Collision Kinematics

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Simple knowledge check:

- DPA stands for:
  1. Displacements per atom
  2. Damage per atom
  3. Displacement potential of an atom
  4. Down plane acceleration
- The energy transferred to a PKA can be calculated given:
  1. The mass and energy of the incident particle
  2. The velocity and angle of the particles
  3. The mass of the interacting particles, the scattering angle, and the initial energy of the incident particle
  4. The mass of the interacting particles, the incident angles, and the initial velocity of the incident particle
- Fluence is a good unit to determine the material damage due to radiation
  1. True
  2. False

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Outline

Interatomic potentials:

- Asymptotic energy
- Collision kinematics
- Scattering integral

Goal:

1. Describe a collision between any species
2. Develop the relationship between impact parameter and scattering angle
3. Find the distance of the closest approach as a function of potential

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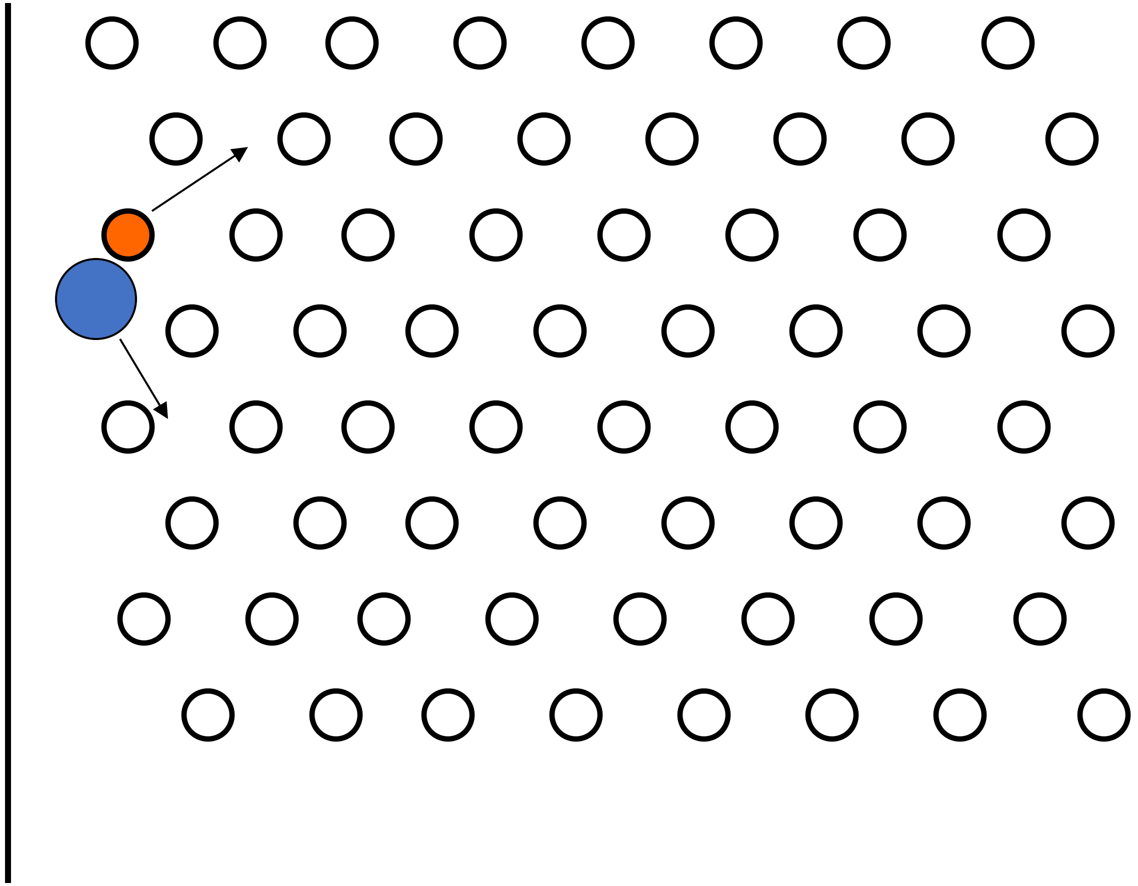
Radiation Damage: the basics

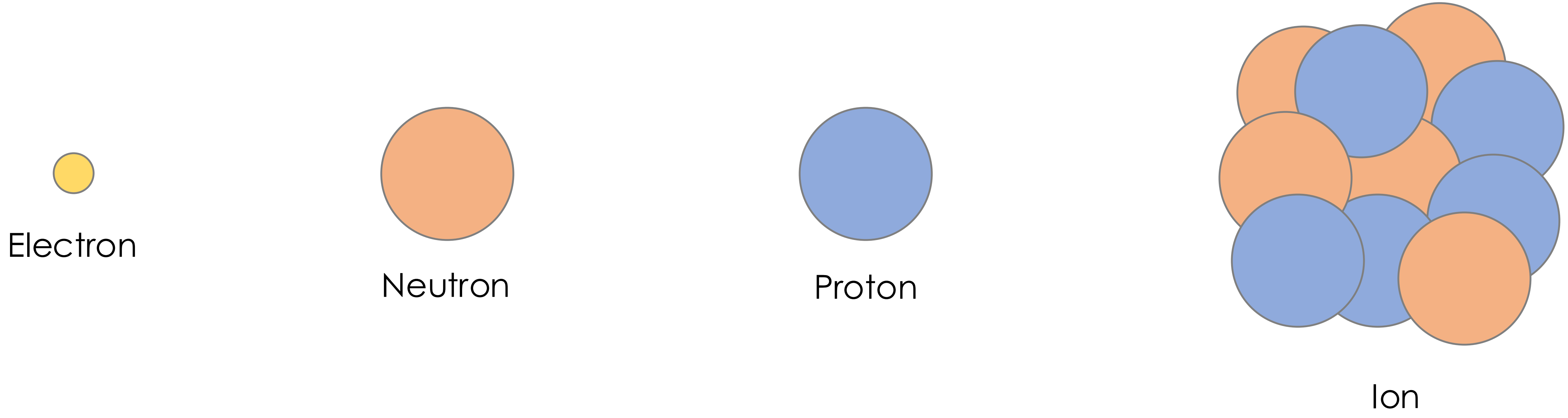
- All of radiation damage boils down to a common step: **collisions between energetic particles and atoms composing a material**

T=



Source: T.R. Allen

What's the difference?



Why is this difference important for radiation damage?

Collision kinematics

- Remember for neutron-atom collisions:

$$T = \frac{\gamma}{2} E_i (1 - \cos \phi)$$

- For ion-atom collisions, there are several differences
  1.
  2.
  3.

