Computational Physics

Lecture-13

M. Reza Mozaffari

Physics Group, University of Qom

Contents

- Basis Concepts
- Numerical Differentiation
- Numerical Integration
- Numerical Finding Root
- Classical Scattering

Classical Scattering

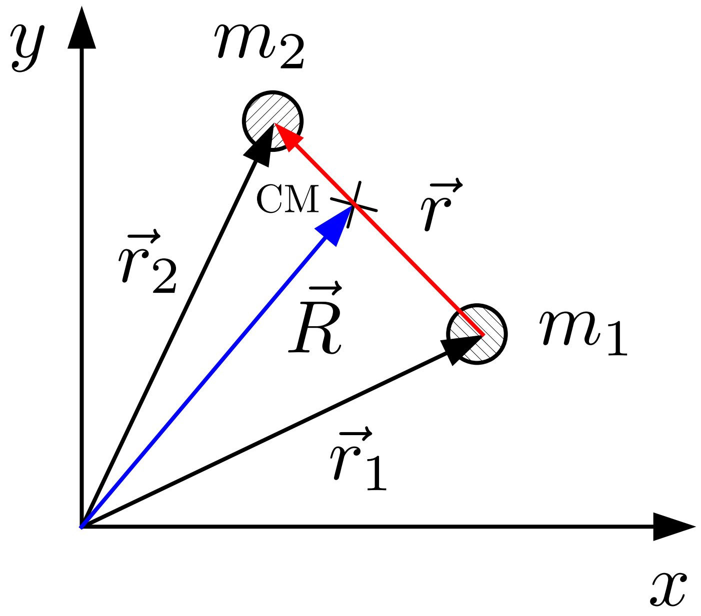
- **Central Forces**

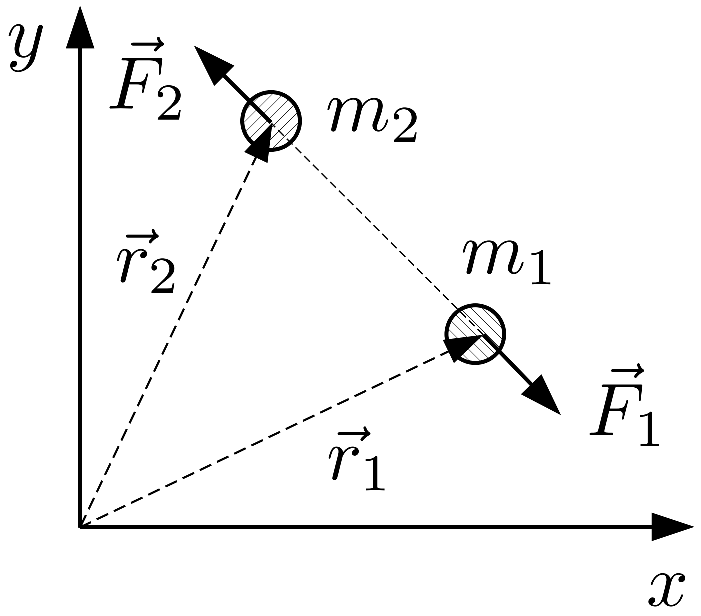
$$\begin{cases} \vec{r} = \vec{r}_2 - \vec{r}_1 \\ (m_1 + m_2)\vec{R} = m_1\vec{r}_1 + m_2\vec{r}_2 \end{cases}$$

$$\begin{cases} \vec{r}_1 = -\dfrac{\mu}{m_1}\vec{r} + \vec{R} \\ \vec{r}_2 = +\dfrac{\mu}{m_2}\vec{r} + \vec{R} \end{cases}$$

$$M = m_1 + m_2$$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$





$$\begin{cases} \vec{F}_1 = m_1 \dfrac{\mathrm{d}^2\vec{r}_1}{\mathrm{d}t^2} \\ \vec{F}_2 = m_2 \dfrac{\mathrm{d}^2\vec{r}_2}{\mathrm{d}t^2} \end{cases}$$

$$\vec{F}_2 = -\vec{F}_1 = \vec{F}(\vec{r})$$

Classical Scattering

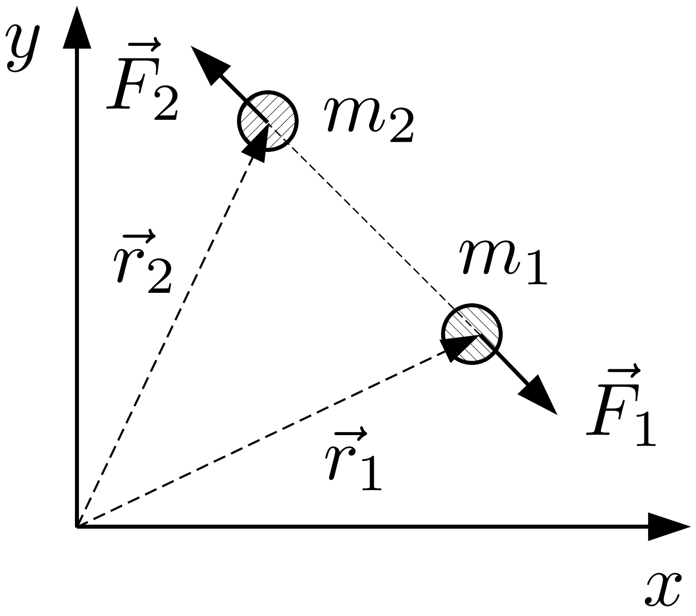
- **Central Forces**

$$\begin{cases} \vec{r}_1 = -\dfrac{\mu}{m_1}\vec{r} + \vec{R} \\ \vec{r}_2 = +\dfrac{\mu}{m_2}\vec{r} + \vec{R} \end{cases}$$

$$M = m_1 + m_2$$

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$\begin{cases} \vec{F}_2 = \mu\dfrac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} + m_2\dfrac{\mathrm{d}^2\vec{R}}{\mathrm{d}t^2} \\ \vec{F}_2 = \vec{F}(\vec{r}) = F(\vec{r})\hat{e}_r \end{cases}$$



$$\vec{F}_1 = m_1\frac{\mathrm{d}^2\vec{r}_1}{\mathrm{d}t^2}$$

$$\vec{F}_2 = m_2\frac{\mathrm{d}^2\vec{r}_2}{\mathrm{d}t^2}$$

$$\vec{F}_2 = -\vec{F}_1 = \vec{F}(\vec{r})$$

$$F(\vec{r})\hat{e}_r = \mu\frac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} + m_2\frac{\mathrm{d}^2\vec{R}}{\mathrm{d}t^2}$$

$$\begin{cases} F(\vec{r})\hat{e}_r = \mu\dfrac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} \\ \dfrac{\mathrm{d}^2\vec{R}}{\mathrm{d}t^2} = 0 \end{cases}$$

