**ATOMIC PROCESSES IN PLASMAS**

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**Outline**
- Introduction: Spectral Line Intensities
  - Survey of Atomic Processes
    - Continuum (free-free & bound-free)
    - Bound-bound Transitions
    - Thermodynamic Equilibrium and Detailed Balance
  - Laboratory and Astrophysical Plasma Regimes
  - Modeling Approximations
    - Local Thermodynamic Equilibrium
    - Level-Population Kinetic Equations
    - Approximations: Coronal, Collisional-radiative,
      Line trapping, Nubular (photo-ionized), Transient

**Spectral Line Intensities**
- Line transition from upper level j to lower level i
- Intensity (ph s⁻¹ cm⁻³) emitted in plasma \( I_j = \eta A_j \)
- The Einstein coefficient for spontaneous emission \( A_j(s⁻¹) \) is a constant of nature, e.g., in dipole approximation \( A_j = (4/3\pi)|\langle r | j | i \rangle|^2 \)
- Diagnostics come from population of upper levels \( \eta_j(T_e,n,\nu_j,\ldots) \) and mostly from line ratios
  - \( I_j / I_i = \eta_j / \eta_i (T_e, n, \nu_j, \nu_i, \ldots) \)
  - Absolute line flux (photons s⁻¹ cm⁻²)
  - \( F_j = \int I_j dV / 4\pi d^2 = \eta A_j V / 4\pi d^2 \)

**Survey of Atomic Processes**
- Basically, all permutations on reactions of ions, electrons, and photons
- Two body reactions and three some
- Resulting in ionization, recombination, excitation, de-excitation, emission, and absorption of photons
- Not all processes are relevant for a given plasma
- The challenge of plasma spectroscopy is to identify the important processes for a given plasma

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**Line Resolved Spectra**

**Continuum Processes**
- Bremsstrahlung (braking radiation)
  - \( X^+ + e^- \rightarrow X^+ + e^- + hv \)
  - Bremsstrahlung spectrum (erg s⁻¹ cm⁻³ Hz⁻¹)
    - \( \varepsilon_{ff} = 6.8 \times 10^{-16} (n_e n_i)^2 / T_e^{3/2} \) e⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻⁻~-~-~
  - becomes increasingly important with density, with charge, and maximal for \( \lambda_{\text{max}} \sim T_e / 10^7 K \) (\( g_u \approx 1 \))
- Inversely, Bremsstrahlung absorption
  - Absorption coefficient
    - \( \alpha_c = 3.7 \times 10^{20} (n_e n_i^2 / \sqrt{\nu T_e^{3/2}}) (1 - e^{-\nu / \nu_{\text{max}}}) g_{nu} \) cm⁻¹
  - Negligible for X-ray frequencies (\( \nu > 10^{17} \) Hz)
**Continuum Processes (2/4)**

- Bound-free processes
- Electron impact (collisional) ionization
  \[ X^{(q)} + e^- \rightarrow X^{(q+1)} + 2e^- \]
  - Inversely, three body recombination
  \[ X^{(q+1)} + 2e^- \rightarrow X^q + e^- \]
  - Excess energy goes to (other) free electron
  - Rate of TBR \( \sim n_e^2 \), hence less important for low-density (astrophysical) plasmas

**Continuum Processes (3/4)**

- Photo-ionization
  \[ X^{(q)} + h\nu \rightarrow X^{(q+1)} + e^- \]
  - Inversely, radiative recombination
  \[ X^{(q+1)} + e^- \rightarrow X^q + h\nu \]
  - Excess energy expelled by photon
  - Auto-ionization from doubly- or inner-shell (Auger) excited levels,
    \[ X^{(q+1)} \rightarrow X^q + h\nu \]
  - Electron impact (collisional) recombination
    \[ X^{(q+1)} + e^- \rightarrow X^q + e^- \]
    - ion absorbs excess energy
    - radiationless resonant process - well defined \( E(e) \)

**Continuum Processes (4/4)**

- Di-electronic recombination - 2 step process
  \[ X^{(q+1)} + e^- \rightarrow X^q \rightarrow X^{(q+1)} + e^- \]
  - Same initial and final states as RR
  - Quantum interference? \( \alpha_{rec} \sim |\alpha| \phi_{1s2}^+ + |\alpha| \phi_{1s2}^f \)
  - Inverse Autoionization - also 2 step process
    \[ X^{(q)} + h\nu_{id} \rightarrow X^{q+1} + e^- \]
    - Important only with energetic photons/electrons

