Chapter II:
Interactions of ions with matter
Trajectories of α particles of 5.5 MeV

Source: SRIM
www.srim.org
Incident proton on Al: Bohr model

\[
v = v_0 \rightarrow E_p = 0.025 \text{ MeV}
\]

\[
\text{relativistic effect} \rightarrow E_p = 938 \text{ MeV}
\]

\[
\text{Al, } \rho = 2.70 \text{ g/cm}^3
\]
Contents

• Quantum model of the electronic stopping force
  - Intermediate velocities
  - Large velocities
  - Small velocities

• Nuclear stopping force (small velocities)

• Range and Bragg curve
Transferred energy: Classical oscillator (1)

• Before to look for quantum processing $\rightarrow$ details about classical processing: electron = classical harmonic oscillator with pulsation $\omega_0 \rightarrow e^-$ bound to its site by a spring force with modulus $-m\omega_0^2 r \rightarrow$ motion equation $\rightarrow$

$$\frac{d^2 \vec{r}}{dt^2} + \omega_0^2 \vec{r} = -\frac{e}{m} \vec{E}(\vec{r}, t)$$

with $\vec{E}(\vec{r}, t)$ the electric field generated by the projectile (perturbation)

• No-linear equation $\rightarrow$ simplification $\rightarrow$

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r}(t), t) \equiv \vec{E}(t)$$
Transferred energy: Classical oscillator (2)

• By supposing the absence of electric field at \( t = -\infty \) and \( r(-\infty) = 0 \) → a particular solution of the equation is →

\[
\vec{r}(t) = -\frac{e}{m\omega_0} \int_{-\infty}^{t} dt' \vec{E}(t') \sin \omega_0(t - t')
\]

• By supposing that the electric field \( \Delta \) after the distance of closest approach → it is possible to find a time \( t_1 \) for which the electric acting on the e\(^{-} \) becomes negligible → for \( t > t_1 \) → we can extend the maximal bound of the integration to \( +\infty \) because the contributions of the integration are negligible for \( t_1 < t' < +\infty \)
Transferred energy: Classical oscillator (3)

- In this case the solution is:

\[ \mathbf{r}(t) = -\frac{e}{m\omega_0}(\mathbf{C} \sin \omega_0 t - \mathbf{S} \cos \omega_0 t) \]

with

\[ \mathbf{C} = \int_{-\infty}^{+\infty} dt' \mathbf{E}(t') \cos \omega_0 t' \quad \text{et} \quad \mathbf{S} = \int_{-\infty}^{+\infty} dt' \mathbf{E}(t') \sin \omega_0 t' \]

- To determine the energy lost by the projectile to the oscillator:

\[ \mathbf{v}_e(t) = -\frac{e}{m}(\mathbf{C} \cos \omega_0 t + \mathbf{S} \sin \omega_0 t) \]
Transferred energy: Classical oscillator (4)

• Thus the transferred energy $T$ is →

$$T = -\frac{e^2}{2m} (\vec{C}^2 + \vec{S}^2)$$

• That can be also written →

$$T = -\frac{e^2}{2m} \left| \int_{-\infty}^{+\infty} dt' \vec{E}(t') e^{i\omega_0 t'} \right|^2$$
Classical oscillator: Dipolar approximation (1)

• We consider the Coulomb field generated by the incident particle →
  \[ \vec{E}(\vec{r}, t) = -\nabla \Phi(\vec{r}, t) \]
  with \( \Phi, \vec{R} \) and \( \vec{v} \) the potential, trajectory and velocity of the particle:

  \[ \Phi(\vec{r}, t) = \frac{e_1}{|\vec{r} - \vec{R}(t)|} \]
  et

  \[ \vec{R} = \vec{p} + \vec{v} t \]

• We note that

  \[ \vec{p} \cdot \vec{v} = 0 \]
Classical oscillator: Dipolar approximation (2)

- We consider the Fourier transforms at 1 and 3 dimensions →

\[
f(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \, f(t) e^{-i\omega t}
\]

\[
f(\overrightarrow{q}) = \frac{1}{(2\pi)^3} \int_{-\infty}^{+\infty} d^3 \overrightarrow{r} \, f(\overrightarrow{r}) e^{-i \overrightarrow{q} \cdot \overrightarrow{r}}
\]

- To obtain the Fourier transform of the potential → we use the relation →

\[
\frac{1}{r} = \frac{1}{(2\pi)^2} \int_{-\infty}^{+\infty} d^3 \overrightarrow{q} \frac{1}{q^2} e^{i \overrightarrow{q} \cdot \overrightarrow{r}}
\]
Classical oscillator: Dipolar approximation (3)

- The electric field can be thus written →

\[
\overrightarrow{E}(\overrightarrow{r}, t) = -\frac{i e_1}{(2\pi)^2} \int_{-\infty}^{+\infty} d^3\overrightarrow{q} \frac{\overrightarrow{q}}{q^2} e^{[i \overrightarrow{q} \cdot (\overrightarrow{r} - \overrightarrow{p} - \overrightarrow{v} t)]}
\]