Classical Scattering

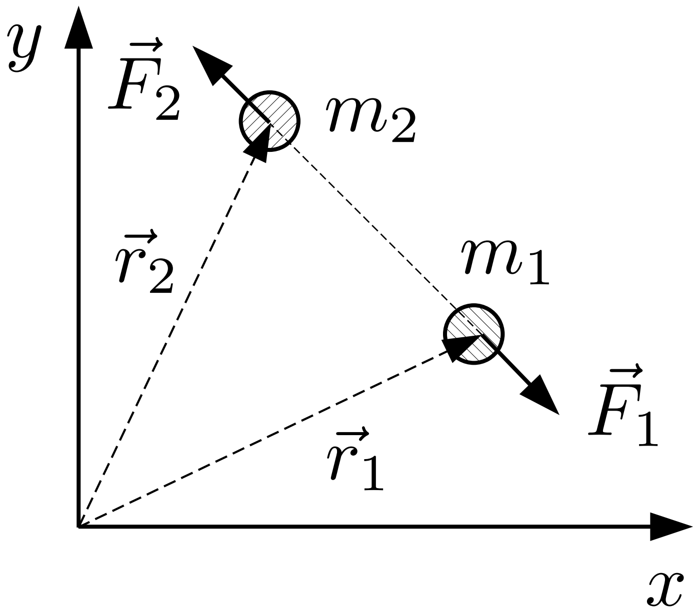
- Central Forces

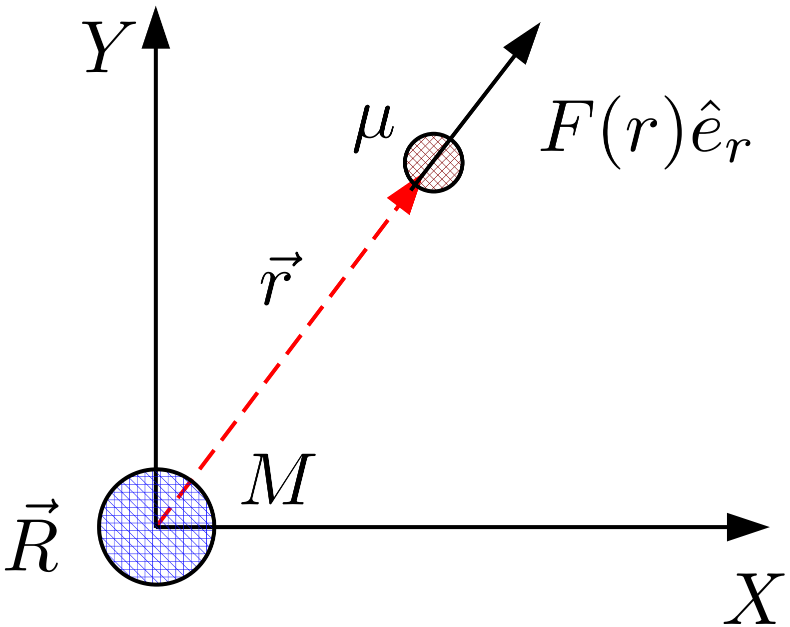
$$\begin{cases} \vec{F}_1 = m_1 \dfrac{\mathrm{d}^2\vec{r}_1}{\mathrm{d}t^2} \\ \vec{F}_2 = m_2 \dfrac{\mathrm{d}^2\vec{r}_2}{\mathrm{d}t^2} \end{cases}$$

$$\begin{cases} F(\vec{r})\hat{e}_r = \mu \dfrac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} \\ \dfrac{\mathrm{d}^2\vec{R}}{\mathrm{d}t^2} = 0 \end{cases}$$

Here, we have assumed that

$$\vec{V} = \frac{\mathrm{d}\vec{R}}{\mathrm{d}t} = 0$$



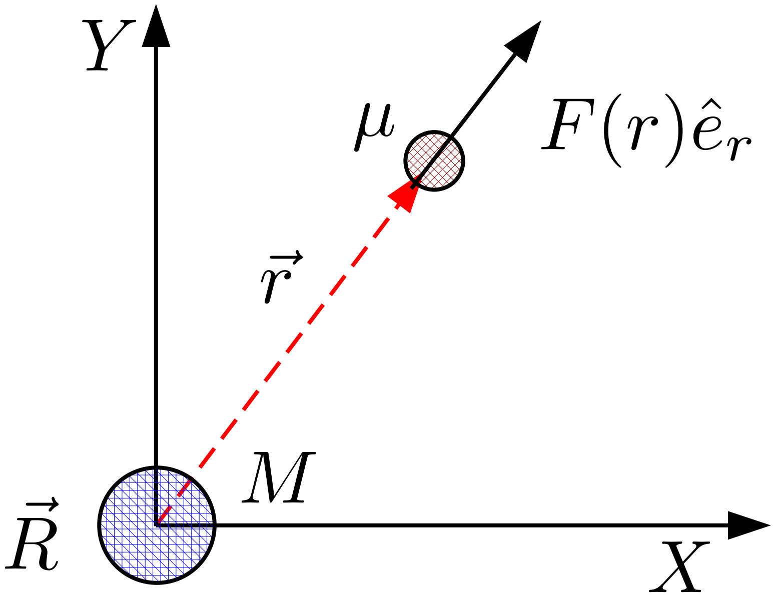


Classical Scattering

- **Central Forces**

$$\begin{cases} F(\vec{r})\hat{e}_r = \mu \dfrac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} \\ \dfrac{\mathrm{d}^2\vec{R}}{\mathrm{d}t^2} = 0 \end{cases}$$

$$\begin{cases} \vec{r} = r\hat{e}_r, \quad \dfrac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \dot{r}\hat{e}_r + r\dot{\phi}\hat{e}_\phi \\ \dfrac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} = (\ddot{r} - r\dot{\phi}^2)\hat{e}_r + (2\dot{r}\dot{\phi} + r\ddot{\phi})\hat{e}_\phi \end{cases}$$



$$\begin{cases} \mu(\ddot{r} - r\dot{\phi}^2) = F(r) \\ \mu(2\dot{r}\dot{\phi} + r\ddot{\phi}) = 0 \end{cases}$$

$$\xRightarrow{\times r} \mu(2\dot{r}\dot{\phi} + r\ddot{\phi}) = 0 \Rightarrow \mu(2r\dot{r}\dot{\phi} + r^2\ddot{\phi}) = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mu r^2\dot{\phi}) = 0$$