**Dielectronic Recombination**

- Initial (free e-) Capture Final (doubly excited) (stabilization)
- Electron beam
- continuum
- L-shell
- X-shell

**DR of H-like Kr with EBIT**

![Experiment vs. Fit](Hu+13)

**Bound-Bound Transitions**

- Spontaneous photon (line) emission
  \[ X^{(q)} \rightarrow X^{(q-1)} + h\nu \]
  - Inversely, photo-excitation (~ resonant scattering)
    \[ X^{(q-1)} + h\nu \rightarrow X^{(q)} \]
  - Induced photon emission
    \[ X^{(q)} + h\nu_{ij} \rightarrow X^{(q+1)} + 2h\nu_{id} \]
  - Electron impact (collisional) excitation
    \[ X^{(q)} + e^- \rightarrow X^{(q+1)} + e^- \]
  - Inversely, electron impact de-excitation
    \[ X^{(q+1)} + e^- \rightarrow X^{(q)} + e^- \]
  - Resonant excitation via di-electronic capture
    \[ X^{(q+1)} + e^- \rightarrow X^{(q+1)} + 2e^- \]

**Related Notes**

- Close coupling methods treat \( X^q + e^- \) as one quantum mechanical system with both bound and continuum states
- Complicates the atom, but resonant processes (RE, EA) arise more naturally
- Ion-ion collisions much less important due to both repelling charges and low ion velocities (\( Q \sim v \))
- Charge exchange collisions with neutrals important in low-charge plasmas, and in interfaces of ionized and neutral gas
- Astrophysical scenarios include solar wind, supernova remnants, and in interactions of neutral gas with cosmic rays (Galactic center)

**Thermodynamic Equilibrium and Detailed Balance**

- In Thermodynamic Equilibrium (TE), the level populations and spectrum are governed by statistical physics and the 5 equations: Boltzmann, Planck, Kirchoff, Saha, Maxwell-Boltzmann
- In terms of atomic processes, each reaction is balanced by its inverse reaction
- The principle of detailed balance is used to derive relations between transition rates in TE, but since the resulting expressions involve only atomic quantities, the relations hold in any plasma
Detailed Balance: Example

- Auto-ionization and di-electronic capture (DC) (level i) \( X^{+\alpha} \rightleftharpoons X^{+\alpha+1} + e^- \) (level i)
- In TE the rates \( (\text{cm}^{-3}\text{s}^{-1}) \) are balanced locally
  \( n_i \sigma_i = n_e \sigma_{\text{DC}}(i,T) \)
- But in TE also, the populations are given by the Saha + Boltzmann equations
  \( n_i/n_e = (g_i/2g_j)(2\pi/mkT)^{3/2}E_i^{1/2} \exp[-E_i/kT] \)
  \( \Rightarrow \sigma_{\text{DC}}(i,T) = (g_i/2g_j)(2\pi/mkT)^{3/2}E_i^{1/2} \exp[-E_i/kT] A_{\text{DC}} \)
- Since this is a relation between atomic quantities it is general and valid in any plasma.

Laboratory and Astrophysical Plasma Regimes

- Collisionally dominated plasma
- Net full TE: Equilibrium between collisional processes only, but not radiation field
- TE properties hold except Planck spectrum, e.g., \( n_i/n_e = (g_i/2g_j) \exp[-E_i/kT] \) (Maxwell, Saha, Kirchoff)
- For collisional de-excitation to dominate over radiative decay for excited level \( (j,j_i) \)
  \( \beta_i \gg A_i \)
  Requires high density \( \rho \) Wilson criterion
  \( n_e \gg 4.8\times10^{31}q_i^2(4/7k_\text{B}eV)^{3/2} \text{ cm}^{-3} \)
- How does this depend on specific level \( j \)?
- Clearly, invalid for most astrophysical plasmas except (the important) stellar atmospheres

Local Thermodynamic Equilibrium

- Non-LTE brute-force: Include all processes in transition-rate matrix
- For each level \( i \) \( \text{dn}/\text{dt} = + \) (populating) - (depleting) rates
- \( J_i \) may require proper radiative transfer
- Need to solve set of \( N \) linear equations
- For \( N \) levels, how many independent equations?