- For small movements from the equilibrium → dipolar approximation →

\[
e^{i \overrightarrow{q} \cdot \overrightarrow{r}} \approx 1 + i \overrightarrow{q} \cdot \overrightarrow{r} \approx 1
\]

- The Fourier transform of the electric field can be written in the dipolar approximation →

\[
\overrightarrow{E}(\omega) = -\frac{i e_1}{(2\pi)^2} \int_{-\infty}^{+\infty} d^3\overrightarrow{q} \frac{\overrightarrow{q}}{q^2} e^{-i \overrightarrow{q} \cdot \overrightarrow{p}} \delta(\omega - \overrightarrow{q} \cdot \overrightarrow{v})
\]
Classical oscillator: Dipolar approximation (4)

- The integration is usually made by choosing the $x$ axis along the projectile velocity and the $y$ axis along the impact parameter →

$$\vec{E}(\omega) = -\frac{e_1 \omega}{\pi v^2} \left( i K_0 \left( \frac{\omega_j 0 p}{v} \right), K_1 \left( \frac{\omega_j 0 p}{v} \right), 0 \right)$$

with $K_0$ and $K_1$, the modified Bessel functions of order 0 and 1

- Thus $T$ becomes →

$$T = \frac{2e_1^2 e^2}{mv^2 p^2} f_{dist}(p)$$

with

$$f_{dist}(p) = \left[ \frac{\omega_0 p}{v} K_0 \left( \frac{\omega_0 p}{v} \right) \right]^2 + \left[ \frac{\omega_0 p}{v} K_1 \left( \frac{\omega_0 p}{v} \right) \right]^2$$

- For $(\omega_0 p/v) \ll 1 \rightarrow f_{dist} \approx 1 \rightarrow$ we find again the Bohr result
Semi-classical model for the stopping power: $v_0 \ll v \ll c$ (1)

• Semi-classical model developed by Bethe (1930) → the motion of the nucleus is analyzed by classical mechanics and the motion of bound electrons by quantum mechanics → the electrons are no more considered as classical oscillators but occupy quantum states in the target atom.

• We consider a target atom with $Z_2$ electrons (with mass $m$) and the stationary states $|j\rangle$ of energies $\epsilon_j$, with $j$ that represent a full set of quantum numbers and $j = 0$ for fundamental state → the resonant frequencies for an atom in its initial state are given by

$$\hbar \omega_{j0} = \epsilon_j - \epsilon_0$$

• The electrons are at rest during the → $v \gg v_0$
Semi-classical model for the stopping power: \( v_0 \ll v \ll c \) (2)

- For a loss energy \( Q \) by the incident ion → Bethe considered:

\[
S = \sum_j \int Q d\sigma_R f_{j0}(Q)
\]

- \( \sigma_R \) is the Coulomb cross section for a transferred energy \( Q \) (\( R \) is for Rutherford)
- The functions \( f_{j0}(Q) \) are called generalized oscillator forces (GOS) that include all quantum effects for the stopping cross section and that describe the transition probabilities between different states for a given transferred energy \( Q \)
- Determination of \( f_{j0}(Q) \)?
Resolution of Schrödinger’s equation (1)

• The electronic motion is controlled by Schrödinger’s equation depending on time →

\[(H + V) \Psi(\vec{r}, t) = i\hbar \frac{d\Psi(\vec{r}, t)}{dt}\]

with \(H\), the Hamiltonian of an isolated atom of the target, \(\Psi\), the wave function depending on time for a bound state of the atom, \(V\), the potential describing the interaction with the given projectile is given by

\[V(\vec{r}, t) = \sum_{\nu=1}^{Z_2} \frac{-e_1 e}{\vec{r}_\nu - \vec{R}(t)}\]

where \(\vec{r}\) is for \((\vec{r}_1, ..., \vec{r}_{Z_2})\) with \(\vec{r}_\nu\) the position operator of the \(\nu^{th}\) electron and \(\vec{R} = \vec{p} + \vec{v} t\), the trajectory of the projectile.
Resolution of Schrödinger’s equation (2)

• The wave function depending on time $\Psi$ can be developed according to stationary waves $\rightarrow$

$$\Psi(\vec{r}, t) = \sum_j c_j(t) e^{-i\epsilon_j t} |j\rangle$$

where $|j\rangle$ are solutions of:

$$H |j\rangle = \epsilon_j |j\rangle$$

• Within the framework of the first order perturbations method ($1^{\text{st}}$ order Born approximation) $\rightarrow$ the $c_j$ coefficients can be developed as power of the perturbation potential $V$ $\rightarrow$

$$c_j(t) = \delta_{j0} + c_j^{(1)}(t) + c_j^{(2)}(t) + \ldots$$
Resolution of Schrödinger’s equation (3)

with

\[ \delta_{j0} = \begin{cases} 
1 & \text{for } j = 0 \\
0 & \text{for } j \neq 0 
\end{cases} \]

and

\[ c_{j}^{(1)}(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} dt' e^{i\omega_{j0}t'} \langle j|V(\vec{r}, t')|0\rangle \]

\[ c_{j}^{(2)}(t) = \left( \frac{1}{i\hbar} \right)^2 \sum_{k} \int_{-\infty}^{t} dt' e^{i\omega_{jk}t'} \langle j|V(\vec{r}, t')|k\rangle \]

\[ \times \int_{-\infty}^{t'} dt'' e^{i\omega_{k0}t''} \langle k|V(\vec{r}, t'')|0\rangle \]

and so on... (remark $\rightarrow$ fundamental state at $t = -\infty$)
Resolution of Schrödinger’s equation (4)

