Atomic collisions

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Collision (excitation)

Continuum

Main binary quantity: cross section \( \sigma(E) \) [cm\(^2\)]

Effective area for a particular process

\[
\sigma(E) = \int f(E, \theta, \phi) d\Omega
\]

\( f \) is the scattering amplitude

Process rate in plasmas:

\[
R[s^{-1}] = N(\sigma v) = N \int \sigma(E) v f(E) dE
\]

Direct and inverse

Quantum mechanics tells us that characteristics of direct and inverse processes are related

\( \Delta E \) is the excitation threshold

Klein-Fockel formula:

\[
\Omega_{ij}(E + \Delta E) = \Omega_{ij}(E)
\]

Ratios:

\[
\Omega_{ij}(E + \Delta E) \sigma_{exc}(E + \Delta E) = \sigma(E)\sigma_{exc}(E)
\]

Milne formula for photoionization/photorecombination:

\[
h\omega = E + E_f
\]

\[
A + h\nu \rightarrow A^\prime + e
\]

Order of cross sections

- General order
  - optically allowed > optically forbidden > spin forbidden
  - OA: long-distance, similar to E1 radiative transitions
  - The larger \( \Delta l \), the smaller cross section
- L-like ions: 2s \( \rightarrow \) 2p excitation

Collision in plasmas

• More than one particle: collisions!
• Elastic, inelastic

Number of collisions per unit time:

\[
n[1/cm^3] \cdot v[cm/s] \cdot Area[cm^2] \sim [1/s]
\]

Equilibrium plasma: \( T_e = T_i \)

\[
v_e = \sqrt{\frac{M}{m_e}} \]

Basic Parameters

Cross sections are probabilities

- Classically: \( \sigma(E, E') = \int \rho(E, E', \rho) 2\pi d\rho \)
- Typical values for atomic cross sections
  - \( \sigma_0 \sim 5 \cdot 10^{-16} \text{ cm}^2 \)
- Collision strength \( \Omega \) (dimensionless, on the order of unity):
  \[
  \sigma_0(E) = \frac{\pi \sigma_0}{\rho(E)}
  \]
  - Ratio of cross section to the de Broglie wavelength squared
  - Symmetric w/r to initial and final states

Types of transitions for excitation

- Optically(dipole)-allowed
  - Examples in He I:
  - \( 1s^2 1S \rightarrow 1s2s^1P \)
  - \( 1s2s^1S \rightarrow 1s4d^3D \)

- Spin-forbidden (EXCHANGE!)
  - \( 1s2s^1S \rightarrow 1s4d^3D \)

From cross sections to rates

Rate coefficients for an arbitrary energy distribution function

\[
\langle \sigma v \rangle = \int \sigma(E) v f(E) dE \rightarrow \left( \frac{8 \pi f(E) \sigma(E)}{m_e^2 v} \right)^{1/2} \int E \sigma(E) e^{-E/T} dE
\]

Effective collision strength:

\[
\begin{align*}
\Omega_i(E) &= \int 2\pi E f(E) dE \\
\Omega_i(E) &= \int 2\pi E f(E) dE \\
\langle \sigma v \rangle &= \frac{8 \pi f(E) \sigma(E)}{m_e^2 v} \\
\sigma_i(E) &= \frac{8 \pi f(E) \sigma(E)}{m_e^2 v} \\
\end{align*}
\]

Often only threshold is important:
van Regemorter-Seaton formula

- Optically-allowed excitations
  \[ X = E/\Delta E_{ij} \quad \sigma_{\gamma}(E) = \frac{8\pi}{\sqrt{3}} \frac{\alpha}{\Delta E_{ij}} \left| g(X) \right|^2 \frac{f_\gamma}{X} \]

- Gaunt factor

\[ X \rightarrow \omega : g(X) = \frac{\sqrt{3}}{2\pi} \sin(X) \quad \sigma'(E) = \frac{6.51 \times 10^{-18} \ln(X)}{\left[ \Delta E_{ij}/\alpha \right]^2} \frac{f_\gamma}{X} \left[ \text{cm}^{-1} \right] \]

"Recommended" Gaunt factors:

Atoms:
\[ g(\omega = 0, X) = \left[ \frac{0.53 - 0.51}{X} - \frac{0.68}{X^2} \right] \sin(X) \]

Ions:
\[ g(\omega = 0, X) = \left[ \frac{0.55 - 0.51}{X} - \frac{0.68}{X^2} \right] \sin(X) \]

Scaling of Excitations

- n-scaling
  - f-n, ΔE-n^3, σ-n^4
  - Into high n
    - f-n^0, ΔE-n^6, σ-n^3

- Z-scaling
  - Δn=0
    - f-Z^1, ΔE-Z, σ-Z^4, <σ> = Z^2
  - Δn=0
    - f-Z^0, ΔE-Z^3, σ-Z^4, <σ> = Z^3

Direct and Exchange

Direct channel

\[ \Delta E \]

Exchange channel

\[ \Delta E \]

Resonances in excitation

Direct excitation

Intermediate states

Intermediate AI states

Collisional Methods and Codes

- Plane-wave Born
- Coulomb-Born (better for highly-charged ions)
- Distorted-wave method
- Close-coupling (CC) methods
  - Convergent CC (CCC)
  - R-matrix (with PS, Dirac, etc.)
  - B-splines
  - Time-Dependent CC
- Relativistic versions are available

Ionization cross sections

\[ \sigma_{\text{ion}}(n, E) = 2.76 \pi n^2 \frac{R^2_0}{n^4} \left( \frac{\ln(E/E_0)}{E} \right) \frac{1}{Z^3} \frac{\ln X}{X} \]

Lotz formula:

Same theoretical methods as for excitation: Born, Coulomb-Born, DW, CC, CCC, RMPS...
3-Body Recombination

\[ A + e \leftrightarrow A^+ + e + e \]

3-body rate coefficient \( \alpha_{3\text{body}}(T_e) \) from ionization rate coefficient \( S_e(T_e) \):

\[
\alpha_{3\text{body}}(T_e) = \frac{g_e}{2g_{e+1}} \left( \frac{2\pi \hbar}{m_e} \right)^{3/2} \exp \left[ \frac{E_e}{T_e} \right] S_e(T_e)
\]

Rates from rate coefficients: \( n_e S_e(T_e) \) but \( n_e^2 \alpha_{3\text{body}}(T_e) \)

Likes high-n states; \( \alpha(T_e) \propto 1/T_e^{3/2} \)

Selection rules

- Examples of Al states: \( 1s2s^2, 1s^22p^1l \) (high n)
- Same old rule: before = after
- \( A^{**} \rightarrow A^+ + eI \)
  - Exact: \( P_J = P_i; \Delta J = 0 \)
  - Approximate (LS coupling): \( \Delta S = 0, \Delta L = 0 \)

Radiative Recombination

\[ A^{2+} + e \rightarrow A^{(2+)+1} + h\nu \]

(hv = E + l)

Semiclassical Kramers cross section:

\[
\sigma_{\text{semi}}(E) = \frac{64\pi^2 e^4}{3\hbar^2 m_e^4} \left( \frac{E}{T_e} \right)^3 a_0^2
\]

Quantummechanical cross section:

\[
\sigma_{\text{QM}}(E) = \sigma_{\text{semi}}(E) G_0^2(E)
\]

Cross section Z-scaling:

\[
\sigma \propto \left( \frac{\hbar}{Z} \right)^2 \alpha \left( \frac{1}{Z^2} \right)
\]

Radiative recombination

\[ A^{(2+)+1} \rightarrow A^{2+} + \nu \]

DR step 1: dielectronic capture

\[ A^{2+} + e \rightarrow A^{2+} + h\nu \]

Ion recombined

Excitation-Autoionization

\[ 3s23p63d104s2 Xe^{24+}: \text{Pindzola et al, 2011} \]

\[ 3p3d Ti^{24+}: \text{van Zoest et al, 2004} \]

IP

When EA is important:

- Few electrons on the outermost shell
- Mid-Z multielectron ions
- ...but less important for higher Z (radl)

EA in ionization cross sections is not required for detailed modeling with Al states!