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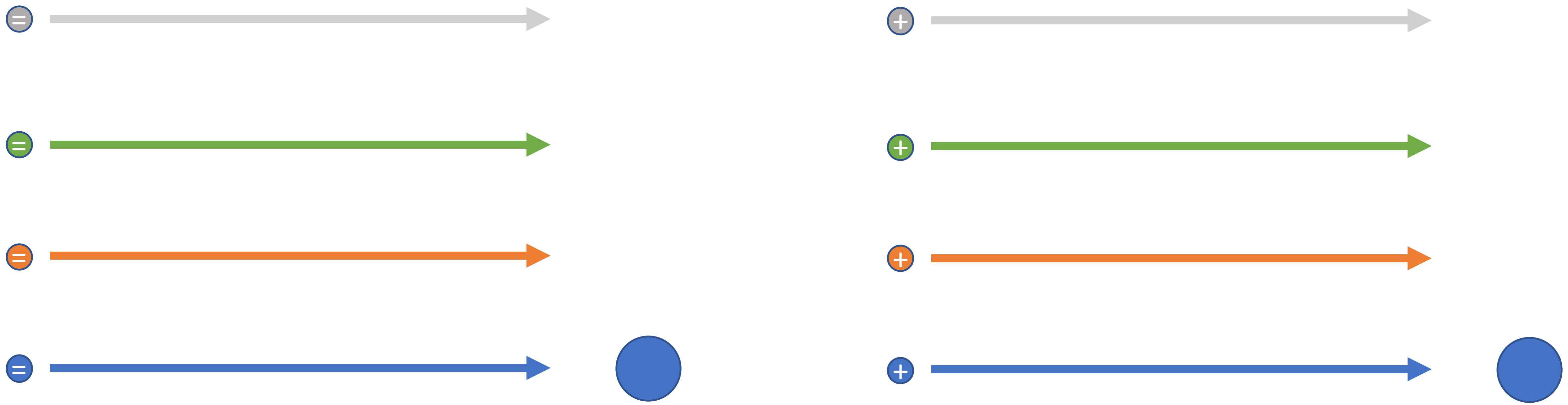
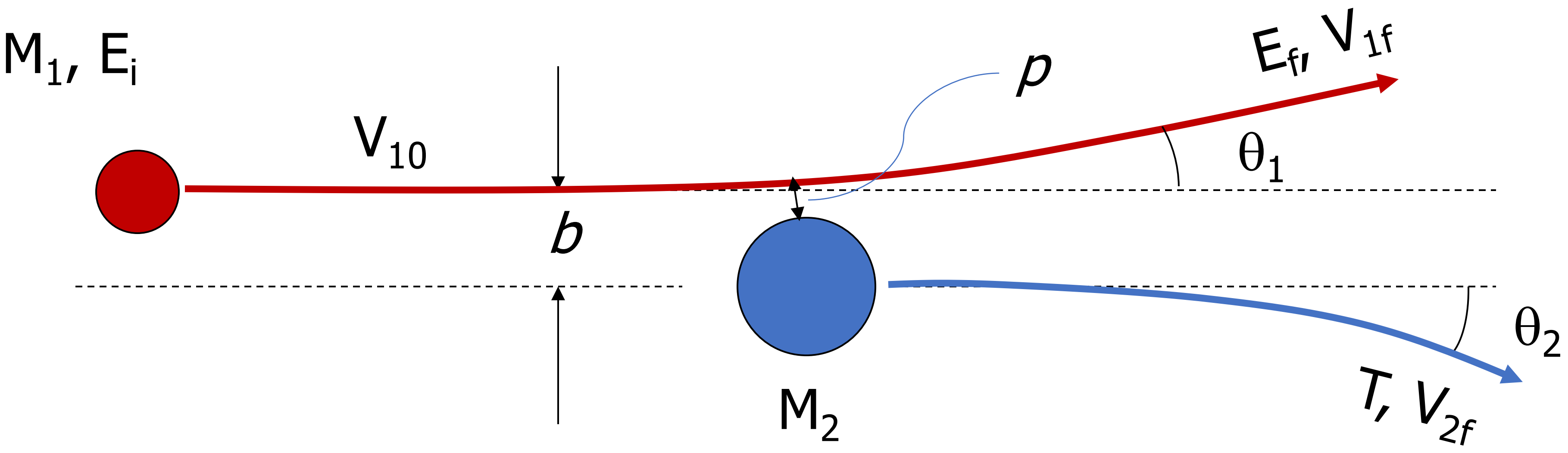
Simple thought experiment for ion-atom collisions

