# Fast Evaluation of Ionization Cross Sections for Ion-Atom Collisions in High Energy Ion Beams

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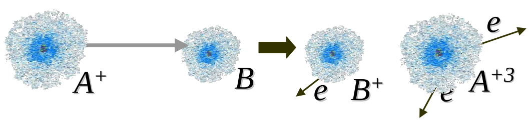
## In Collaboration with

- **Theory** (PPPL):
  - E. A. Startsev, R. C. Davidson,
  - S. R. Kecskemeti, A. Bin-Nun, T. Bender
- **Experiment**
  - D. Mueller and L. Grisham (PPPL)
  - R. L. Watson, V. Horvat, K. E. Zaharakis, and Y. Peng (Cyclotron Institute, TX A&M University)
- **Atomic electron functions**
  - T. Koga (Muroran Institute of Technology, Japan)

## Ion-atom Stripping Cross Sections

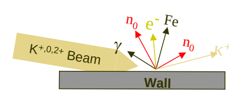



- **Ion – atom collisions occur**
  - Injector
  - Accelerator
  - Fusion chamber

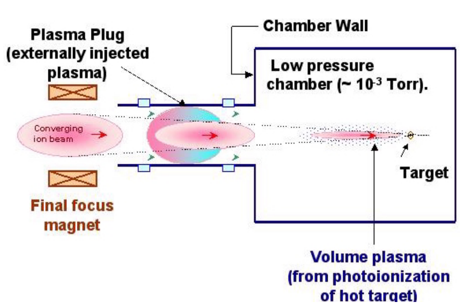
## Ion-atom collisions produce electrons and set vacuum requirements

Ion Beam hitting gas or walls creates electrons and gas.

Collective interaction of the ion beam with electrons produce two stream (hose) instability which leads to beam loss.




## Plasma Neutralizes Ion Beam Charge and Provides Tight Focus




## Outline

- **Motivation**
  - Why study cross sections?
  - What do we have to do?
- **Experimental Results**
  - Multi Electron Stripping
  - Extensive data base for theory validation
- **Theory**
  - Theoretical approaches to cross section evaluation
  - New fit formula

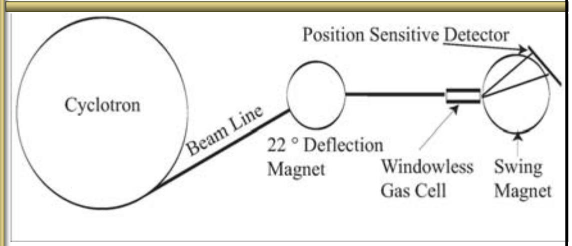
## Motivation: **Why study cross sections**

- Heavy Ion Fusion needs data for ion-atom collisions
  - low charged state
  - Speed up to 0.2c
  - Various pairs of ion and atoms
- No experimental data until driver is build
- Need to rely on theory

## Motivation: **What do we have to do?**

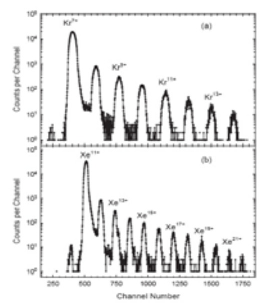
- Collect as much experimental data for ion-atom stripping cross sections
- Validate theory
- Build atomic codes

## Experiments on TX A&M Cyclotron




- Ion beams 3.4-38 MeV/amu
- Limited range of Z/M

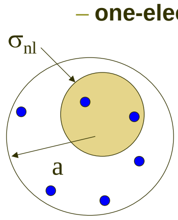
## Clear Evidence of Multiple Electron Stripping




- Charge distributions $Kr^{+7}$ and $Xe^{+11}$
  - 3.4MeV/amu
  - $N_2$ 4mTorr gas
- Peak ~ gas pressure =>
  - Single event of multiple electron loss
  - not many collisions

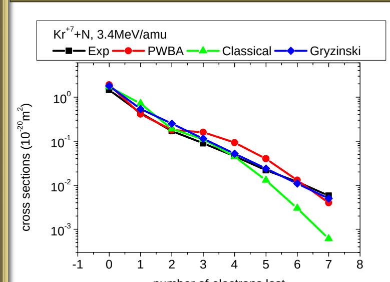
## Multiple Electron Stripping in Ions with Many Electrons