Atomic Level-Population Kinetic Equations

Coronal Approximation

- High-\( T \)
- Low-\( n \)
- Optically-Thin Plasmas \( (J_i = 0) \)

Coronal Approximation

- Rates \( (n_i^2) \ll \) Rates \( (n_i) \ll \) Rates (spontaneous)
  - 3-body recombination not important
  - Collisional processes from excited levels dominated by spontaneous radiative decays
  - Left with collisional processes from ground levels and radiative processes from excited levels
- Atomic processes: Coll. ionization (including EA), radiative recombination (including DR), collisional excitation, radiative decay (including cascades)
- Ions basically in their ground state
- Ionization decoupled from excitation
Coronal Approximation (2/3)
- Leads to very simple expressions
  - Steady state excitation
    \[ n_i Q_i(T) = n_e \sum A_{ji} \Rightarrow n_i = \frac{n_e Q_i(T)}{\sum A_{ji}} \]
  - Unlike LTE (Boltzmann), depends on rates & not \( n_e \)
  - Line ratios independent of density
  - Steady state ionization balance
    \[ n_q \alpha_{q+1}(T) = n_{q-1} \alpha_{q-1}(T) \]
  - Since for \( q=0 \)
    \[ n_0 \alpha_{0+1}(T) = n_{-1} \alpha_{-1+1}(T) \]
  - The general solution is:
    \[ \frac{n_0}{n_i} = \frac{S_{q+1}(T)}{\alpha_{q+1}(T)} \]

Coronal Approximation (3/3)
- Effect can be approximated by transmission
  - Affects level populations, and obviously spectrum
  - Only resonant lines?
  - Other absorption
    - Resonant scattering: line photons can be absorbed and re-emitted, unless strong velocity shear
      - How do populations & ionizations compare with LTE? Are they higher? lower?
  - Normalize and assume no particle losses (laboratory)

Coronal Approximation (4/5)
- Approximation breaks down for
  - Meta-stable levels (forbidden decay)
  - Close (high) lying levels \( Q_i = E_i^0, S_j = E_j^{-2} \)
  - Effect of "continuum lowering" to "thermal limit" where high-lying levels \( \Rightarrow \) LTE, and are more likely to be excited or ionized than to decay radiatively
  - Effect other than density with same result?
  - These high lying levels effectively become part of the continuum \( q+1 \) via electron impact ionization, thus modifying the ionization balance equations

Coronal Approximation (5/5)
- The higher \( n_e \), the more levels depart from "coronal" and tend to "thermal"
- Requirement for small effect is used to determine validity of approximation, say \( \frac{S_{\text{thermal}}}{S} \)
  - Results in another Wilson criterion
    \[ n_e < 4 \times 10^{21} q^{-4} (kT/1\text{keV})^4 \text{ cm}^{-3} \]
  - Intermediate densities (laboratory plasmas) hardest to model
  - How do populations & ionizations compare with LTE? Are they higher? lower?

Coronal Regime
- Intermediate density, but optically thin
  - Includes cascades and collisional transitions to/from excited levels
    \[ n_i A_{ji} = n_e \sum Q_i(T) = n_e \sum A_{ji} \]
  - Need to solve transition matrix (for ionization?)
  - Normalize and assume no particle losses (laboratory)

Collisional-Radiative Model (2/3)
- Unlike coronal, excited levels can be (depending on \( T_e, n_e \)) significantly populated
  - Provides density sensitive line ratios
  - Forbidden lines in laboratory plasmas?
  - Can you think of alternative density diagnostics?

Collisional-Radiative Model (3/3)
- Resonant scattering line photons can be absorbed and re-emitted, unless strong velocity shear
  - Other absorption "hazards", how important?
  - Only resonant lines?
  - Affects level populations, and obviously spectrum
  - Effect can be approximated by transmission corrections (escape-factor) to rates: \( \eta A_{ji} T_{ci} \)
    \[ 0 < T_{ci} = \exp\{-N (n_e^2/mc^2) f_i \Phi(v)\} < 1 \]
  - \( N = \int n_i d\ell \) column density, \( f_i \) - oscillator strength, and \( \Phi(v) \) - profile, generally Voigt profile, but dominated by Doppler broadening
  - Think of geometrical effects in extended sources
**Nebulae**

- Plasma at least moderately optically thick to external source, but density still low
- Steady state ionization determined not by temperature, but by balance between photo-ionization (~Fλ spectrum) and recombination (nₑ)
  \[ \eta \int F \sigma_i^\text{PI}(E) \, dE = n_\text{i} \eta_\text{r} n_\text{e}(T_\text{e}) \]
- Ionization \( n_\text{i} / n_\text{e} \sim k \eta_\text{r} \sim L / n^2 \sim T_\text{e} \)
- Unlike coronal approximation, does depend on density. Where else does ionization depend on \( n_\text{e} \)?
- With no other energy source, \( T_\text{e} \) not an independent parameter, depends on photo-heating and cooling

**Nebular Approximation (a/3)**

- \( T_\text{e} \) insufficient for electron impact excitation / ionization
- Lines (\& RRC) then driven by RR and PE
- Depend on optical depth
- Line ratios may depend on ionization balance (not decoupled)
- Why PE more effective than PI?