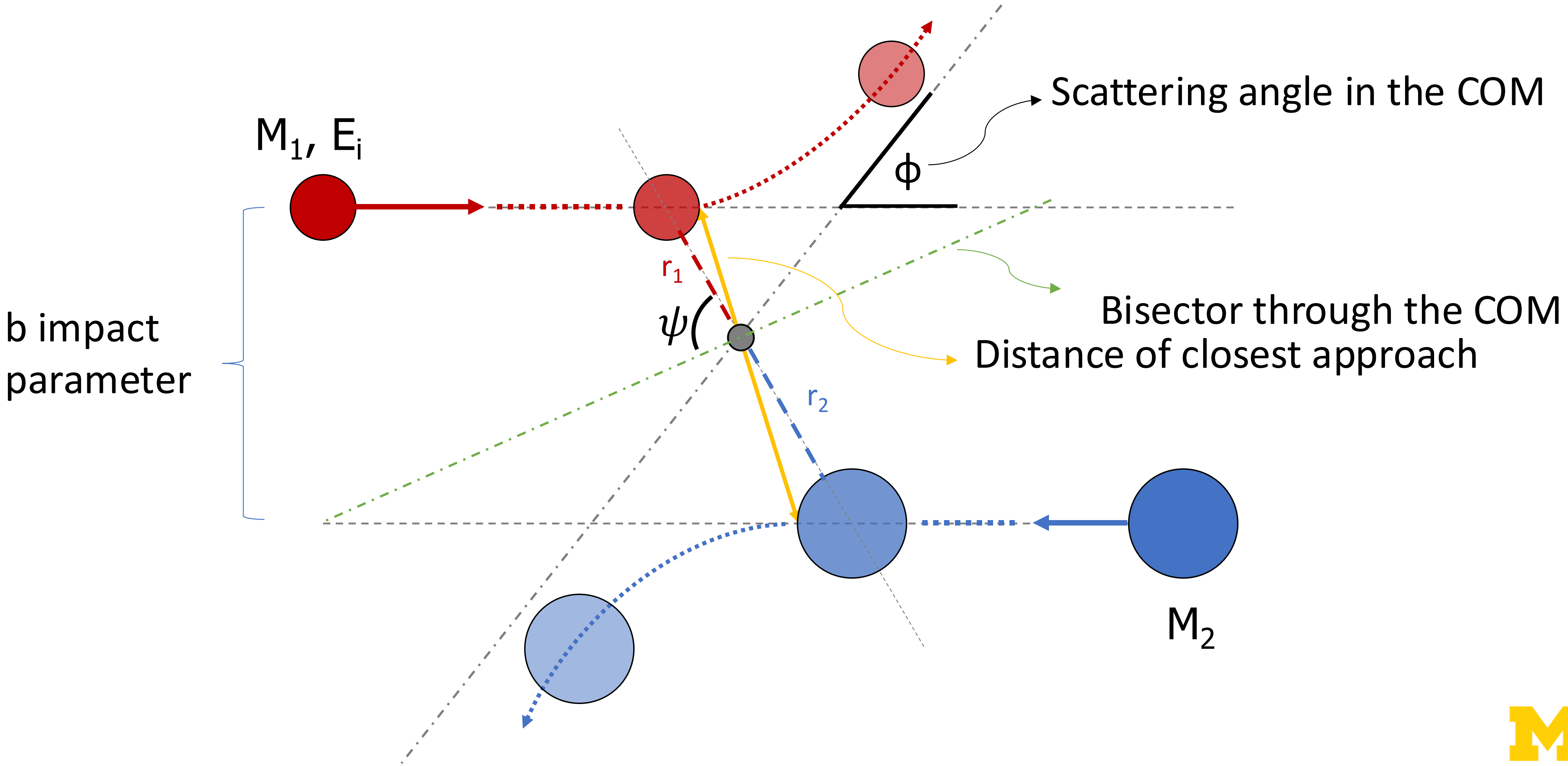


Collision kinematics (Lab Frame)

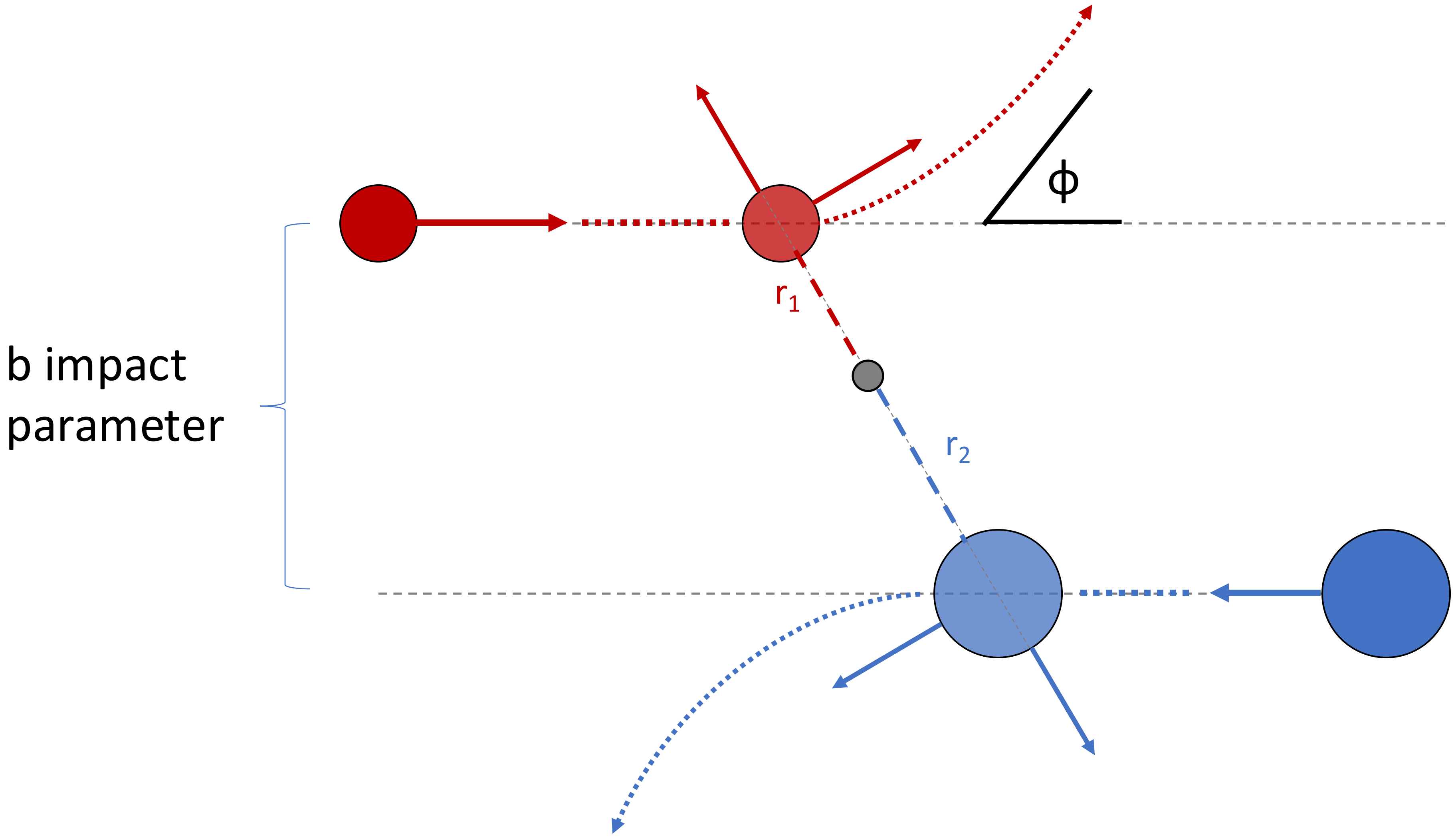


In lab frame of reference, it is clear that the resulting energy transferred, **<u>T</u>**, must be a function of the impact parameter, **<u>b</u>**

Collision kinematics (COM frame)



Collision kinematics (COM frame)



