Ionization Cross Sections for Ion-Atom Collisions in High Energy Ion Beams

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Talk Outline

- **Revision of cross section calculated by use of the Rutherford formula**
  - for more details see our tutorial review
  - I.D. Kaganovich, E. A. Startsev and R. C. Davidson, "Scaling cross sections for ion-atom impact ionization", http://www.pppl.gov/pub_report/2003/PPPL-3819.pdf; http://arXiv.org/abs/physics/0407140
- **Filamentation (Weibel) instability**
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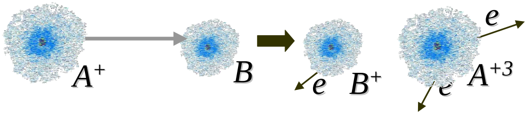
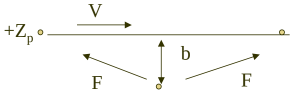
Definition of Electron Loss Events



1) **from neutral gas: ionization**
2) **from projectile ion: stripping**
   1) **Target is charged => long range interaction**
   2) **Target is neutral => no long range interaction**

Thompson's Treatment (1912)

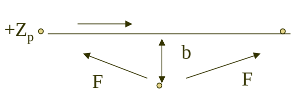


$$\Delta p_{||} = 0$$

$$\Delta p_\perp = \int_{-\infty}^{\infty} F_\perp dt$$

- **Fully stripped ion pass near atomic electron (assumed free).**
- **σ=πb², where b is maximum impact parameter leading to ionization.**

Thompson's Treatment (1912) cnt'd



$$\Delta p_\perp(b) = \int_{-\infty}^{\infty} F_\perp dt = \frac{2e^2 Z_p}{Vb}$$

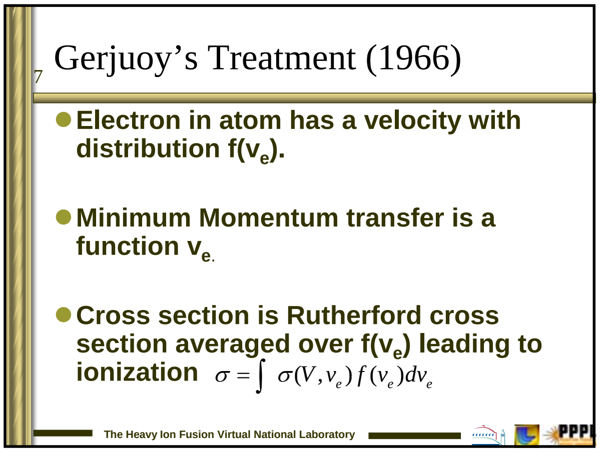
Momentum transfer as a function of impact parameter for Coulomb interaction.

$$(\Delta p_\perp)^2 / 2m = I$$

Momentum transfer needed for ionization with ionization potential I.

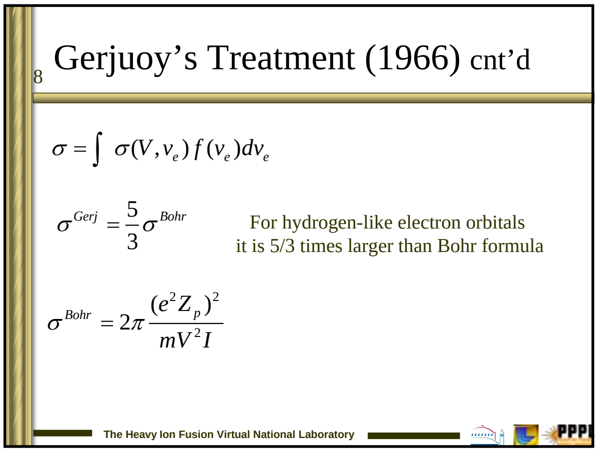
$$\sigma^{Bohr} = 2\pi \frac{(e^2 Z_p)^2}{mV^2 I}$$

Thompson – Bohr formula



Gerjuoy’s Treatment (1966)

- **Electron in atom has a velocity with distribution f(v_e).**
- **Minimum Momentum transfer is a function v_e.**
- **Cross section is Rutherford cross section averaged over f(v_e) leading to ionization** $\sigma = \int \sigma(V, v_e) f(v_e) dv_e$