- Multiple electron stripping occurs if
  - number of electron ● ($N_{nl}$)
  - one-electron cross section $\sigma_{nl}$




$$N_{nl}\ \sigma_{nl} > \pi a^2$$

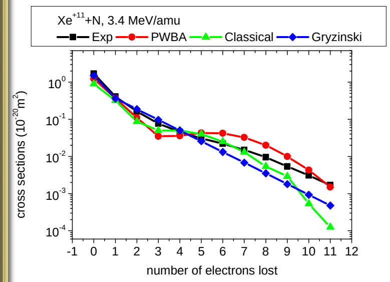
## Multiple Electron Losses Cross Sections 3.4MeV/amu $Kr^{+7}$ in $N_2$




$Kr^{+7}$ has 29 electrons

Average number of electron lost per collision 1.9

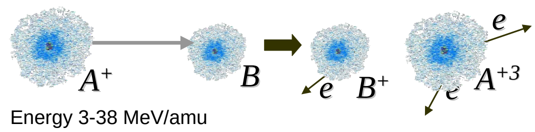
## Multiple Electron Losses Cross Sections 3.4 MeV/amu $Xe^{+11}$ in $N_2$




**$Xe^{+11}$ has 43 electrons**

**Average number of electron lost per collision 2.0**

## Extensive Experimental Data Base for Theory Validation



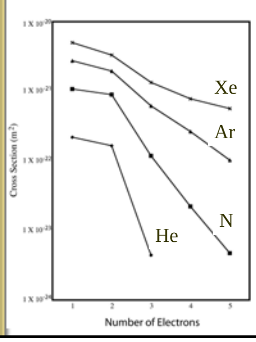

Energy 3-38 MeV/amu

Kr 7+ and Xe $^{+11}$ in $N_2$;

Ar $^{+6}$, Ar $^{+8}$, $He^{+}$, N $^{+6}$ — all in He, $N_2$, Ar and Xe.

- See, D. Mueller, et al., Laser and Particle Beams **20**, 551 (2002); Physics of Plasmas, **8**, 1753 (2001).

## Electron Loss Cross Sections for 10.2 MeV/amu $Ar^{+6}$ in Various Gases




**Average number of electron lost per collision:**

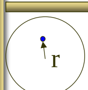
- **He 1.45**
- **N 1.57**
- **Ar 1.77**
- **Xe 1.96**

## Theoretical Approaches to Cross Sections Evaluation

**Solving for 3D Schrödinger equation for electron wave-functions in many electron system is impossible => approximations**

- **Classical description of electron motion**
- **N. Bohr**
  - K. Dan. Vidensk. Selsk. Mat.-Fys. Medd., (1948)
- **Quantum mechanical**
  - **Born approximation**
- **H. Bethe**
  - Ann. Phys. (Leipz.) (1930)

## Qusiclassical approach can predict easily ionization potentials of most elements




$$V(r) = V_{TF}(r) + \frac{1}{r} + V_{exch}(r) - \frac{(l+1/2)^2}{r^2}$$

$$V_{TF}(r) = \frac{Z}{r} X\left(\frac{Z^{1/3} r}{0.885}\right) \qquad V_{exch}(r) = 0.34\sqrt{V_{TF}}$$

$$\oint \sqrt{E_{n,l} - V(r)}\,dr = 2\pi\hbar(n_r + 1/2)$$

- **$E_{n,l}$ gives orbital binding energy (ionization potential) $n=n_r+l$**

## Qusiclassical approach can predict easily ionization potentials of most elements

Argon, Ar Z=18

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

$$\oint p_r dr = 2\pi\hbar(n_r + 1/2)$$

| Electron state | Exact $E_{n,l}$, eV | Quasi-Classical $E_{n,l}$, eV |
|---|---|---|
| 3S | 29.2 | 28.3 |
| 2S | 324 | 301 |
| 1S | 3200 | 3073 |
| | | |
| 3P | 15.8 | 14.8 |
| 2P | 247 | 240 |

## Comparison of Experiment with Calculations

**Table. The total electron-loss weighted cross-sections of $He^{+}$ on 30MeV/amu compared with the calculated cross sections in units of $10^{-22}$ $m^2$.**

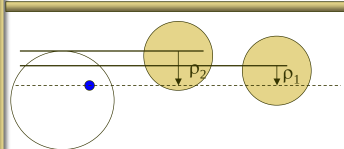
| Target | Experiment | Theory Born | Theory Classic |
|---|---|---|---|
| He | 0.4±0.1 | 0.30 | 0.69 |
| N | 1.9±0.1 | 2.4 | 4.1 |
| Ar | 7.3±0.4 | 9.0 | 11.5 |
| Xe | 23.±1. | 47 | 36 |