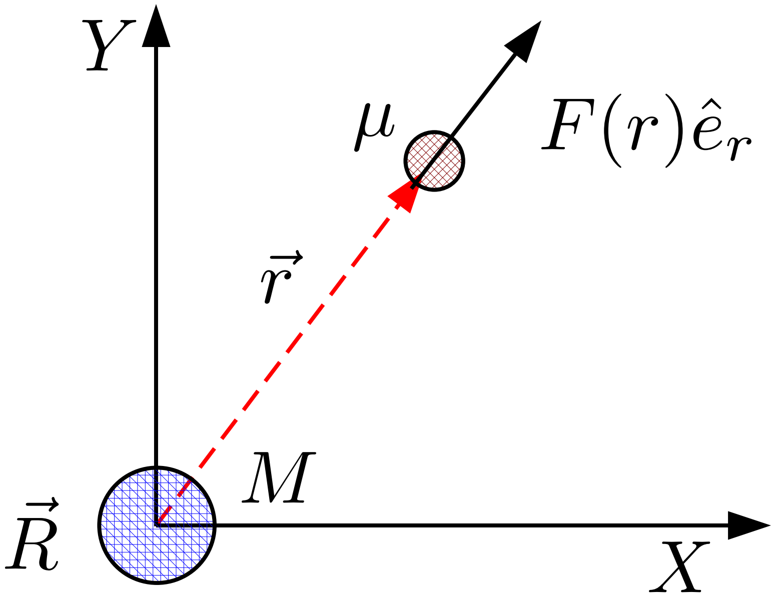
Classical Scattering

- **Central Forces**

$$\begin{cases} \mu(\ddot{r} - r\dot{\phi}^2) = F(r) \\ \dfrac{\mathrm{d}}{\mathrm{d}t}(\mu r^2 \dot{\phi}) = 0 \end{cases}$$

$$\begin{cases} \vec{L} = \mu \vec{r} \times \vec{v} = \mu r^2 \dot{\phi} \hat{z} = L_z = l \\ \dfrac{\mathrm{d}}{\mathrm{d}t}(\mu r^2 \dot{\phi}) = 0 \end{cases} \Rightarrow l = \mu r^2 \dot{\phi}$$

Conservation of angular momentum



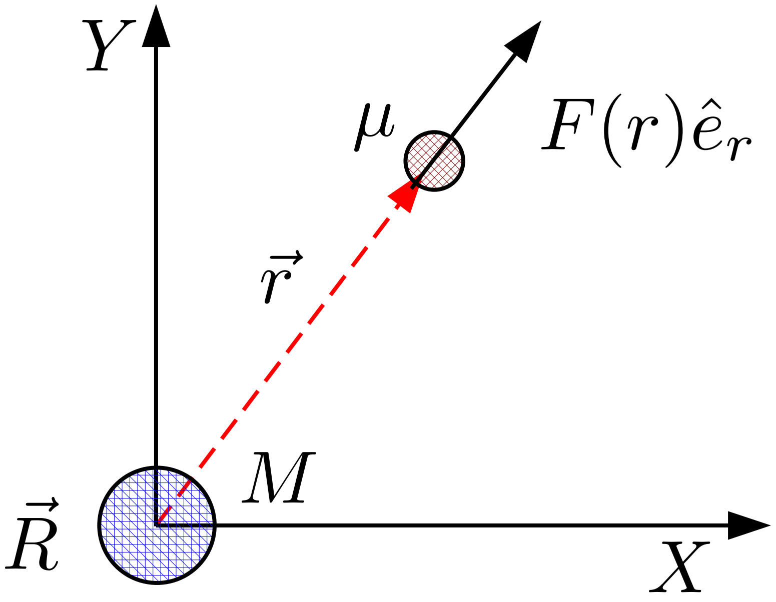
$$\begin{cases} \mu(\ddot{r} - r\dot{\phi}^2) = F(r) \Rightarrow \mu\ddot{r} = F(r) + \mu r \dot{\phi}^2 \\ l = \mu r^2 \dot{\phi} \Rightarrow \dot{\phi} = \dfrac{l}{\mu r^2} \end{cases}$$

$$\mu\ddot{r} = F(r) + \frac{l^2}{\mu r^3}$$

Classical Scattering

- **Central Forces**

$$\begin{cases} \mu\ddot{r} = F(r) + \dfrac{l^2}{\mu r^3} \\ \dot{\phi} = \dfrac{l}{\mu r^2} \end{cases}$$



$$E = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 + U(r)$$

$$\begin{cases} \vec{r}_1 = -\dfrac{\mu}{m_1}\vec{r} + \vec{R} \\ \vec{r}_2 = +\dfrac{\mu}{m_2}\vec{r} + \vec{R} \end{cases} \qquad \begin{cases} \vec{v}_1 = -\dfrac{\mu}{m_1}\vec{v} + \vec{V} \\ \vec{v}_2 = +\dfrac{\mu}{m_2}\vec{v} + \vec{V} \end{cases}$$

$$F(r) = -\frac{\mathrm{d}U}{\mathrm{d}r}$$

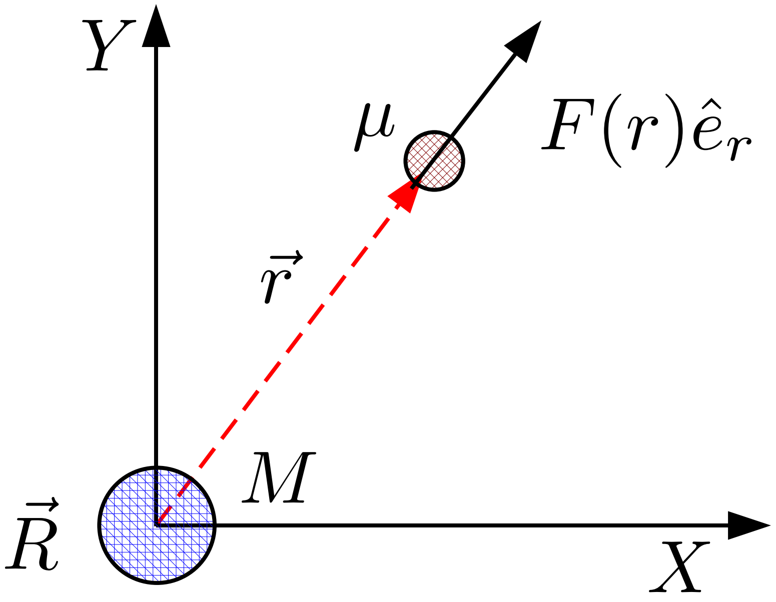
$$E = \frac{1}{2}MV^2 + \frac{1}{2}\mu v^2 + U(r)$$