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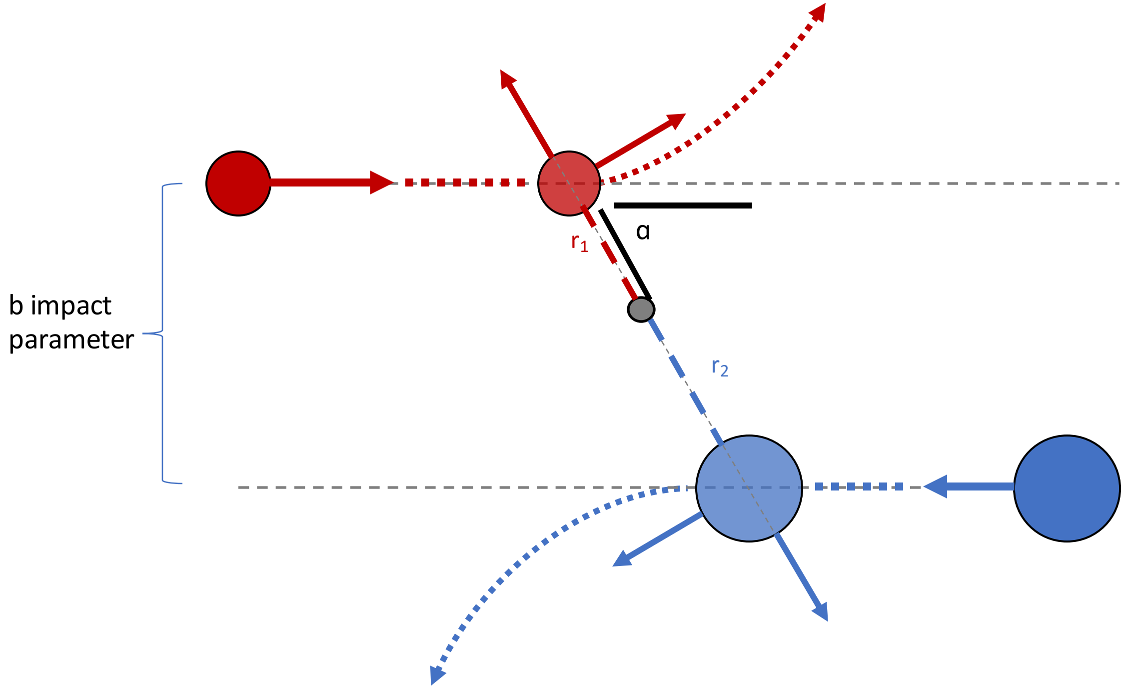
Collision kinematics (COM frame)



- Asymptotic kinetic energy: $$\Sigma = \frac{m_2}{m_1 + m_2} E_i$$

- Total angular momentum

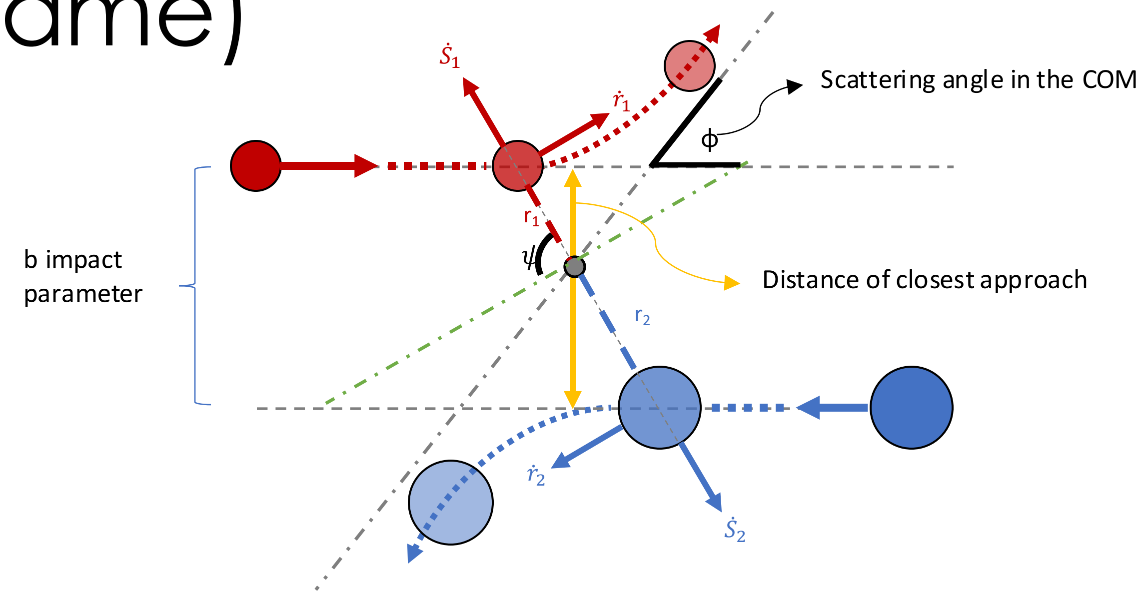
$$L = r_1 \sin\alpha\, m_1 v_c + r_2 \sin\alpha\, m_2 v_{CM}$$

- From last lecture:

- Therefore:

- Result:

Collision kinematics (COM frame)



- Total energy of the system:

$$\Sigma = V(r) + \frac{1}{2}m_1 v_c^2 + \frac{1}{2}m_2 V_c^2$$

- Velocity: $v_c = \sqrt{\dot{r}_1^2 + r_1^2\dot{\psi}^2}$

- Conservation of total energy during the collisions

$$\Sigma = V(r_1 + r_2) + \frac{1}{2}m_1\left(\dot{r}_1^2 + r_1^2\dot{\psi}^2\right) + \frac{1}{2}m_2\left(\dot{r}_2^2 + r_2^2\dot{\psi}^2\right)$$

- Result:

$$\boldsymbol{\Sigma = V(r) + \frac{1}{2}\left(\frac{m_1 m_2}{m_1 + m_2}\right)\left(\dot{r}^2 + r^2\dot{\psi}^2\right)}$$

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Collision kinematics (COM frame)

- Change of variables:

$$\dot{r} = \frac{dr}{dt} = \frac{dr}{d\psi}\dot{\psi}$$

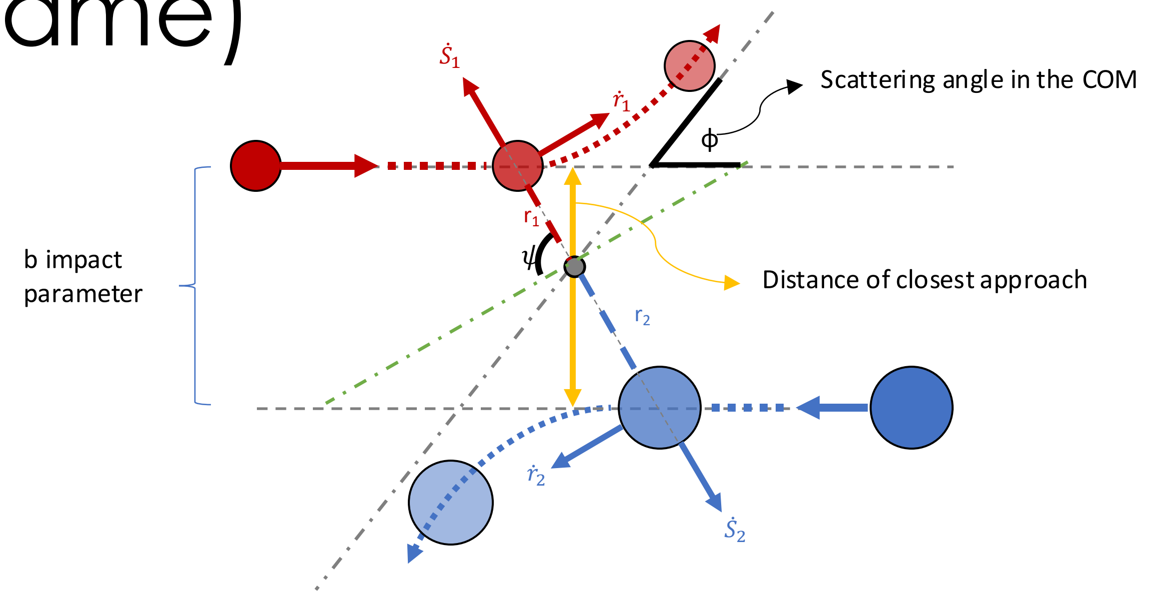
$$\Sigma = V(r) + \frac{1}{2}\left(\frac{m_1 m_2}{m_1 + m_2}\right)\left(\left(\frac{dr}{d\psi}\right)^2 + r^2\right)\dot{\psi}^2$$

- Angular conservation of momentum

$$L = v_\ell\left(\frac{m_1 m_2}{m_1 + m_2}\right)b = m_1 r_1^2\dot{\psi} + m_2 r_2^2\dot{\psi} \rightarrow \dot{\psi} = v_\ell b/r^2$$

- Time-independent orbit equation

$$\boldsymbol{\Sigma = V(r) + \frac{1}{2}\left(\frac{m_1 m_2}{m_1 + m_2}\right)\left(\left(\frac{dr}{d\psi}\right)^2 + r^2\right)\left(\frac{v_\ell b}{r^2}\right)^2}$$



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Collision kinematics (COM frame)

- Using Σ and $E_i = \frac{1}{2} M_1 v_\ell^2$:

$$\frac{d\psi}{dr} = \frac{b}{r^2} \frac{1}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}$$

$$\int_{\frac{\phi}{2}}^{\frac{\pi}{2}} d\psi = \frac{\pi}{2} - \frac{\phi}{2}$$

$$\boldsymbol{\phi = \pi - 2 \int_{\infty}^{p} \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}}$$

- This relates the impact parameter b to the scattering angle, ϕ, in the COM

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Collision kinematics (COM frame)

$$\boldsymbol{\phi = \pi - 2\int_{\infty}^{p} \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}}$$

- At the distance of closest approach:

$$\left.\frac{dr}{d\psi}\right|_{\frac{\pi}{2}} = 0 \Rightarrow \boldsymbol{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2} = 0}$$

- If V(r) is specified, then p(b) can be found!

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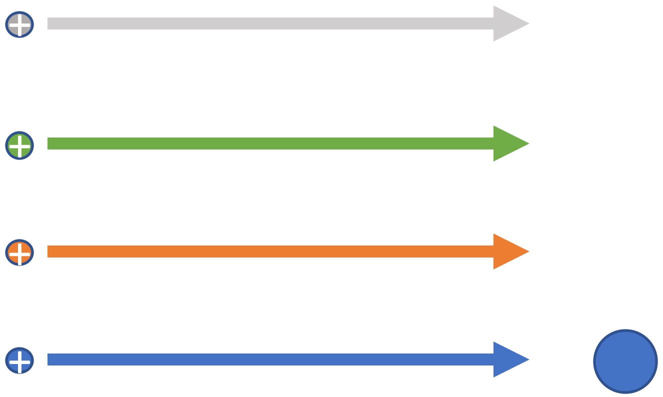
Importance of Interatomic Potentials:

- Required to estimate the number of displaced atoms produced by a primary knock-on atom
- Needed to capture the physics of energy loss for a charged particle
- Used to determine the mean free paths for the displacement of atoms
- Used in the determination of focusing and channeling



$$\phi = \pi - 2\int_{\infty}^{p} \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}$$

There exists no single function that describes all interactions between atoms

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Interactions between ions and atoms requires use of interatomic potentials

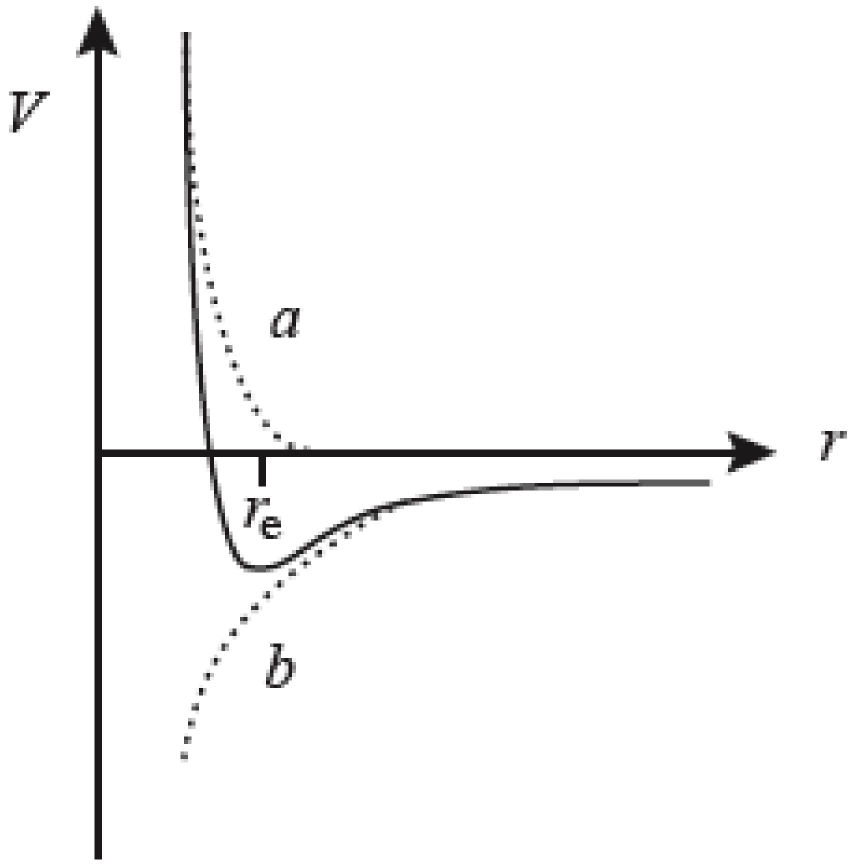
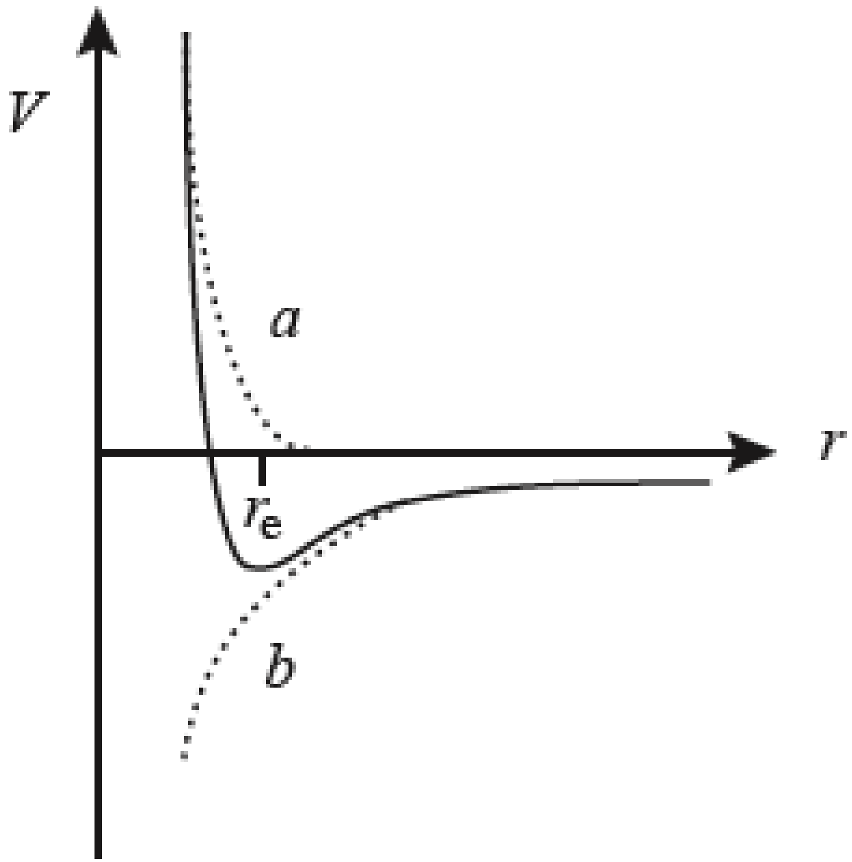