FF+BF at Alcator C-mod: 1 eV, H

Edge: n=1

n=2

n=3

Lumma et al (1997)
Dielectronic capture + autoionization = no recombination

\[ \Delta E(\Delta n = 0) \ll \Delta E(\Delta n \neq 0) \approx 13.6 eV \cdot \Delta^2 \]

Continuum

Bound states

\[ A^{(2s+1)S} + e \rightarrow A^{(2p+1)P} + e \]

DC and AI are direct and inverse

\[ A^{(2s+1)S} + e \rightarrow A^{(2p+1)P} + h\nu \]

Stabilizing transition: Mostly x-rays

Dielectronic Recombination

Example: \( \Delta n = 0 \) for Fe XX \( 2s^2 2p^3 \)

\[ 2s^2 2p^4 S_{3/2} + e \rightarrow 2s^2 2p^6 (P_{3/2})_{nl} \]

\[ 2s^2 2p^4 S_{1/2} + e \rightarrow 2s^2 2p^6 (P_{1/2})_{nl} \]

\[ 2s^2 2p^4 S_{1/2} + e \rightarrow 2s^2 2p^6 (P_{3/2})_{nl} \]

\( \Delta E(\Delta n = 0) \ll \Delta E(\Delta n \neq 0) \approx 13.6 eV \cdot \Delta^2 \)

Dielectronic Recombination

Examples:

\[ 1s^2 + e \rightarrow 1s2pnl \rightarrow 1s^2 nl + h\nu \]

\[ 1s^2 2s^2 + e \rightarrow 1s^2 3pnl \rightarrow 1s^2 2pnl + h\nu \]

\[ 1s^2 2s^2 + e \rightarrow 1s^2 3s^2 \rightarrow 1s^2 2s^2 + h\nu \]

\[ 1s^2 2s^2 + e \rightarrow 1s^2 3p^2 \rightarrow 1s^2 2p^2 + h\nu \]

\[ 1s^2 2s^2 + e \rightarrow 1s^2 3s^2 \rightarrow 1s^2 2s^2 + h\nu \]

Is DR important?..

Answer: YES

Burgess (1964) was the first to show importance of DR for solar corona ionization balance

There exist a number of recommended formulas for rate coefficients of variable quality; \( Z < 30 \)

\( \alpha \) \( \propto \) \( T \), \( n \approx 0.77 \)

Higher \( l \) values are preferentially populated but it depends on collision energy

Neutral beams: \( E \approx 100 \text{ keV} \) \( \Rightarrow \) heavy particle collisions are of highest importance

Energy levels in He-like Ar

- Ground state: \( 1s^2 \, ^1S_0 \)
- Two subsystems of terms
  - Singlets \( 1s1n \, ^1L_J \) (example \( 1s3d \, ^1D_2 \))
  - Triplets \( 1s1n \, ^3L_J \) (example \( 1s2p \, ^3P_{0,1,2} \))
- Radiative transitions within each subsystem are strong, between systems depend on \( Z \)
### He-like Ar Levels and Lines

#### 1s2l'lnl satellites
- 1s2l's'\text{S}_{l'/2}
- 1s22p':
  - 1s22p(2P)\text{P}_{1/2,3/2}
  - 1s22p(2P)\text{P}_{1/2,3/2,5/2}
- 1s2p':
  - 1s2p(3P)\text{P}_{1/2,3/2,5/2}
  - 1s2p(3P)\text{P}_{1/2,3/2,5/2,7/2}
- 1s2lnl:
  - Closer and closer to W
  - Only 1s2l2l can be reliably resolved
  - Contribute to W line profile

### Z-scaling of A's
- W[E1]: A(1s^2 \text{1S}_0 - 1s2p \text{1P}_1) \propto Z^4
- Y[E1]: A(1s^2 \text{1S}_0 - 1s2p \text{3P}_1)
  - \propto Z^{10} for low Z
  - \propto Z^8 for large Z
  - \propto Z^4 for very large Z
- X[M2]: A(1s^2 \text{1S}_0 - 1s2p \text{3P}_2) \propto Z^8
- Z[M1]: A(1s^2 \text{1S}_0 - 1s2s \text{3S}_0) \propto Z^{10}

### Databases for Collisions
- IAEA
- NIFS
- TIPbase
- CCC Database
- CAMDB
- …

### NIFS database