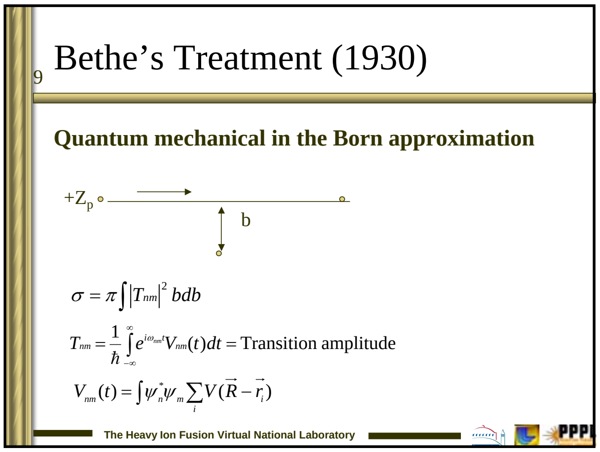
Gerjuoy’s Treatment (1966) cnt’d

$$\sigma = \int \sigma(V, v_e) f(v_e) dv_e$$

$$\sigma^{Gerj} = \frac{5}{3}\sigma^{Bohr}$$

For hydrogen-like electron orbitals it is 5/3 times larger than Bohr formula

$$\sigma^{Bohr} = 2\pi \frac{(e^2 Z_p)^2}{mV^2 I}$$



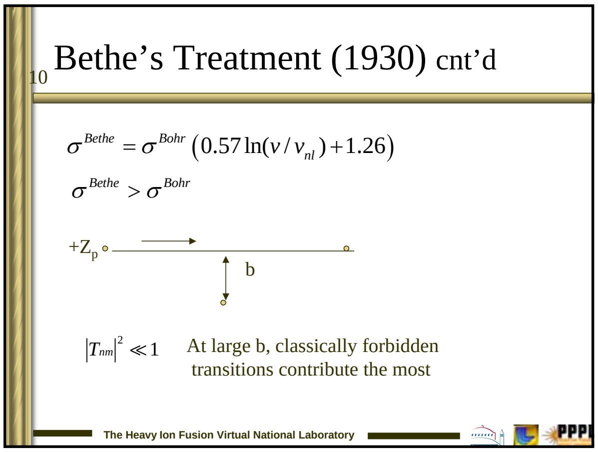
Bethe’s Treatment (1930)

Quantum mechanical in the Born approximation

$$\sigma = \pi \int |T_{nm}|^2 \, b db$$

$$T_{nm} = \frac{1}{\hbar}\int_{-\infty}^{\infty} e^{i\omega_{nm}t} V_{nm}(t) dt = \text{Transition amplitude}$$

$$V_{nm}(t) = \int \psi_n^* \psi_m \sum_i V(\vec{R} - \vec{r}_i)$$

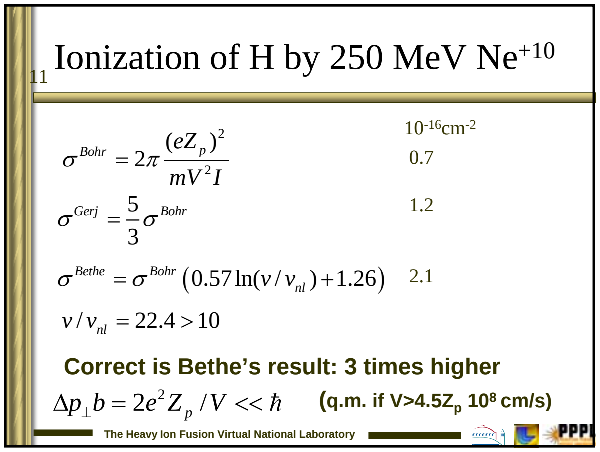


Bethe’s Treatment (1930) cnt’d

$$\sigma^{Bethe} = \sigma^{Bohr}\left(0.57\ln(v/v_{nl}) + 1.26\right)$$

$$\sigma^{Bethe} > \sigma^{Bohr}$$

$|T_{nm}|^2 \ll 1$ At large b, classically forbidden transitions contribute the most



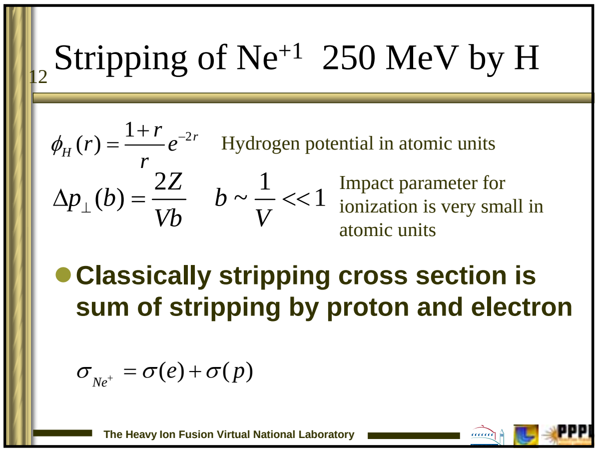
Ionization of H by 250 MeV Ne^{+10}

	10^{-16}cm^{-2}
$\sigma^{Bohr} = 2\pi \frac{(eZ_p)^2}{mV^2 I}$	0.7
$\sigma^{Gerj} = \frac{5}{3}\sigma^{Bohr}$	1.2
$\sigma^{Bethe} = \sigma^{Bohr}\left(0.57\ln(v/v_{nl}) + 1.26\right)$	2.1