$$\vec{V} = 0: \quad E = \frac{1}{2}\mu v^2 + U(r)$$

Classical Scattering

- **Central Forces**

$$\begin{cases} \mu\ddot{r} = F(r) + \dfrac{l^2}{\mu r^3} \\ \dot{\phi} = \dfrac{l}{\mu r^2} \end{cases}$$



$$E = \frac{1}{2}\mu v^2 + U(r)$$

$$\vec{r} = r\hat{r}, \qquad \frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = \dot{r}\hat{e}_r + r\dot{\phi}\hat{e}_\phi$$

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{1}{2}\mu r^2\dot{\phi}^2 + U(r)$$

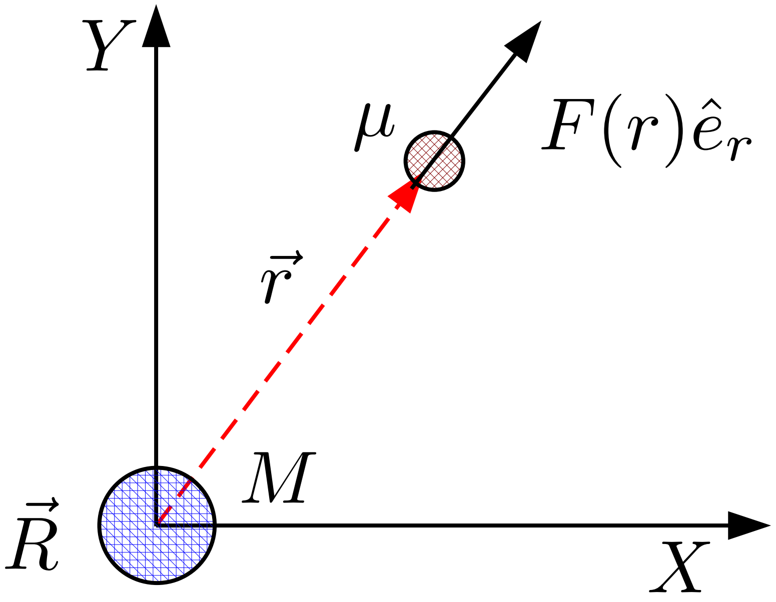
$$\Downarrow \quad \dot{\phi} = \frac{l}{\mu r^2}$$

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{l^2}{2\mu r^2} + U(r)$$

Classical Scattering

- **Central Forces**

$$\begin{cases} \mu\ddot{r} = F(r) + \dfrac{l^2}{\mu r^3} \\ \dot{\phi} = \dfrac{l}{\mu r^2} \end{cases}$$



$$E\left[r(t)\right] = \frac{1}{2}\mu\dot{r}^2 + \frac{l^2}{2\mu r^2} + U(r)$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = 0$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \mu\dot{r}\ddot{r} - \frac{l^2}{\mu r^3}\dot{r} + \frac{\mathrm{U(r)}}{\mathrm{d}r}\dot{r}$$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \dot{r}\left(\mu\ddot{r} - \frac{l^2}{\mu r^3} - F(r)\right) = 0$$