Figure 1.8 in Was, pg. 20

Interactions between ions and atoms requires use of interatomic potentials



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Interactions between ions and atoms requires use of interatomic potentials

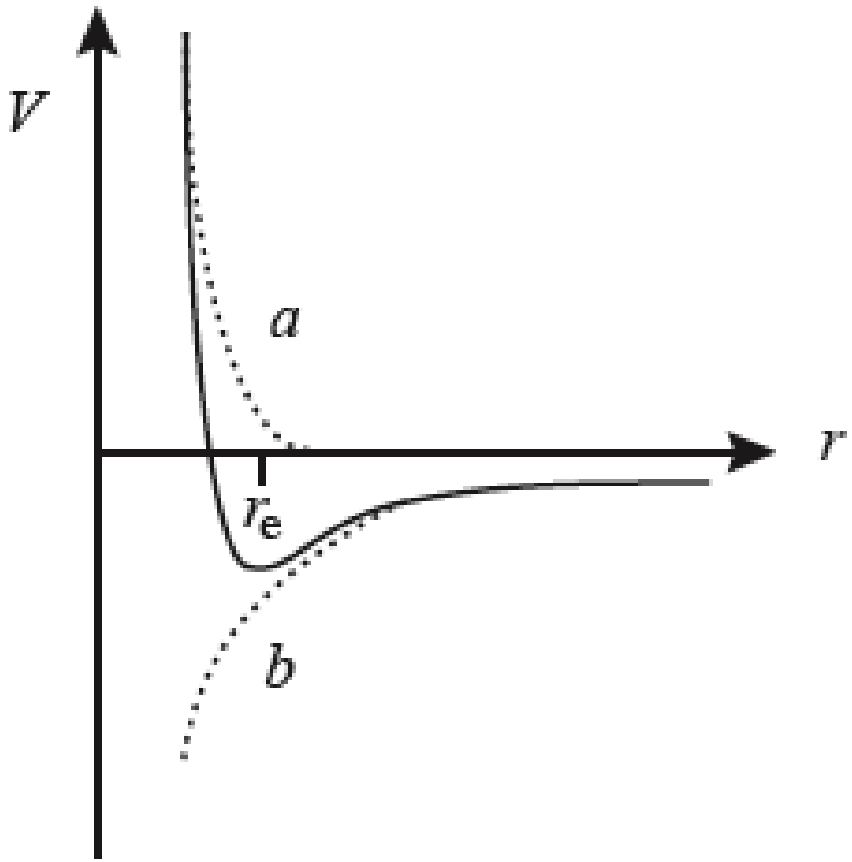


Figure 1.8 in Was, pg. 20

Interactions between ions and atoms requires use of interatomic potentials

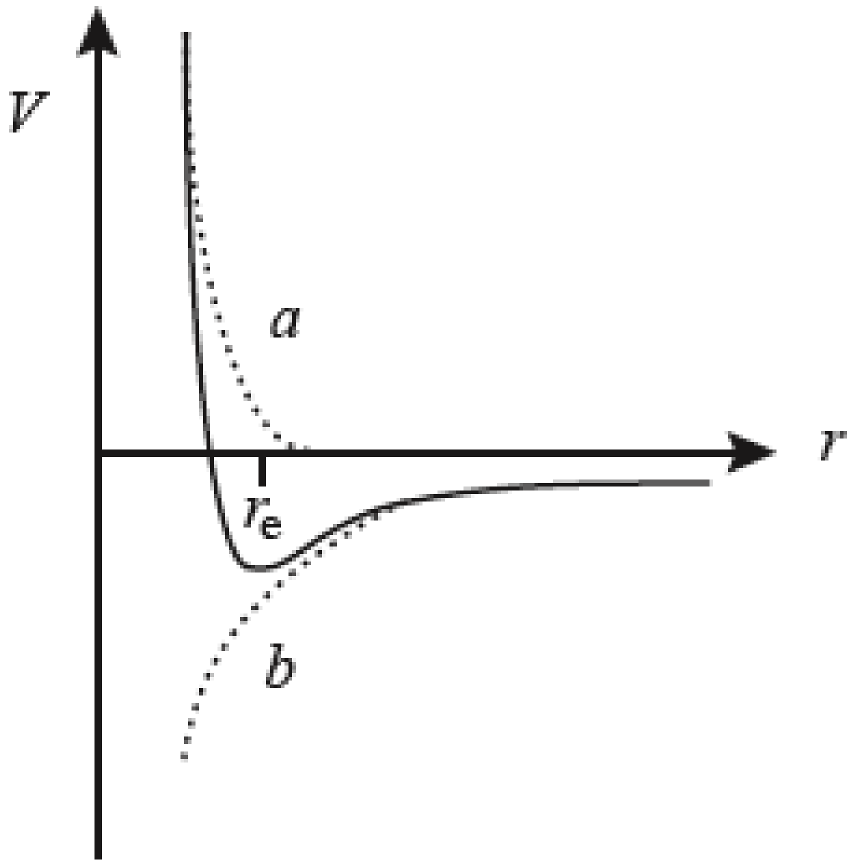
