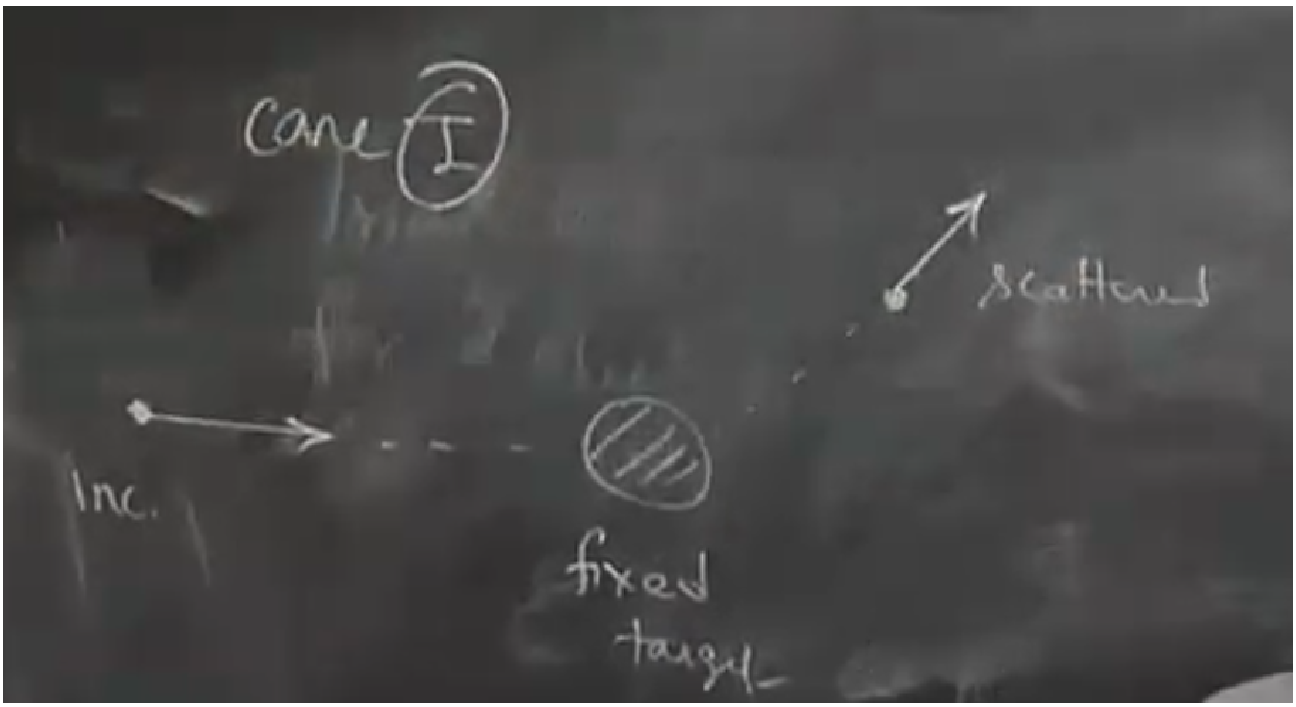
# Scattering

## Assumptions:

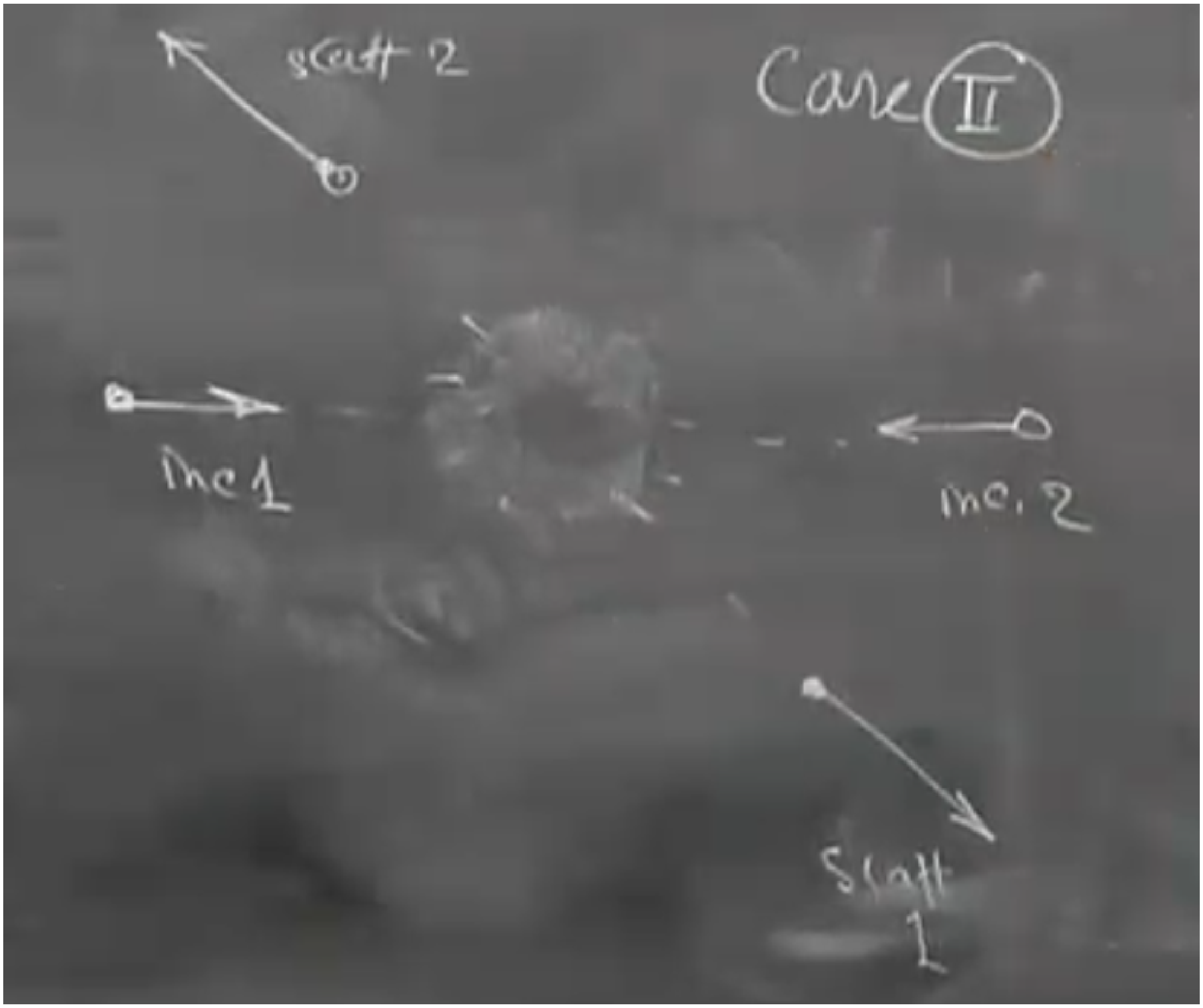
1. We assumes collisions are none-relativistic
2. Elatistic Scattering
3. No new particle created

The geometry of the scattering:

- Cast I



- Case 2




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

Cast 2:

$$H = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\vec{r}_1-\vec{r}_2) \$\$ We can change this to center of mass coord$$

\begin{align}
\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}}
\end{align}

$$This gives$$

H = -\frac{\hbar^2}{2M}\nabla{R}^2-\frac{\hbar^2}{2m}\nabla{r}^2+V(\vec{r})
\tag{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 ![[