• Within the framework of the first order perturbations method → only coefficients $c_j^{(1)}(\infty)$ are important → they are the transition amplitudes → important to calculate them

• By inserting in $c_j^{(1)}(\infty)$ the explicit expression of the potential, by considering the Fourier transform and by integrating on $t'$ →

$$c_j^{(1)}(\infty) = \frac{-e_1 e}{i \pi \hbar} \int \frac{dq}{q^2} e^{i \overrightarrow{q} \cdot \overrightarrow{P}} F_{j0}(\overrightarrow{q}) \delta(\omega_{j0} - \overrightarrow{q} \cdot \overrightarrow{v})$$

with

$$F_{j0}(\overrightarrow{q}) = \left\langle j \left| \sum_{\nu=1}^{Z_2} e^{i \overrightarrow{q} \cdot \overrightarrow{r}_\nu} \right| 0 \right\rangle$$

We note $Q = \frac{\hbar^2 q^2}{2m}$
Transition probabilities

- The transition probabilities are given by (Postulate IV) →

  \[ P_j(p) = |\langle j|\Psi(\infty)\rangle|^2 \]

- And thus within the framework of the first order perturbations method →

  \[ P_j(p) = \left| c_j^{(1)}(\infty) \right|^2 \]

- Attention → \( c_j^{(1)}(\infty) \neq 0 \) for \( \omega_{j0} < q\nu \) → condition son \( Q \) →

  \[ \omega_{j0}^2 < q^2\nu^2 \Rightarrow 2m\nu^2Q > (\epsilon_j - \epsilon_0)^2 \]
Approximation of distant collisions – Dipolar approximation (1)

- We consider the $c_j^{(1)(\infty)}$ at large $p$ (distant collisions) $\rightarrow$ we use the dipolar approximation $\rightarrow$

$$e^{i \vec{q} \cdot \vec{r}} \simeq 1 + i \vec{q} \cdot \vec{r}$$

- We thus obtain

$$F_{j0}(\vec{q}) \simeq i \vec{q} \left\langle j \middle| \sum_{\nu = 1}^{Z_2} \vec{r}_\nu \right| 0 \right\rangle$$

- Within this approximation and choosing the $x$ axis along the velocity of the projectile and the $y$ axis along the impact parameter $\rightarrow$

$$c_j^{(1)}(\infty) = - \frac{2e_1 e \omega_{j0}}{i \hbar v^2} \left\langle j \middle| \sum_{\nu} \vec{r}_\nu \right| 0 \right\rangle$$

$$\times \left( i K_0 \left( \frac{\omega_{j0} p}{v} \right), K_1 \left( \frac{\omega_{j0} p}{v} \right), 0 \right)$$
Approximation of distant collisions –
Dipolar approximation (2)

with $K_0$ and $K_1$, the modified Bessel functions of 0 and 1 order

- The transitions probabilities thus become →

$$P_j(p) = -\frac{2e_1^2e^2 Z_2}{mv^2p^2\hbar\omega_{j0}} f_{j0}$$

$$\times \left\{ \left[ \frac{\omega_{j0}p}{\nu} K_0 \left( \frac{\omega_{j0}p}{\nu} \right) \right]^2 + \left[ \frac{\omega_{j0}p}{\nu} K_1 \left( \frac{\omega_{j0}p}{\nu} \right) \right]^2 \right\}$$

- The quantity $f_{j0}$ is called the dipolar oscillator force and has as expression →

$$f_{j0} = \frac{2m}{3\hbar^2 Z_2} (\epsilon_j - \epsilon_0) \left| \langle j | \sum_{\nu} \frac{\mathbf{r}}{r_{\nu}} | 0 \rangle \right|^2$$

with the sum rule of Thomas-Reiche-Kuhn: $\sum_j f_{j0} = 1$
Comparison classical ↔ semi-classical

• We consider the mean transferred energy $T_{moy}$ as

$$T_{moy}(p) = \sum_j P_j(p) \hbar \omega_{j0}$$

• By comparing this expression with the classical result →

$$T = \frac{2e_1^2 e^2}{mv^2 p^2} f_{dist}(p)$$

$$f_{dist}(p) = \left[ \frac{\omega_0 p}{v} K_0 \left( \frac{\omega_0 p}{v} \right) \right]^2 + \left[ \frac{\omega_0 p}{v} K_1 \left( \frac{\omega_0 p}{v} \right) \right]^2$$