$$v/v_{nl} = 22.4 > 10$$

Correct is Bethe’s result: 3 times higher

$\Delta p_\perp b = 2e^2 Z_p / V << \hbar$ **(q.m. if V>4.5Z$_p$ 10^8 cm/s)**



Stripping of Ne^{+1} 250 MeV by H

$\phi_H(r) = \frac{1+r}{r} e^{-2r}$ Hydrogen potential in atomic units

$\Delta p_\perp(b) = \frac{2Z}{Vb}$ $b \sim \frac{1}{V} << 1$ Impact parameter for ionization is very small in atomic units

- **Classically stripping cross section is sum of stripping by proton and electron**

$$\sigma_{Ne^+} = \sigma(e) + \sigma(p)$$

The Born Approximation Formulary

$$\sigma = \int_0^\infty P(q)\frac{d\sigma}{dq}dq \qquad P_{nm}(q) = \int \sum_i e^{i\vec{q}\cdot\vec{r}} \psi_n^*(A)\psi_m(A)dA$$

P is the probability of transition due to momentum transfer q
dσ/dq is differential cross section for transfer of momentum q.

$$\frac{d\sigma}{dq} = \frac{8\pi}{v^2}\frac{Z_s(q)^2 + Z_{AS}(q)^2}{q^3}$$

$$Z_S(q) = Z - \sum_{j=1}^{N} F_{jj}(q) \quad Z_{AS}(q) = N - \sum_{j=1}^{N} |F_{jj}(q)|^2 \quad F_{jj}(q) = \langle j\,|\exp(i\vec{q}\cdot\vec{r})|\,j\rangle$$

F is the form factor – the FFT of the electron density of orbital

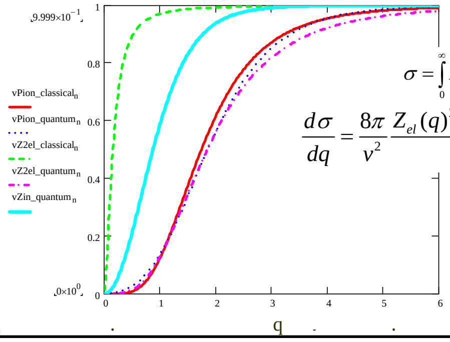
The Born Approximation Formulary cnt'd

$$\frac{d\sigma}{dq} = \frac{8\pi}{v^2}\frac{Z_{el}(q)^2 + Z_{in}(q)^2}{q^3}$$

For fully stripped target, $Z_{el}(q)=Z_t$ $Z_{in}(q)=0$ and cross section is the Rutherford cross section.

For target with electrons Z_{el} is effective charge of nucleus screened by electrons, Z_{in} describes scattering by electrons of the target.

Classical Versus Quantum Approaches for Stripping of Ne^{+1} 250 MeV by H



$$\sigma = \int_0^\infty P(q)\frac{d\sigma}{dq}dq$$

$$\frac{d\sigma}{dq} = \frac{8\pi}{v^2}\frac{Z_{el}(q)^2 + Z_{in}(q)^2}{q^3}$$

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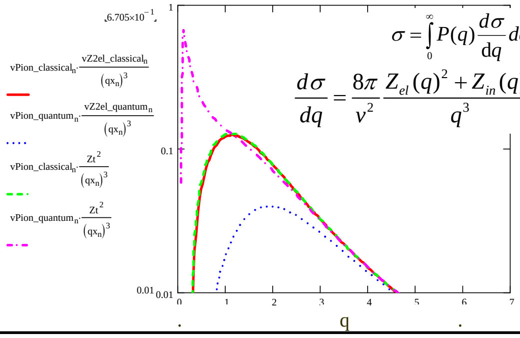

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$$\frac{d\sigma}{dq} = \frac{8\pi}{v^2}\frac{Z_{el}(q)^2 + Z_{in}(q)^2}{q^3}$$

Stripping of Ne^{+1} 250 MeV by H

	10^{-19}cm^{-2}
$\sigma^{Bohr}(p) = 2\pi\frac{(eZ_p)^2}{mV^2 I}$	2.3
$2\sigma_H = 2\frac{5}{3}\sigma^{Bohr}(p)$	7.8 (exact 7.6)
$\sigma^{Bethe}(p)$	6.3
σ_H^{BA}	1.7+3.1=4.8

Correct is the Born Approximation (BA)

4.8 10^{-19}cm^{-2}

Conclusions (1/2)