Conservation of total energy

Classical Scattering

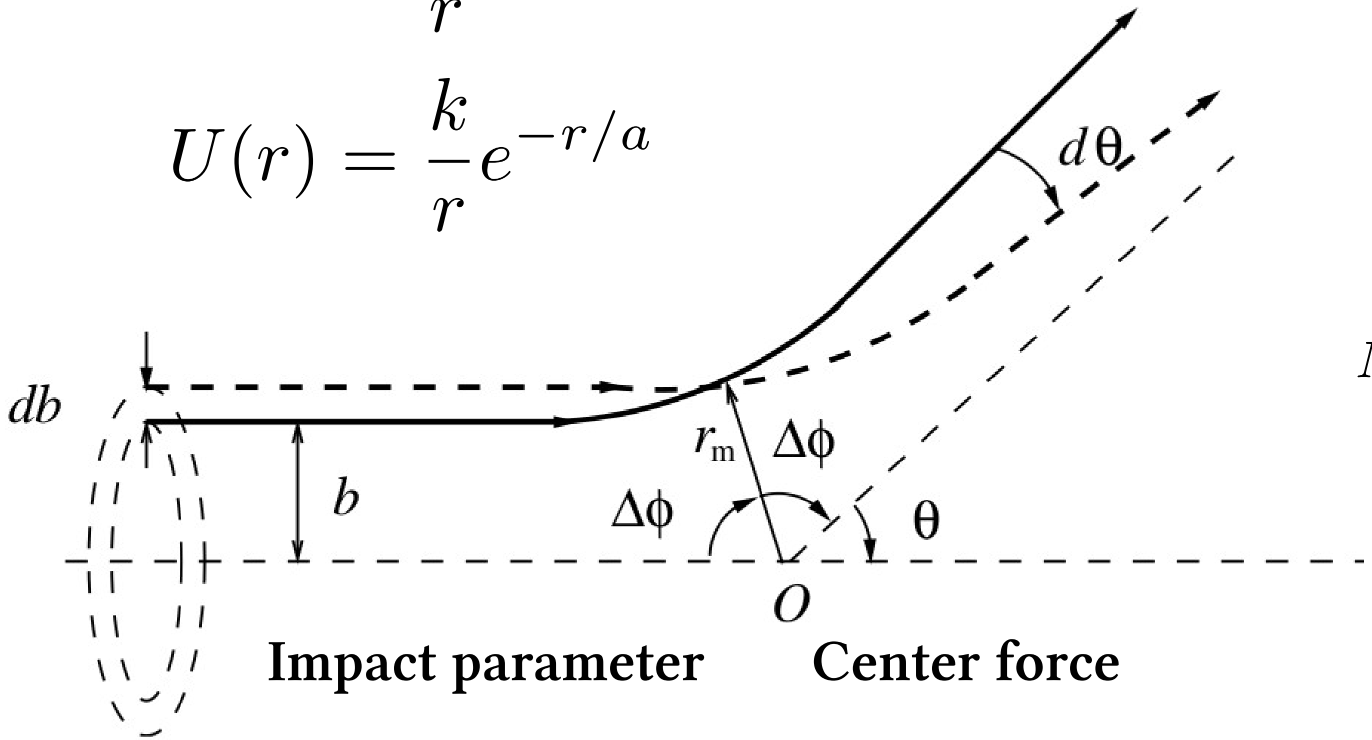
- **Cross section of scattering**

$$U(r) = \frac{k}{r} \qquad k > 0$$

$$U(r) = \frac{k}{r}e^{-r/a}$$

$$\begin{cases} \dot{\phi} = \dfrac{l}{\mu r^2} \\ E = \dfrac{1}{2}\mu \dot{r}^2 + \dfrac{l^2}{2\mu r^2} + U(r) \end{cases}$$

$$\lim_{M/m\to\infty} \mu = \lim_{M/m\to\infty} \frac{Mm}{M+m} \to m$$



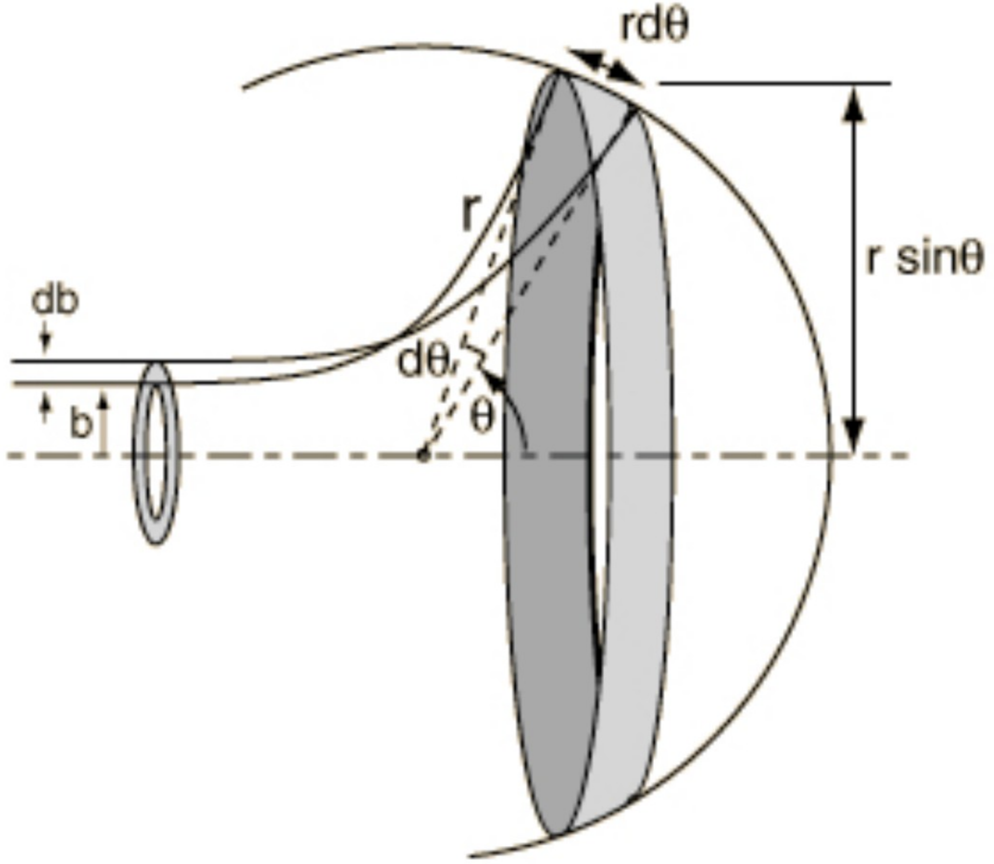
Impact parameter   Center force

$$r \to \pm\infty : \quad E = \frac{1}{2}mv_0^2$$

$$r \to \pm\infty : \quad l = mbv_0$$

Classical Scattering

- **Cross section of scattering**



- The number of particles scattered per unit time between θ and $\theta + \mathrm{d}\theta$ is equal to the number incident particles per unit time between b and $b + \mathrm{d}b$.

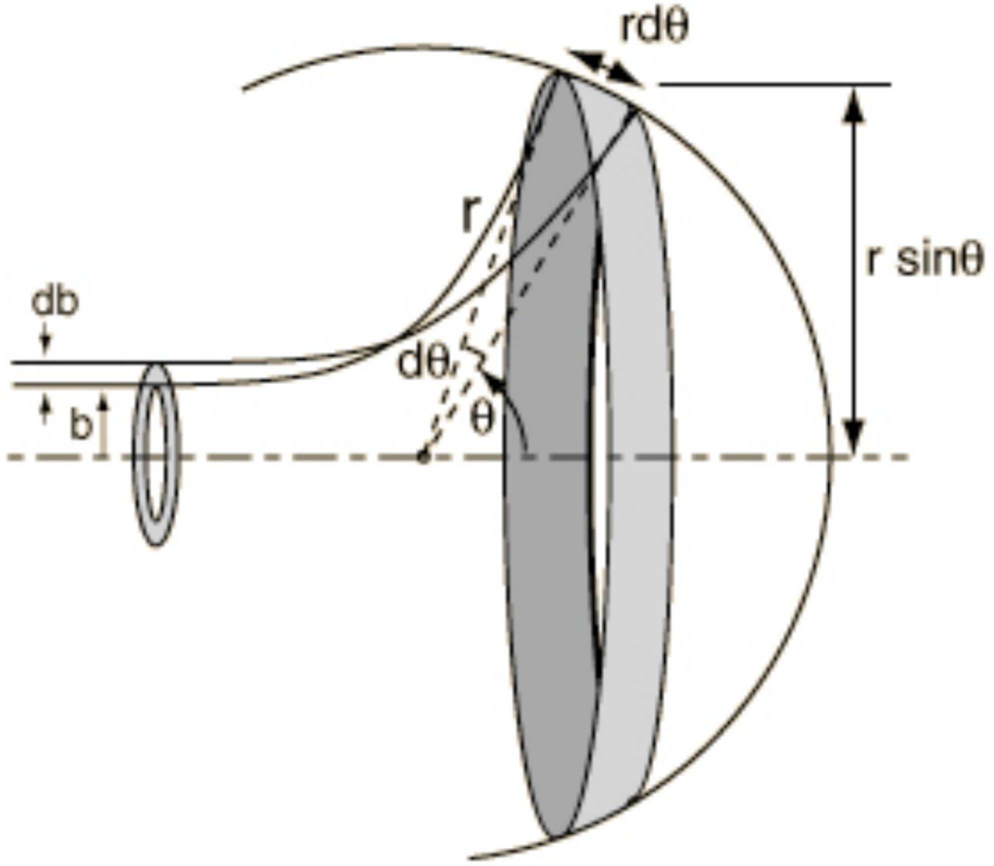
- For incident flux Φ, the number of particles scattered into the solid angle $\mathrm{d}\Omega = 2\pi \sin\theta \mathrm{d}\theta$ per unit time is given by