• Equal expression with

$$f_{dist}(p) = \sum_j f_{j0} \left[ \frac{\omega_{j0} p}{v} K_0 \left( \frac{\omega_{j0} p}{v} \right) \right]^2 + \left[ \frac{\omega_{j0} p}{v} K_1 \left( \frac{\omega_{j0} p}{v} \right) \right]^2$$
Beyond distant collisions

• To generalize the previous $f_{j0}$ functions to large values of $Q$, Bethe sets out →

$$f_{j0}(Q) = \frac{1}{Z_2} \frac{\epsilon_j - \epsilon_0}{Q} |F_{j0}(\vec{q})|^2$$

called generalized oscillator forces

• At the limit of small $Q$ values →

$$f_{j0}(Q) \bigg|_{Q \sim 0} = f_{j0}$$
Stopping power: Bethe equation: $v_0 \ll v \ll c \ (1)$

- Necessary distinction between distant and close collisions (via $p$) ↔ collisions with large or small transferred momentum (via $q$) ↔ collisions with or small transferred energy (via $Q$)

- Splitting of the integral:

$$S = \sum_j \int Q d\sigma_R f_{j0}(Q)$$

into 2 parts in relation to $Q_0$ → For $Q < Q_0$ → dipolar approximation is valid ($Q_0$) →

$$S_{dist} = \sum_j f_{j0} \int_{(\epsilon_j - \epsilon_0)^2/2mv^2}^{Q_0} Q d\sigma_R$$
Stopping power: Bethe equation: \( v_0 \ll v \ll c \) (2)

• For \( Q > Q_0 \rightarrow \) it is necessary to determine the upper bound of the integral \( \rightarrow \) for an ion interacting with an \( e^- \) \( (m_1 \gg m) \rightarrow \)

\[
T_{\text{max}} = \gamma E
= \frac{4m_1 m}{(m_1 + m)^2} \frac{m_1 v^2}{2}
\approx 2mv^2
\]

• That gives \( \rightarrow \)

\[
S_{\text{close}} = \int_{Q_0}^{2mv^2} Q d\sigma_R \sum_j f_{j0}(Q)
\]
Stopping power: Bethe equation: $v_0 \ll v \ll c$ (3)

- Bethe demonstrated that →
  \[ \sum_j f_{j0}(Q) = 1 \]

- We have thus →
  \[ S_{\text{close}} = \int_{Q_0}^{2mv^2} Q d\sigma_R \equiv \sum_j f_{j0} \int_{Q_0}^{2mv^2} Q d\sigma_R \]

- By combining close and distant collisions →
  \[ S = S_{\text{close}} + S_{\text{dist}} = \sum_j f_{j0} \int_{(\epsilon_j - \epsilon_0)/2mv^2}^{2mv^2} Q d\sigma_R \]
Stopping power: Bethe equation: \( v_0 \ll v \ll c \) (4)

- By considering the explicit expression of \( d\sigma_R \rightarrow \)

\[
d\sigma_R = 2\pi \frac{e_1^2 e_2^2}{m_2 v^2} \frac{dQ}{Q^2}
\]

- We thus obtain

\[
S = \frac{4\pi e_1^2 e_2^2}{m v^2} Z_2 \sum_j f_{j0} \ln \frac{2m v^2}{\epsilon_j - \epsilon_0}
\]
Stopping power: Bethe equation: \( v_0 \ll v \ll c \) (5)

- The stopping power equation of Bethe is usually written as:

\[
S_e = \frac{4\pi e_1^2 e^2}{mv^2}Z_2 \ln \frac{2mv^2}{I}
\]

with \( I \) defined as the mean excitation energy such as:

\[
\ln I = \sum_j f_{j0} \ln (\epsilon_j - \epsilon_0)
\]

- Let’s recall the application conditions:

\[
m_1 \gg m, \quad v \gg v_0 \Rightarrow mv^2 \gg \hbar \omega_0
\]
Bethe equation versus Bohr equation

\[ S_e = \frac{4\pi Z_2 e_1^2 e^2}{mv^2} L_e \]

with \[ L_e = \ln \frac{Cmv^3}{|e_1 e|\omega_0} \] from Bohr

with \[ L_e = \ln \frac{2mv^2}{I} \] from Bethe
Principal dependences of the stopping force

\[- \left( \frac{dE}{dx} \right)_{elec} = NS_e = \frac{4\pi e_1^2 e^2}{mv^2} NZ_2 \ln \frac{2mv^2}{I} \]

\[\frac{4\pi e_1^2 e^2}{mv^2} \quad \text{Principal dependence in the velocity} \]

\[NZ_2 \quad \text{Principal dependence in the material} \]

\[\ln \frac{2mv^2}{I} \quad \text{Weak dependence in the velocity and in the material} \]
Mean logarithmic excitation energy (1)