- **Ionization of H by 250 MeV Ne^{+10}**
  - The Bohr formula 0.7 10^{-16}cm^{-2}, Gerjou 1.2 10^{-16}cm^{-2}
  - The Bethe formula **2.1 10^{-16}cm^{-2}**
- **Quantum mechanics gives larger cross section due classically forbidden transitions at large impact parameters**

$$\sigma^{Bethe} = \sigma^{Bohr}\left(0.57\ln(v/v_{nl}) + 1.26\right)$$

Conclusions (2/2)

- **Stripping of Ne^{+1} 250 MeV by H**
  - The Bohr formula 2x 2.3, Gerjou- 7.8 10^{-19}cm^{-2}
  - The Born approx. for H **4.8**, for proton 6.3 10^{-19}cm^{-2}

Collision with H can be viewed as collision with separate electron and proton, but

in quantum mechanics the proton screening by an electron has to be accounted for and reduces the proton cross section by a factor of two.

If Projectile Energy E >$2Z_t I_p$kev/amu the Description Has to Be Quantum Mechanical!

Here Z_t is effective charge of the target and I_p is the ionization potential of the projectile electron orbital.

- Quantum vs classical mechanics gives
  - larger ionization cross sections by fully stripped projectiles
    - due absence of long range interactions and classically forbidden transitions at large impact parameters
  - smaller stripping cross sections by neutral atoms
    - due absence of long range interactions and classically forbidden transitions at large impact parameters and
    - failure of the assumption of classical mechanics that an electron can be localized at very small impact parameters due uncertainty principle.
  - I. D. Kaganovich, et al., "Phys. Rev. A **68**, 022707 (2003), http://arxiv.org/abs/physics/0304112

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Simple Derivation of Plasma Frequency

E=4πenδx

$$m\frac{d^2\delta x}{dt^2} = -eE$$

$$m\frac{d^2\delta x}{dt^2} = -4\pi e^2 n\delta x \quad => \quad \omega_p^2 = \frac{4\pi e^2 n}{m}$$

Electron plasma frequency

Simple Derivation of Filamentation Instability

B=$4\pi e n_b V_b \delta x/c$

$$M_b\frac{d^2\delta x}{dt^2} = \frac{eV_b}{c}B$$

$$M\frac{d^2\delta x}{dt^2} = \frac{4\pi e^2 V_b^2 n_b}{c^2}\delta x => \quad \gamma^2 = \frac{4\pi e^2 n V_b^2}{Mc^2} = \omega_{pb}^2\beta^2$$

Increment of filamentation instability is the ion plasma frequency times beta.

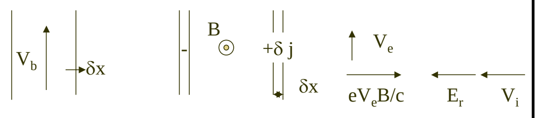
Account of the Electron Return Current

- **Electron current tends to neutralize magnetic field if** δx>skin depth=c/ω_p

$$\gamma^2 = \omega_{pb}^2\beta^2\frac{1}{1+\omega_{pe}^2/k^2c^2}$$

=>increment decreases for kc/ω_p<1

Account of the Background Ion Radial Displacement



There is uniform neutralizing electron current $V_e n_e$.

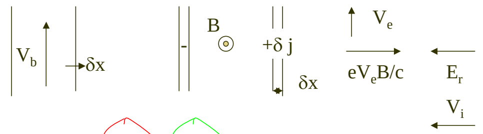
Radial Electric field build up,

it expels the background plasma (ion and electrons) away from δ j, thus,

it reduces the electron return current and

increasing magnetic field and instability.

Account of the Background Ion Radial Displacement Enhances Instability



$$\gamma^2 = \frac{\omega_{pb}^2 \boxed{(\beta - \beta_e)^2} + \boxed{\omega_{pi}^2 \beta_e^2}}{1 + \omega_{pe}^2 / k^2 c^2}$$

Effect of radial electric field on electrons and ions

For light ions like H: $\omega_{pb}^2/\omega_{pi}^2 = M/M_p = 20$ and the second term is larger if $\beta_e \sim \beta_b$ ($n_e \sim n_b$).

Example for NDC **Ne^{+1} in H**

$$\gamma^2 = \frac{\omega_{pb}^2 (\beta - \beta_e)^2 + \omega_{pi}^2 \beta_e^2}{1 + \omega_{pe}^2 / k^2 c^2}$$

3kA Ne^{+1} 250 MeV in H

100m of neutralized drift

$$\frac{L}{V_b}\gamma = \frac{L}{V_b}\omega_{pb}\beta = 0.1 \qquad \frac{L}{V_b}\gamma = \frac{L}{V_b}\omega_{pi}\beta = 0.5$$

H ions are fixed, H ions move and $n_e = n_b$