$$N \mathrm{d}\Omega = N 2\pi \sin\theta \mathrm{d}\theta = 2\pi b \mathrm{d}b \Phi$$

$$\frac{N}{\Phi} = \frac{b}{\sin\theta} \left| \frac{\mathrm{d}b}{\mathrm{d}\theta} \right|$$

Classical Scattering

- **Cross section of scattering**



$$\begin{cases} \dfrac{N}{\Phi} = \dfrac{b}{\sin\theta}\left|\dfrac{\mathrm{d}b}{\mathrm{d}\theta}\right| \\ \dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \dfrac{N}{\Phi} \end{cases} \Longrightarrow \boxed{\dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \dfrac{b}{\sin\theta}\left|\dfrac{\mathrm{d}b}{\mathrm{d}\theta}\right|}$$

For classical Coulomb scattering,

$$U(r) = \frac{k}{r}$$

particle follows hyperbolic trajectory. In this case, a straightforward calculation obtains the Rutherford formula:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right| = \frac{k^2}{16E^2}\frac{1}{\sin^4\theta/2}$$

Classical Scattering

- **Cross section of scattering**

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

$$\begin{cases} \dot{\phi} = \dfrac{l}{mr^2} \\ E = \dfrac{1}{2}m\dot{r}^2 + \dfrac{l^2}{2mr^2} + U(r) \\ r \to \pm\infty : \quad E = \dfrac{1}{2}mv_0^2 \\ r \to \pm\infty : \quad l = mbv_0 \end{cases}$$

$$\frac{1}{2}m\dot{r}^2 + \frac{l^2}{2mr^2} + U(r) = E = \frac{1}{2}mv_0^2$$

$$\frac{1}{2}m\dot{r}^2 = E - \frac{l^2}{2mr^2} - U(r)$$

$$\frac{1}{2}m\dot{r}^2 = E\left(1 - \frac{l^2}{2Emr^2} - \frac{U(r)}{E}\right)$$

$$\frac{1}{2}m\dot{r}^2 = \frac{1}{2}mv_0^2\left(1 - \frac{b^2}{r^2} - \frac{U(r)}{E}\right)$$

$$\dot{r}^2 = v_0^2\left(1 - \frac{b^2}{r^2} - \frac{U(r)}{E}\right)$$

$$\dot{r} = \pm v_0\sqrt{1 - \frac{b^2}{r^2} - \frac{U(r)}{E}}$$

Classical Scattering

- **Cross section of scattering**

$$\begin{cases} \dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \dfrac{b}{\sin\theta}\left|\dfrac{\mathrm{d}b}{\mathrm{d}\theta}\right| \\ \dot{\phi} = \dfrac{l}{mr^2} \\ \dot{r} = \pm v_0\sqrt{1 - \dfrac{b^2}{r^2} - \dfrac{U(r)}{E}} \\ l = mbv_0 \end{cases}$$

$$\dot{r} = \frac{\mathrm{d}r}{\mathrm{d}t} = \pm v_0\sqrt{1 - \frac{b^2}{r^2} - \frac{U(r)}{E}}$$

$$\dot{\phi} = \frac{\mathrm{d}\phi}{\mathrm{d}t} = \frac{l}{mr^2}$$

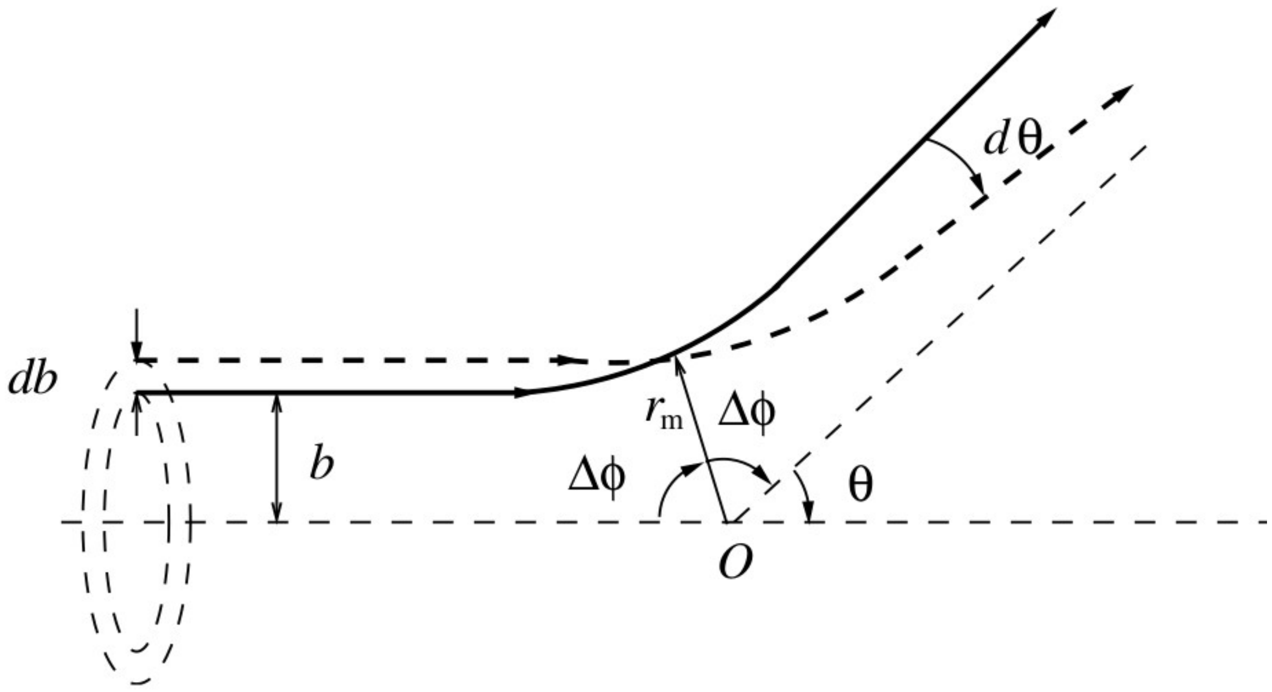
$$\frac{\dot{r}}{\dot{\phi}} = \frac{\mathrm{d}r}{\mathrm{d}\phi} = \pm\frac{mv_0 r^2\sqrt{1 - \frac{b^2}{r^2} - \frac{U(r)}{E}}}{l}$$