• The mean logarithmic excitation energy $I$ only depends on the medium (not on the projectile)
• Difficult calculations → obtained from experiment
• $I$ is in the logarithmic part of → not necessary to be known with precision
• $I$ linearly varies (approximately) with $Z$ → atomic model of Thomas-Fermi (atomic electrons = “gas”)
• The irregularities in the variation with $Z$ are due to the shell structure of the atom
• Usually → evaluation of $I$ with an empirical equation
Mean logarithmic excitation energy (2)

\[
\frac{I}{Z} = \begin{cases} 
12 + 7/Z & Z < 13 \\
9.76 + 58.8Z^{-1.19} & Z \geq 13
\end{cases}
\]
For composite materials → the stopping power of the material can be approximated by the sum of the stopping powers of its elementary constituents → identical relation for the mean excitation energies

Bragg’s additivity rule for \( n \) materials \( i \):

\[
NZ = \sum_{i}^{n} N_i Z_i
\]

\[
NZ \ln I = \sum_{i}^{n} N_i Z_i \ln I_i
\]

\( Z_i \) is the atomic number of the atoms of type \( i \), \( N_i \) is the number of atoms of type \( i \) per volume unit and \( N = \sum_{i} N_i \) is the total number of atoms per volume unit

Approximate rule → can lead to important mistakes
Bethe-Bloch equation: \( v_0 < v \sim c \) (1)

Many corrections to the Bethe equations → Bethe-Bloch equations (in the Born approximation)

\[
S_e = \frac{4\pi r_e^2 mc^2}{\beta^2} Z z^2 L(\beta)
\]

Standard reference expression for the electronic stopping power with 
\( \beta = v/c, \ z = e_1/e, \ r_e = e^2/(mc^2) \) (\( r_e \): classical radius of the electron)

\[
L(\beta) = L_0(\beta) = \frac{1}{2} \ln \left(\frac{2mc^2 \beta^2 \mathcal{W}_m}{1 - \beta^2}\right) - \beta^2 - \ln I - \frac{C}{Z} - \frac{\delta}{2}
\]

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Bethe-Bloch equation: $\nu_0 < \nu \simeq c$ (2)

- With $W_m$ the maximum energy transferred during 1 collision to a free electron (non-approximated relativistic expression) →

$$W_m = \frac{2mc^2\beta^2}{1 - \beta^2} \left[ 1 + \frac{2m}{m_1(1 - \beta^2)^{1/2}} + \left( \frac{m}{m_1} \right)^2 \right]^{-1}$$

- For $m_1 \gg m$ → we well find $2m\gamma_1^2v^2$
Relativistic correction: $\nu \simeq c$ (1)

- When $\nu \simeq c$ or $\beta = \nu/c \simeq 1 \rightarrow$ relativistic corrections have to be done to previous expression $\rightarrow$ term $\gamma_1 = (1-\beta^2)^{-1/2}$
- We also have $\rightarrow p_{\text{max}} \sim \gamma_1 \nu/\omega_0 \rightarrow$ of the upper bound of the impact parameter when $\nu \rightarrow$
- A complete relativistic classical calculation (as for quantum) shows that $E$ becomes $\rightarrow$

\[
\overrightarrow{E}(\omega) = -\frac{e_1 \omega}{\pi \gamma_1 \nu^2} \left( \frac{i}{\gamma_1} K_0 \left( \frac{\omega_0 \rho}{\gamma_1 \nu} \right), K_1 \left( \frac{\omega_0 \rho}{\gamma_1 \nu} \right), 0 \right)
\]

- We have thus a relativistic modification of $f_{\text{dist}}(p) \rightarrow$

\[
f_{\text{dist}}(p) = \frac{1}{\gamma_1^2} \left[ \frac{\omega_0 \rho}{\gamma_1 \nu} K_0 \left( \frac{\omega_0 \rho}{\gamma_1 \nu} \right) \right]^2 + \left[ \frac{\omega_0 \rho}{\gamma_1 \nu} K_1 \left( \frac{\omega_0 \rho}{\gamma_1 \nu} \right) \right]^2
\]
Relativistic correction: \( v \approx c \) (2)

- And thus a modification of the principal dependence in velocity leads to:
  \[
  \frac{4\pi e_1^2 e^2}{mv^2} \Rightarrow \frac{4\pi e_1^2 e^2}{m\gamma_1^2 v^2} = \frac{4\pi e_1^2 e^2}{mv^2} (1 - \beta^2)
  \]

- Moreover the momentum of the incident particle becomes \( m\gamma_1 v \) leads to:
  \[
  T_{max} = 2m\gamma_1^2 v^2
  \]

- And thus we have a modification of the logarithmic term leads to:
  \[
  \ln \frac{2mv^2}{I} \Rightarrow \ln \frac{2m\gamma_1^2 v^2}{I} = \ln \frac{2mv^2}{I(1 - \beta^2)}
  \]

- The combination of all modifications implies that \( S \uparrow \) when \( v \uparrow \)
Density correction (1)

• Density correction $\rightarrow -\delta/2$

• In the Bethe equation $\rightarrow$ interactions with isolated atoms $\rightarrow$ valid for low density gas