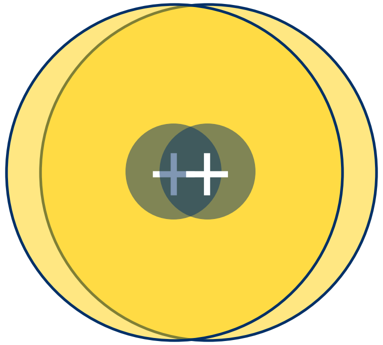
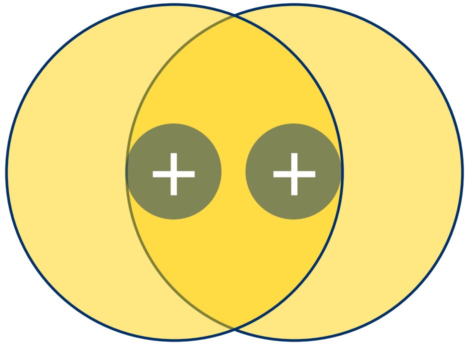


Figure 1.8 in Was, pg. 20

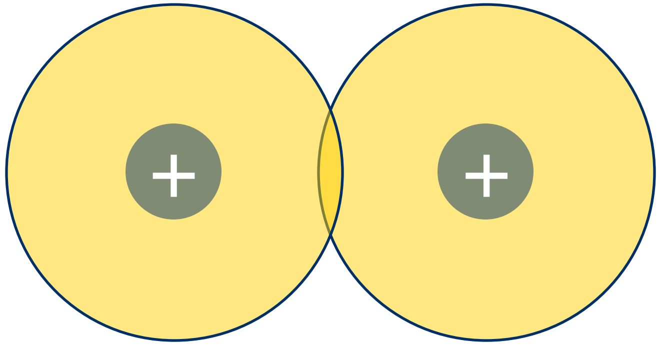
A visual of what this looks like…



R<K-shell radius
(Coulomb)



K-shell radius<R<Lattice Constant
(Screened Coulomb)



<R<Lattice Constant
(Born-Mayer)

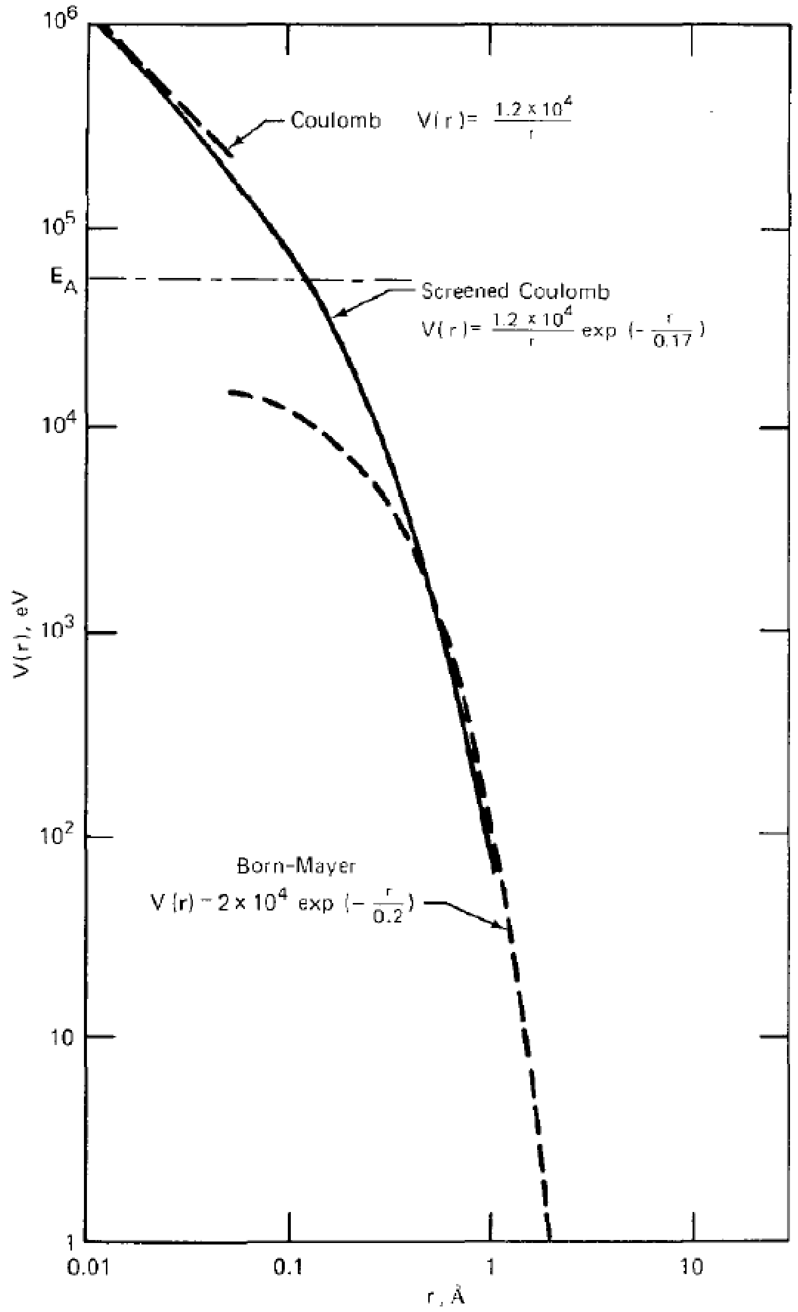
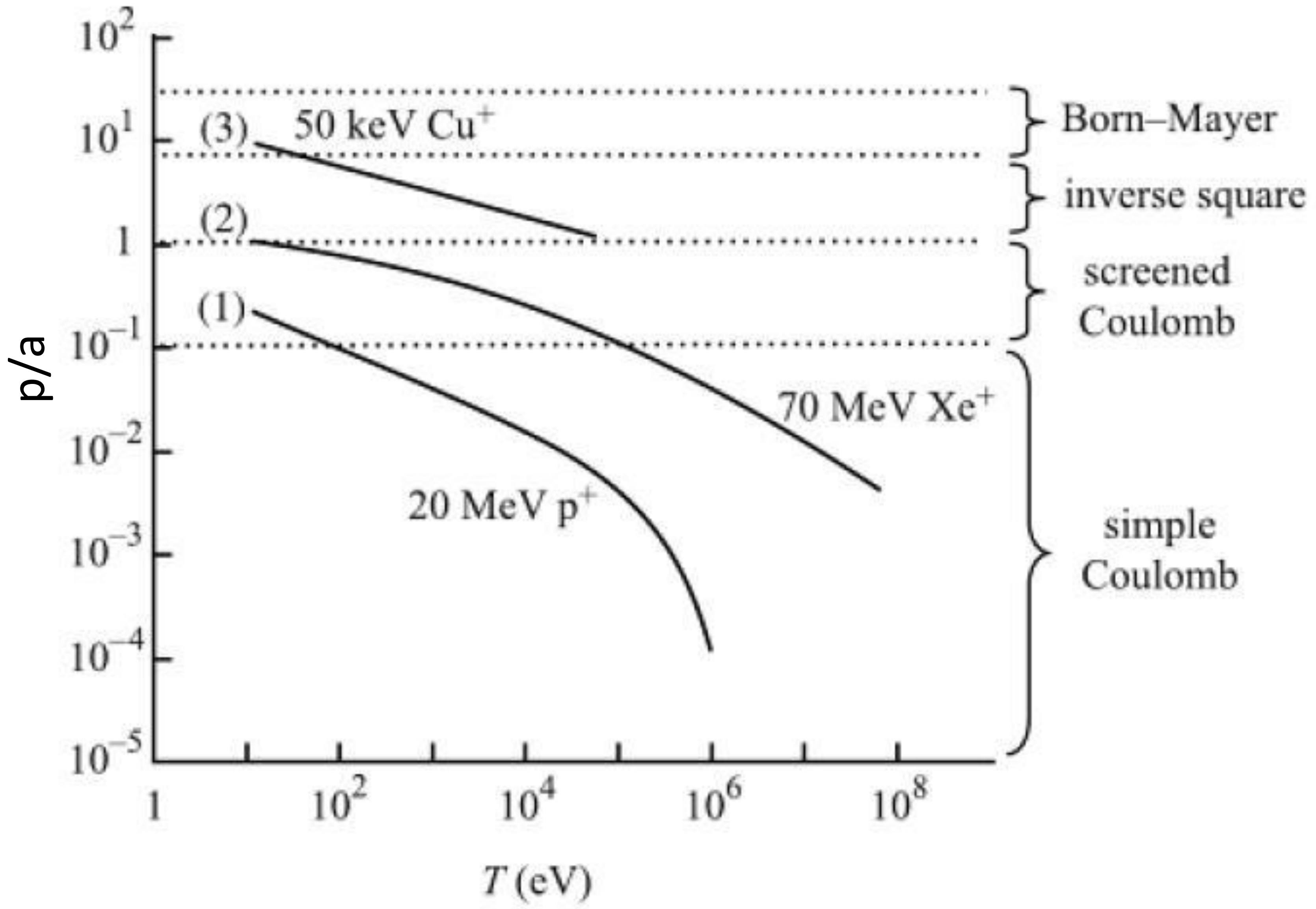