$$\frac{\mathrm{d}r}{\mathrm{d}\phi} = \pm\frac{r^2\sqrt{1 - \frac{b^2}{r^2} - \frac{U(r)}{E}}}{b}$$

Classical Scattering

- **Cross section of scattering**

$$
\begin{cases}
\dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \dfrac{b}{\sin\theta}\left|\dfrac{\mathrm{d}b}{\mathrm{d}\theta}\right| \\
\pm\dfrac{b}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}\mathrm{d}r = \mathrm{d}\phi
\end{cases}
$$



Deflection angle : $\theta = \pi - 2\Delta\phi$

$$
\Delta\phi = b\int_{r_m}^{\infty}\frac{\mathrm{d}r}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}} = -b\int_{\infty}^{r_m}\frac{\mathrm{d}r}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}
$$

$$
1-\frac{b^2}{r_m^2}-\frac{U(r_m)}{E} = 0
$$

Classical Scattering

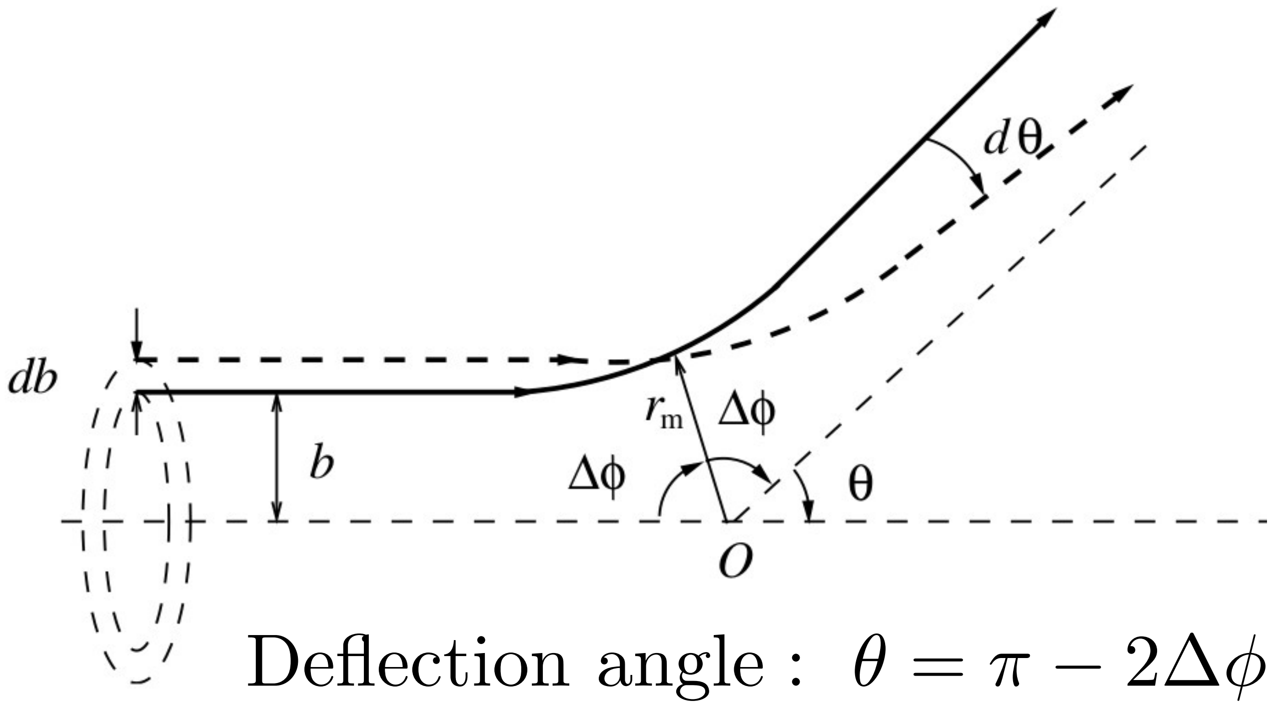
- **Cross section of scattering**

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

$$\Delta\phi = b\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}$$

$$1-\frac{b^2}{r_m^2}-\frac{U(r_m)}{E}=0$$

$$\pi = 2b\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}}}$$



Deflection angle : $\theta = \pi - 2\Delta\phi$

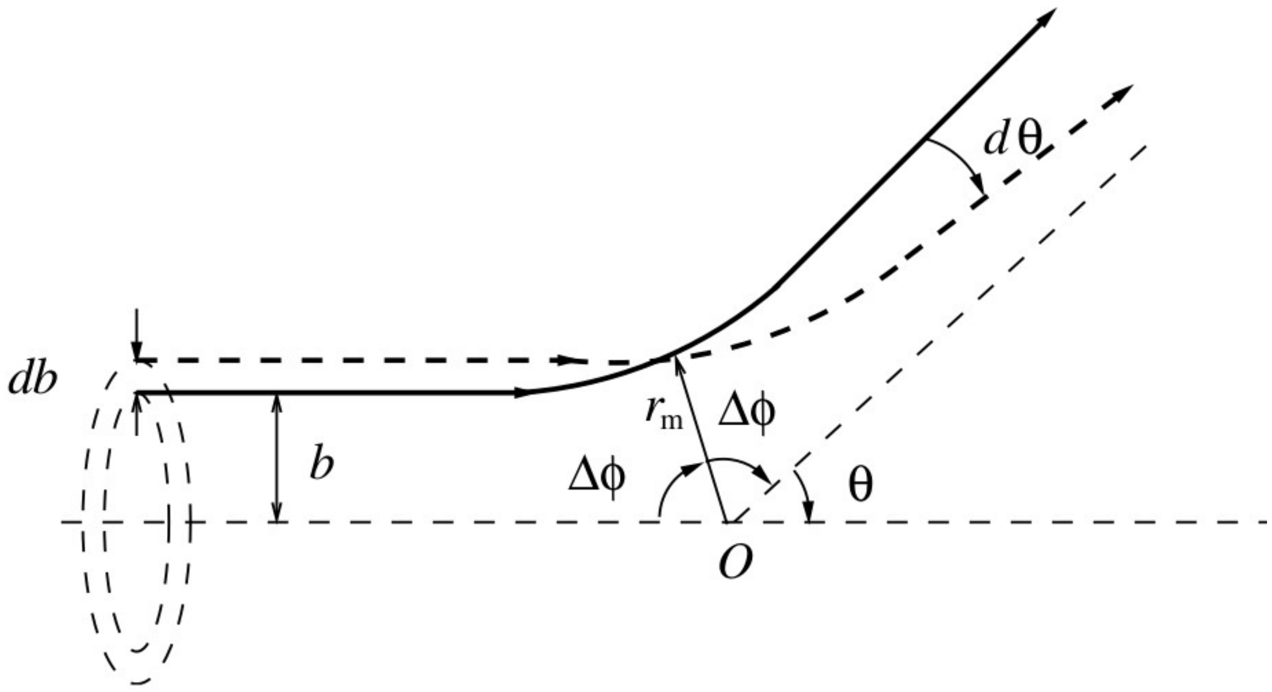
$$\theta = \pi - 2b\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}$$

$$\forall\, b \to r_m, \theta, \frac{d\sigma}{d\Omega}$$