• In condensed matter (solid) $\rightarrow$ the interactions can get done with a large amount of atoms at once $\rightarrow$ we have to consider collective effects

• Model of Fermi (1940) $\rightarrow$ matter assimilated to a gas of oscillators submitted to the electric field of the particle

• Incident charged particle $\rightarrow$ polarization of matter $\rightarrow$ the electric field due to the charged particle disturb the atoms $\rightarrow$ they get a dipolar electric momentum $\rightarrow$ production of an electric field opposed to the field due to the charged particle $\rightarrow$ reduction of the electric field due to screening effect of the dipoles
Density correction (2)

• The polarization implies that distant atoms are submitted to a weaker electric field → their contribution to the stopping power is then reduced

• The density effect particularly appears for high energies because of the factor $\gamma_1$ in $\rho_{\text{max}}$ that increases the mistake made by ignoring polarization of the medium → $v \uparrow \rightarrow \rho_{\text{max}} \uparrow \rightarrow \delta/2 \uparrow \rightarrow S \downarrow$

• The density correction can be written →

$$\frac{\delta}{2} = \ln \frac{\hbar \omega_p}{I} + \ln \gamma_1 \beta - \frac{1}{2}$$

with $\omega_p$, the plasma pulsation for an electronic density $n = NZ$ ($\varepsilon_0$: dielectric constant) →

$$\omega_p = \sqrt{\frac{ne^2}{\varepsilon_0 m}}$$
Density correction (3)

• Relativistic and density corrections cancel each other out → Fermi’s plateau
Shell correction (1)

• Shell correction $\rightarrow -C/Z$
• Bethe and Bohr equations supposed $v \gg v_0$ (velocity of the atomic electrons) $\rightarrow$ the evaluation of $I$ is based on this assumption $\rightarrow$ mean $I$ value
• When it is not the case ($v \downarrow$) $\rightarrow$ it is necessary to explicitly calculate the ions-electrons interactions for each electron shell and for each electron binding energy
• When $v \downarrow$ $\rightarrow$ contribution to $S$ of internal electrons (first K, then L, ...) $\downarrow$
• “Mean” correction that reduces $S$ (maximal correction = 6%) $\rightarrow$ = for all charged particles (including electrons) $\rightarrow$ only dependent on medium and velocity
Shell correction (2)

1. The method of the hydrogenous wave functions (HWF: bound e\textsuperscript{-} described by hydrogenous wave functions)
2. The method of the local density approximation (LDA: bound e\textsuperscript{-} are a gas of e\textsuperscript{-} with variable density)
Shell correction (3)
Shell correction (4)

LDA

HWF

\( \frac{C}{Z_2} \) vs. \( \frac{E_p}{Z_2} \) (MeV)

\( Z_2 \) values: 82, 47, 29, 18, 13, 4
Corrections beyond the first order Born approximation

- The stopping number $L_0$ is valid only if the velocity of the projectile is large by comparison to the velocities of the atomic electrons.

- For $v_0 \lesssim v \rightarrow$ the first order Born approximation (necessary for the calculations of Bethe) is no more valid.

- We have to add correction terms to $L_0 \rightarrow$ expansion of $L$ in power of $z \rightarrow$

\[ L(\beta) = L_0(\beta) + zL_1(\beta) + z^2L_2(\beta) \]
Barkas-Andersen correction

- Barkas-Andersen correction $\rightarrow zL_1(\beta)$

- The Barkas-Andersen correction is proportional to an odd power in $z$ (charge of the projectile) $\rightarrow S$ for negative particles is slightly weaker than for positive particles $\rightarrow S \neq$ between particles and corresponding antiparticles

- A positive charge attracts the $e^-$ $\rightarrow$ the interactions $\uparrow \rightarrow S \uparrow$

- A negative charge repulses the $e^-$ $\rightarrow$ the interactions $\downarrow \rightarrow S \downarrow$
Example of Barkas-Andersen effect

Incident proton and antiprotons on silicon
Bloch correction

• Bloch correction $\rightarrow z^2L_2(\beta)$
• Semi-classical model taking precisely into account distant collisions (large impact parameter)
• Generally Bichsel evaluation of the Bloch correction is used:

$$z^2L_2(y) = -y^2[1.202 - y^2(1.042 - 0.855y^2 + 0.343y^4)]$$

where $y = z\alpha/\beta$ and $\alpha = 1/137$ (fine structure constant)
Evaluation of various corrections (1)

Incident proton on aluminium
Evaluation of various corrections (2)

Protons incident on gold →

![Graph showing relative correction vs. proton energy for gold](image)
Stopping cross section for ions at very high velocities

Ultra-relativistic equation of Lindhard-Sørensen (E~ 100 GeV: far beyond normal applications)

\[ L \rightarrow \ln \frac{1.64c}{R\omega_p} \]

R: radius of the projectile, \( \omega_p = (4\pi e^2 N_e/m)^{1/2} \): plasma frequency that quantifies the electronic density