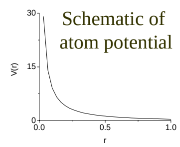
## Comparison of Experiment with Calculations

**Table. The total electron-loss weighted cross-sections of $N^{+6}$ on 38MeV/amu compared with the calculated cross sections in units of $10^{-22}$ $m^2$.**

| Target | Experiment | Theory Born | Theory Classic |
|---|---|---|---|
| He | 0.06±0.01 | 0.044 | 0.046 |
| N | 0.34±0.04 | 0.34 | 0.36 |
| Ar | 1.64±0.03 | 1.58 | 1.58 |
| Xe | 6.29±0.04 | 10.30 | 6.50 |

## Hybrid Method of Cross Sections Calculations




Schematic of atom potential

$\int_{-\infty}^{\infty} V[r(t,\rho_1)]dt > \hbar$ — **Classical mechanics**

$\int_{-\infty}^{\infty} V[r(t,\rho_2)]dt < \hbar$ — **Born approximation of quantum mechanics**

See, I. Kaganovich, et al., Nuclear Instruments and Methods in Physics Research, **544**, 91 (2005); Physics of Plasmas **11** 1229 (2004).

## Results of Hybrid Method: $He^{+}$

**Table. The total electron-loss weighted cross-sections of $He^{+}$ on 30MeV/amu compared with the calculated cross sections in units of $10^{-22}$ $m^2$.**

| Target | Experiment | Theory Born | Theory Classic | Theory Hybrid |
|---|---|---|---|---|
| He | 0.4±0.1 | 0.30 | 0.69 | 0.30 |
| Ar | 7.3±0.4 | 9.0 | 11.5 | 9.1 |
| Xe | 23.±1. | 47 | 36 | 33 |

**Indicates the valid approximation**

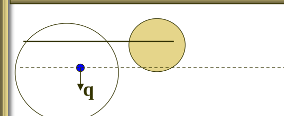
## Results of Hybrid Method: $N^{+6}$

**Table. The total electron-loss weighted cross-sections of $N^{+6}$ on 38MeV/amu compared with the calculated cross sections in units of $10^{-22}$ $m^2$.**

| Target | Experiment | Theory Born | Theory Classic | Theory Hybrid |
|---|---|---|---|---|
| He | 0.06±0.01 | 0.044 | 0.046 | 0.044 |
| Ar | 1.64±0.03 | 1.58 | 1.58 | 1.68 |
| Xe | 6.29±0.04 | 10.30 | 6.50 | 6.9 |

**Indicates the valid approximation**

## Detailed Comparison Between Classical and Quantum Mechanical Calculations




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

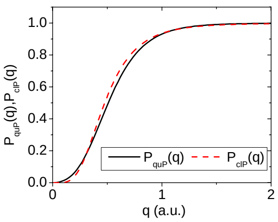
where P(q) is the probability of electron stripping from the projectile when the electron acquires the momentum q, and dσ/dq is the differential cross section for scattering with momentum q.

See, I. Kaganovich, et al., Phys. Rev. A **68**, 022707 (2003)

## The Probability of Electron Stripping From the Projectile

- **Born Approximation**

$$P_{quP}(q)=\int\left|<nl\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}\,|\,\mathbf{k}>\right|^2 d^3\mathbf{k}.$$




- **Classical Mechanics**

$$P_{clP}(q)=\int\Theta\left(\mathbf{q}\cdot\mathbf{v}_e+\frac{q^2}{2m_e}-I_{nl}\right)f(\mathbf{v}_e)\mathbf{d}\mathbf{v}_e.$$

$$f\left(\mathbf{v}_e\right)=Cv_e^2\int\delta\left(\frac{m_e v_e^2}{2}-\frac{e^2 Z_T}{r}+I_{nl}\right)r^2 dr.$$

Classical mechanics prescribes the electron velocity distribution function (EVDF) for hydrogen-like orbitals as a microcanonical ensemble

## The Differential Cross Section for Scattering with Momentum q

- **Born Approximation**

$$\frac{d\sigma}{dq}=8\pi a_0^2\frac{v_0^2(m_e v_0)^2}{v^2}\frac{Z_{quT}^2(q)+N_{eT}(q)}{q^3},$$

$$Z_{quT}(q)=\left|Z_T-\sum_{nl}F_{nlT}(q)\right|,$$

$$N_{eT}(q)=[N_{eT}^{total}-\sum_{nlT}\left|F_{nlT}(q)\right|^2].$$

For Coulomb Potential $Z_{qu}=Z_{cl}$!!!!