Classical Scattering

- **Cross section of scattering**

$$\begin{cases} \dfrac{d\sigma}{d\Omega} = \dfrac{b}{\sin\theta}\left|\dfrac{db}{d\theta}\right| \\ \Delta\phi = b\displaystyle\int_{r_m}^{\infty} \dfrac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}} \\ 1-\dfrac{b^2}{r_m^2}-\dfrac{U(r_m)}{E}=0 \end{cases}$$



Deflection angle : $\theta = \pi - 2\Delta\phi$

Let $U(r) = 0 \Rightarrow \Delta\phi = \pi/2$

$$\pi/2 = b\int_{r_m}^{\infty} \frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}}} \Rightarrow \pi = 2b\int_{r_m}^{\infty} \frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}}}$$

Classical Scattering

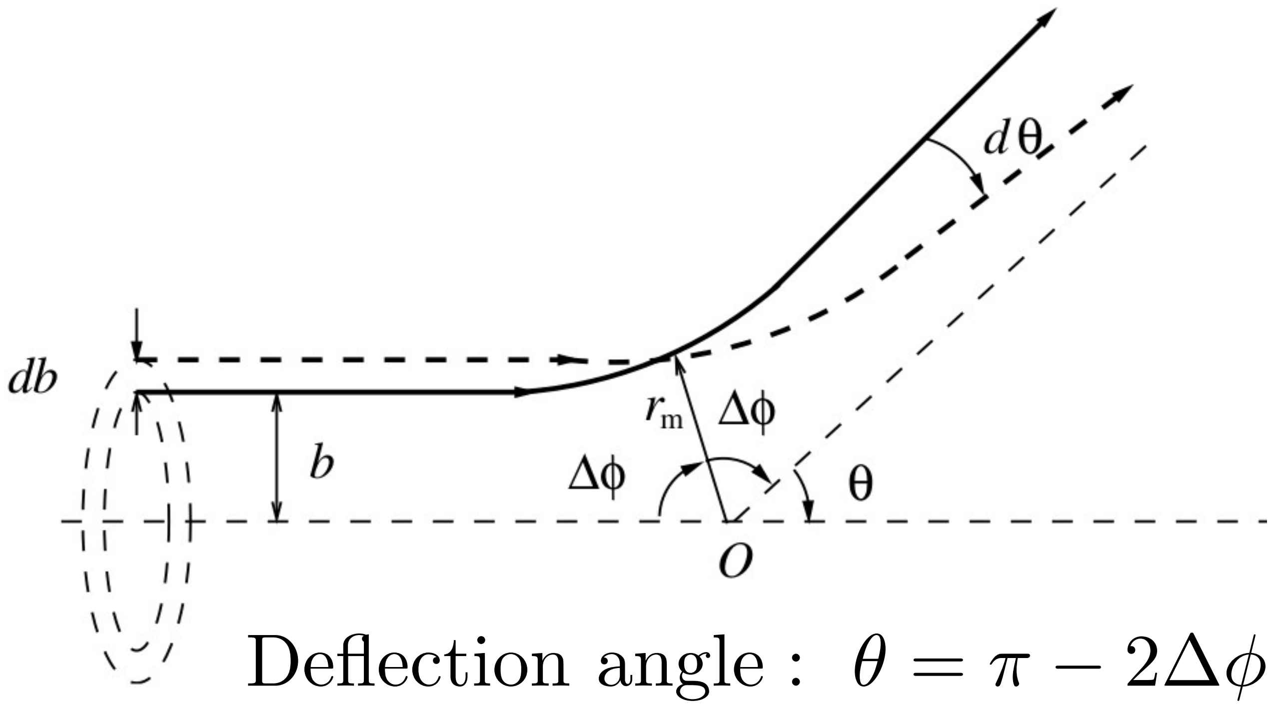
- **Cross section of scattering**

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

$$\Delta\phi = b\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}$$

$$1-\frac{b^2}{r_m^2}-\frac{U(r_m)}{E}=0$$

$$\pi = 2b\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}}}$$



Deflection angle : $\theta = \pi - 2\Delta\phi$

$$\theta = \pi - 2b\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}$$

$$\theta = 2b\left[\int_{b}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}}}-\int_{r_m}^{\infty}\frac{dr}{r^2\sqrt{1-\frac{b^2}{r^2}-\frac{U(r)}{E}}}\right]$$