Attention: for E ↗ the creation of electron-positron pairs becomes predominant
Electronic cross section for ions at small velocities

\[ v \lesssim v_0 \rightarrow \text{Perturbation theory not applicable (no sudden collision)} \]

Moreover, electrons capture by incident projectiles (for example: \( \text{He}^{++} \rightarrow \text{He}^+ \rightarrow \text{He}^0 \)) \( \rightarrow \) charge state of the ion is variable (Thomas-Fermi theory):

\[
\tilde{z}^* = z \left( 1 - e^{-v/(z^2/3 v_0)} \right)
\]

Different theories but not so precise that the Bethe-Bloch theory for large velocities \( \rightarrow \) use of semi-empirical expressions based on a theoretical « trend »

\[ \Rightarrow S_e \propto E^{0.5} \]
Nuclear cross section for ions at small velocities (1)

- Chapter 1 → Nuclear collisions for incidents ions are rare → small contribution to the total stopping power

- Only for incident ions with small velocity → even in that case their contribution is small

- However → They can have effects a posteriori → radiative damages
Nuclear cross section for ions at small velocities (2)
in the center of mass system:
diffusion by angle $\theta$ due to a uncentral potential $V(r)$

\[ S_n = \int T \, d\sigma = \int T \, 2\pi \, p \, dp = 2\pi \gamma E \int \sin^2(\theta/2) \, dp \]  with \[ \gamma = \frac{4m_1m_2}{(m_1 + m_2)^2} \]
Nuclear cross section for ions at small velocities (3)

\[
\frac{m_0}{2} \left[ (\frac{dr}{dt})^2 + r^2 (\frac{d\varphi}{dt})^2 \right] + V(r) = \frac{m_0}{2} v^2 \equiv E_r
\]

\[
m_0 r^2 \frac{d\varphi}{dt} = -m_0 p v
\]

\[
\Rightarrow \theta = \pi - 2 \int_{r_m}^{\infty} dr \frac{p}{r^2} \left( \frac{1}{1 - \frac{V(r)}{E_r}} - \frac{p^2}{r^2} \right)^{-1/2}
\]

with \(E_r\) the initial kinetic energy of the relative motion
Nuclear cross section for ions at small velocities (4)

Interaction potential: \[ V(r) = \frac{z_1 Z_2 e^2}{r} F_s \left( \frac{r}{r_s} \right) \]

The screening function \( F_s(r/r_s) \) takes into account the screening by the atomic electrons (\( r_s \): screening length in the model of Thomas-Fermi) → Adjustment to experimental results → « universal screening function »

\[
F_s(r/r_s) = 0.1818 \exp(-3.2r/r_s) + 0.5099 \exp(-0.942r/r_s) \\
+ 0.2802 \exp(-0.4029r/r_s) + 0.2817 \exp(-0.2016r/r_s)
\]

with \( r_s = 0.88534a_0 (z_1^{0.23} + Z_2^{0.23})^{-1} \) and \( a_0 = 0.529\text{Å} \)
Stopping power for ion: example

Incident proton on aluminium $\rightarrow S = S_{\text{elec}} + S_{\text{nucl}} \approx S_{\text{elec}} = S_{\text{coll}}$
Electronic mass stopping power (1)

• Mass stopping power: ratio between the stopping power and the density $\rho$ of the material (ordinary unit: MeV cm$^2$ g$^{-1}$) →

$$\frac{NS(E)}{\rho} = -\frac{1}{\rho} \frac{dE}{dx}$$

• With $\rho = M_A N/N_A$ ($M_A$ is the molar mass, $N$ is the atomic density and $N_A$ is the Avogadro number) and $M_A = AM_u$ ($A$ is le mass number and $M_u = m_u N_A = 10^{-3}$ kg mol$^{-1}$ is the constant of molar mass and $m_u$ is the atomic mass constant) →

$$-\frac{1}{\rho} \frac{dE_{elec}}{dx} = 4\pi r_e^2 mc^2 \frac{N_A}{M_u} \frac{Z}{A} \frac{z^2}{\beta^2} L(\beta)$$
Electronic mass stopping power (2)

The electronic mass stopping power is the product of 4 factors:

1. The constant factor \(4\pi r_e^2 mc^2 N_A/M_u = 0.307 \text{ MeV cm}^2 \text{ g}^{-1}\) → order of magnitude for the electronic mass stopping power.
2. The factor \(Z/A\) that is included between 0.4 et 0.5 for all stable isotopes (except hydrogen) → weak dependency into the medium.
3. The factor \(\beta^{-2}\) → monotonic decreasing function in ion velocity that tends to 1 for large energies → explain the decrease of the stopping power as a function of the energy.
4. The stopping number \(L(\beta)\) → for \(L(\beta) = L_0(\beta)\) → monotonic increasing function (slow) in the velocity and in \(Z\) (via \(I: -\ln I\)).
Variation of $Z/A$ as a function of $A$
Velocity dependency