Fig. 17.5 Composite potential function for interaction between copper atoms.



Distance of the closest separation as a function of recoil energy for various ions in copper. Source: M.W. Thompson, "Defects and radiation damage in metals", Cambridge U.P., 1969

Potential	Equation	Range of Applicability	Definitions	Eqn in text
Hard sphere	$0 \quad for \;\; r > r_0$ $\infty \;\; for \;\; r < r_0$	$10^{-1}<T<10^{3}$ eV	r_0 = size of atom	(1.46)
Born-Mayer	$V(r) = A\exp(-r/B)$	$10^{-1}<T<10^{3}$ eV $a_0 < r \le r_e$	A,B determined from elastic moduli	(1.47)
Simple Coulomb	$\frac{Z_1Z_2\varepsilon^2}{r}$	light ions of high energy $r << a_0$		(1.48)
Screened Coulomb	$\left(\frac{Z_1Z_2\varepsilon^2}{r}\right)\exp(-r/a)$	Light ions $r < a_0$	a_o = Bohr radius a = screening radius	(1.49)
Brinkman I	$\frac{Z^2\varepsilon^2}{r}e^{(-r/a)}\left(1-\frac{r}{2a}\right)$	$r < a$	$a \cong a_0/Z^{1/3}$	(1.51)
Brinkman II	$\frac{AZ_1Z_2\varepsilon^2\exp(-Br)}{1-\exp(-Ar)}$	$Z > 25$ $r < 0.7r_e$	$A = \frac{0.95\times10^{-6}}{a_o}Z_{eff}^{7/}$ $B = Z_{eff}^{1/3}/Ca_o$ $C \cong 1.5$	(1.52)
Firsov	$\frac{Z_1Z_2\varepsilon^2}{r}\chi\left[\left(Z_1^{1/2}+Z_2^{1/2}\right)^{2/3}\frac{r}{a}\right]$	$r \le a_0$	χ is screening function	(1.56)
TFD Two Center	$\frac{Z^2\varepsilon^2}{r}\chi\left(Z^{1/3}\frac{r}{a}\right)-\alpha Z+\bar{\Lambda}$	$r < r_b\ (3a_0)$	r_b = radius at which the electron cloud density vanishes	(1.57)
Inverse square	$\frac{2E_r}{e}(Z_1Z_2)^{5/6}\left(\frac{a_o}{r}\right)^2$	$a/2 < r < 5a$	E_R = Rydberg energy = 13.6 eV	(1.59)

Summary

- We've accomplished three tasks to get towards a quantification of displacements for a given material system:

Task 1: Determine the energy transferred to the PKA:

$$T = \frac{\gamma}{2} E_i (1 - \cos\phi) \text{ to get } \phi = f(T)$$

Task 2: Determine the scattering angle based on the impact parameter:

$$\phi = \pi - 2\int_{\infty}^{r_0} \frac{b}{r^2} \frac{dr}{\sqrt{1 - \frac{V(r)}{\Sigma} - \frac{b^2}{r^2}}}$$

Task 3: Described V(r) to enable the calculation in Task 2
(simplest is hard sphere)

Next Lecture $\Rightarrow$ $\sigma_s(E_i, T) = 2\pi b \frac{db}{d\phi} \frac{d\phi}{dT}$

Questions?