- **Classical Mechanics**

$$\frac{d\sigma}{dq}=2\pi\rho\frac{d\rho}{dq}.$$

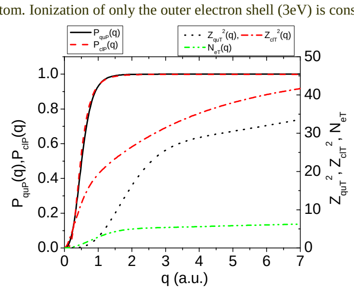
$$q(\rho)=-\frac{2\rho}{v}\int_\rho^\infty\frac{dU_T}{dr}\frac{1}{\sqrt{r^2-\rho^2}}dr,$$

$$Z_{clT}(q)=\frac{qv}{2m_e a_0 v_0^2}\sqrt{-q\rho(q)\frac{d\rho}{dq}},$$

$$\frac{d\sigma}{dq}=8\pi a_0^2\frac{v_0^2(m_e v_0)^2}{v^2}\frac{Z_{clT}(q)^2+N_{eT}^{total}}{q^3}.$$

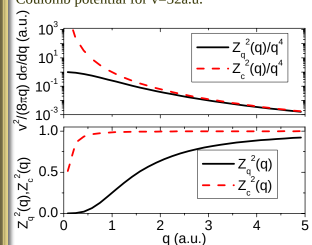
## The Differential Cross Section for Scattering with Momentum q

Shown in the figure is a comparison of the ionization probabilities and the effective charges in quantum and classical mechanics for 3.2GeV $I^-$ ions colliding with a nitrogen atom. Ionization of only the outer electron shell (3eV) is considered.




## The Differential Cross Section for Screened Coulomb Potential $e^{-r}/r$

Plot of the differential cross section for shielded Coulomb potential for v=32a.u.




Quantum tends to the Rutherford cross section for q>>1

$$\frac{d\sigma}{qdq}=\frac{8\pi}{v^2}\frac{1}{(q^2+1)^2}$$

Classical for ρ>>1, q>>2/v

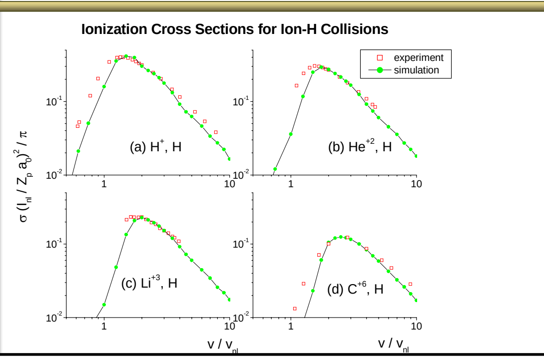
## Detailed Comparison Between Classical and Quantum Mechanical Calculations of Electron Striping by Atomic Nitrogen

| σ, $10^{-16}cm^{-2}$ | Quantum | Classical |
|---|---|---|
| $H^-$, 0.75eV | 0.1 | 1.34 |
| $I^-$, 3eV | 0.08 | 0.47 |
| $Cs^+$, 25eV | 0.045 | 0.1 |

V=32a.u.

Note, for $N^{+7}$ $\sigma_{qu}/\sigma_{cl}=0.57\ln(v/v_{nl})+1.26$

## Classical Calculation Works Well If Projectile Velocity is Comparable to the Electron Orbital Velocity



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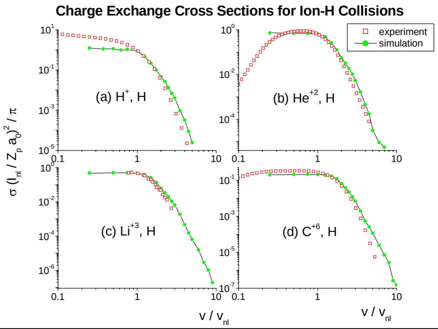



## Developing Simple Fit Formulas

- **Ionization by fully stripped ions**

$$\sigma^{Bohr}(v, I_{nl}, Z_p) = 2\pi Z_p^2 a_0^2 \frac{v_0^2 E_0}{v^2 I_{nl}}.$$

$$\sigma^{Bethe} = \sigma^{Bohr}(v, I_{nl}, Z_p)\left[0.566\ln\left(\frac{v}{v_{nl}}\right)+1.261\right].$$

$$\frac{\sigma(v, I_{nl}, Z_p) I_{nl}^{\ 2}}{2\pi Z_p^2 a_0^2} = F\left(\frac{v_{nl}^2}{v^2}\right).$$