Protons incident on Si → shell and density corrections are neglected in the calculation of $L_0(\beta)$
Electronic mass stopping power: Examples

Protons incident on different media
Influence of the phase

- For large energies → influence of the density correction → large correction for solids and weak correction for gases
- For small energies → influence of chemical and intermolecular bounding → modification of the value of $I$ (example: liquid water: $I = 75.0$ eV and gaseous water: $I = 71.6$ eV)
Range of charged particles (1)

• Charged particles lose their energy in matter → they travel a certain distance in matter → this distance is variable because of aleatory energy losses and deviations (straggling) → different ranges have to be defined:
  – The range $R$ of a charged particle of energy $E$ in a medium is the mean value $\langle l \rangle$ of the length $l$ of its trajectory as it slows down to rest (we do not take into account thermal motion)
  – The projected range $R_p$ of a charged particle of energy $E$ in a medium is the mean value of its penetration depth $\langle d \rangle$ along the initial direction of the particle

• $R_p < R$ due to the sinuous character of trajectories → definition of the detour factor $= R_p/R_{CSDA} < 1$
Range of charged particles (2)

• In CSDA approximation →

\[ R_{CSDA} = \int_0^E \frac{dE'}{NS(E')} \]

• By replacing \( S \) by the Bethe expression (non-relativistic → \( dE = Mvdv \)) →

\[ R_{CSDA} \propto \int_0^v \frac{v^3 dv}{L(v)} \]

• By neglecting the dependency into the velocity for the stopping number →

\[ R_{CSDA} \propto v^4 \propto E^2 \]
Range of charged particles (3)

• In reality → the equation of Bethe (or Bethe-Bloch) is not valid for small velocities → but before to stop small velocities have to be considered

• We consider the empiric equation →

\[ \rho R_{CSDA} = \frac{E^{1.77}}{415} + \frac{1}{670} \]
Range of charged particles: Example

Incident proton on aluminium ($\rho = 2.70 \text{ g/cm}^3$)

http://www.nist.gov/pml/data/star/index.cfm
Detour factor

Incident proton on aluminium

![Graph showing detour factor as a function of kinetic energy (MeV)]
Range approximations

\[ S_e = \frac{4\pi r_e^2 mc^2}{\beta^2} Z z^2 L(\beta) \]

- \( \text{NS}(E) \propto \frac{1}{E} \)
- \( \text{NS}(E)/z^2 \) only depends on \( v \) → if we have particle of mass \( M_i \) and charge \( z_i \):

\[ NS(E) = -\frac{dE}{dx} \Rightarrow -\frac{M_i}{z_i^2} \frac{dv^2}{dx} \propto v^{-2} \]

- For 2 particles \((M_1, z_1)\) and \((M_2, z_2)\) of same velocity:

\[ \frac{R^1_{\text{CSDA}}}{R^2_{\text{CSDA}}} = \frac{M_1 z_2^2}{M_2 z_1^2} \]

Same range for proton and \( \alpha \) of same velocity
Examples of CSDA ranges (1)

- 5.5 MeV α in air: $R_{\text{CSDA}} = 4.2 \text{ cm}$
- 4.0 MeV α in air: $R_{\text{CSDA}} = 2.6 \text{ cm}$
- 5.5 MeV α in aluminium: $R_{\text{CSDA}} = 2.5 \times 10^{-3} \text{ cm}$
- 1 MeV proton in air: $R_{\text{CSDA}} = 2.4 \text{ cm}$
- 4 MeV proton in air: $R_{\text{CSDA}} = 23.6 \text{ cm}$
- 5.5 MeV proton in aluminium: $R_{\text{CSDA}} = 2.3 \times 10^{-2} \text{ cm}$

http://www.nist.gov/pml/data/star/index.cfm
Examples of CSDA ranges (2)

α incident on various media
Bragg curve

- We consider a semi-infinite medium and a beam of identical parallel charged particles with same $E \rightarrow$ they stop after travelling the distance $R_{CSDA}$
- The Bragg curve gives the dose (mean deposited energy per mass unit of the target) as a function of the depth
- At depth $x$, the particle has to cover a distance $d = R_{CSDA} - x$
- The dose $D \propto S \propto 1/v^2 \rightarrow R_{CSDA} \propto v^4$

$$D \propto \frac{1}{\sqrt{d}} = \frac{1}{\sqrt{R_{CSDA} - x}}$$
Example of Bragg curve

- Protons of 700 MeV in water →

- Applications: proton therapy or hadron therapy
Transmission of ions

Transmission probability

Absorber thickness
Strong nuclear interactions

• If ion comes very close to target nucleus → strong nuclear interaction becomes possible → the target nucleus will be broken up

• One particular case: the collision of a high-energy proton with a very heavy nucleus with thus more neutrons than protons (lead: 82 protons and ≈125 neutrons) → the fragments will quickly expel their excess neutrons → production of a large number of secondary neutrons (proton of 1 GeV → on average 25 neutrons in lead)

• This process of neutrons production is called spallation → efficient way to produce neutrons

• All fragments interact with matter