F is a function of only $v/v_{nl}$

## Ionization Cross Sections of Hydrogen by Fully Stripped Ions Experiment Vs Theory

**Classical mechanical calculation**

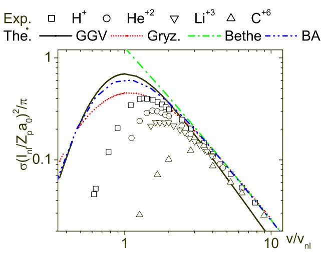
**GGV - the due to Gerjuoy**

**Gryz - the Gryzinski fit**

**Quantum-mechanical calculation**

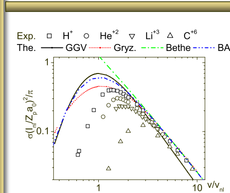
**Bethe – Bethe formula**

**BA- in the Born approximation.**




**All values are in atomic units: the ionization potential $I_H$ =1/2, $v_0$=2.2 $10^8$*cm/s*, $a_0$ =0.529 $10^8$*cm*.**

## Failure of the Gryzinski Formula



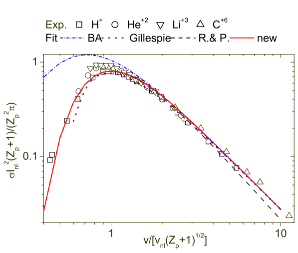

**Applied classical mechanics by averaging Rutherford cross section over atomic electron distribution (EVDF)**

**Took wrong EVDF $\langle v^2 \rangle = \infty$ !**

**Did not account for the electron circulation around nucleus !**

## We Developed New Fit

**Ionization cross sections of *hydrogen* by fully stripped ions showing the scaled experimental data and the theoretical fits**




BA - the Born approximation

Gillespie - Gillespie's fit

"New" denotes the new fit

**Velocity is scaled on**

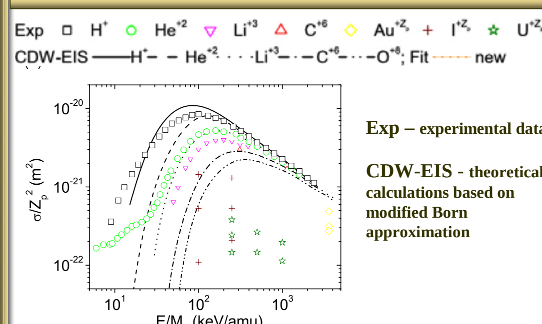
$$v_{nl}\sqrt{Z_p+1}$$

**Cross section - on**

$$I_{nl}^2 (Z_p+1)/Z_p^2$$

See, I. Kaganovich, et al., arxiv. 0407140, Phys. Plasmas **11** 1229 (2004).

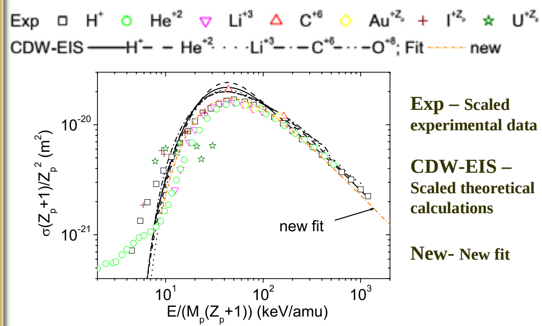
## Ionization Cross Sections of Helium by Fully Stripped Ions Experimental Data




**Exp – experimental data**

**CDW-EIS - theoretical calculations based on modified Born approximation**

# Applying New Fit to He Cross Sections




**Exp** – Scaled experimental data

**CDW-EIS** – Scaled theoretical calculations

**New**- New fit

# Conclusions

- **We have recently investigated theoretically and experimentally the stripping of more than 18 different pairs of projectile and target particles in the range of 3-38 MeV/amu to study the range of validity of both the Born approximation and the classical trajectory calculation.**
- **The new scaling in for the ionization and stripping cross sections of atoms and ions by fully stripped projectiles has been proposed.**
- **We have developed hybrid method, which combine both approximations and helps to identify which method is more trustworthy and produces more reliable results than either of approximations separately.**