**Nebular Approximation (b/3)**

- Absorption
- Emission

**Nebular Approximation (c/3)**

- Individual-species temperature acquisition times through self collisions \( T_\text{i} = T_\text{col} \)
- In velocity-driven excitation (shock) \( T_\text{i} \ll T_\text{eq} \)
- Much longer equilibration time for \( T_\text{e} \sim T_\text{ion} \)
- Ionization times \( \sim 1 / \eta_\text{r} S_\text{i,rrc} \)
- Usually used within coronal approximation (low \( n_\text{e} \))

**Transient Plasma**

- What are the important X-ray plasma time scales?
- Use Coulomb collision theory (Spitzer 1956) - neglecting collective plasma effects
- \( T_\text{e} \) and \( T_\text{i} \) constant, \( T_\text{e} \ll T_\text{ion} \)
- In velocity-driven excitation (shock) \( T_\text{i} \ll T_\text{eq} \)
- Conduction time for \( T_\text{e} \) much shorter than \( T_\text{eq} \)
- Ionization times \( \sim 1 / \eta_\text{r} S_\text{i,rrc} \)
- Usually used within coronal approximation (low \( n_\text{e} \))

**Transient Plasma (2/6)**

- Temporal Hierarchy

\[
\begin{align*}
 t_\text{c,eq} &= 10.4 \left( \frac{k_\text{B} T_\text{e}}{1 \text{keV}} \right)^{3/2} \left( \frac{1 \text{cm}^{-3}}{n_\text{e}} \right) \text{yrs} \\
 t_\text{c,com} &= 530 \left( \frac{k_\text{B} T_\text{com}}{1 \text{keV}} \right)^{3/2} \left( \frac{1 \text{cm}^{-3}}{n_\text{com}} \right) \frac{1}{k_\text{B} T_\text{com}} \text{yrs} \\
 t_\text{ce} &= 23,000 \left( \frac{k_\text{B} T_\text{e}}{1 \text{keV}} \right)^{3/2} \left( \frac{1 \text{cm}^{-3}}{n_\text{e}} \right) \frac{1}{k_\text{B} T_\text{e}} \text{yrs} \\
 t_\text{ion} &= \frac{1}{n_\text{e} \alpha \bar{R}(T_\text{e})} = 100,000 \left( \frac{1 \text{cm}^{-3}}{n_\text{e}} \right) \text{yrs}
\end{align*}
\]

**Transient Plasma (3/6)**

- Transition matrix of electron impact ionization and recombination rates
- In coronal approximation depends on \( T_\text{e} \) and \( n_\text{e} \)
- If rates (\( \lambda \)) constant, analytical solution possible by recasting \( T \) with similar diagonal matrix \( T = S^{-1} \Sigma S \) (eigenvalues \( \lambda \), in diagonal)
- How to normalize?

**Transient Plasma (4/6)**

- Set of independent differential equations (for \( \mathbf{S} \))

\[
\begin{align*}
 \dot{\mathbf{S}} &= \mathbf{S}(\lambda - \Sigma) \mathbf{S} \\
 \dot{\mathbf{T}} &= \mathbf{T}(\lambda - \Sigma) \mathbf{T}
\end{align*}
\]

- Solution: linear combination of exponents
**Transient Plasma (5/6)**

- $n_Q(t)$ is sum of exponentials with typical time scales
- With independent measure of $T_e$, ion ratios can be used to deduce $n_Q(t)$
- Using emission measure and volume estimate, can disentangle time ($t$) from density ($n_e$)

**Transient Plasma (6/6)**

- Slowly approaches steady state
- In last stages only two relevant charge states remain, $n_1$ and $n_{Q-1}(=1-n_1)$
- The rate equation then is simply $\frac{dn_Q}{dt} = n_1(n_{Q-1}S_{Q-1} - n_Q\alpha_Q)$
  whose solution is $n_Q = S/(S + \alpha)(1 - e^{-\alpha_QS\cdot t})$
- Tends exponentially to steady state within times $t_{ss} \approx 1 / n_e(S + \alpha) \approx 10^{12} / n_e$ sec \~\ 100,000 / $n_e$ yrs
- Excited-level lifetimes much shorter <10$^{-8}$s, don’t affect transient ionization/recombination

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**Recap: Models & Diagnostics**

- Coronal model:
  - Temperature (EMD) from charge states - independent of $n$ (and less from inter-ion lines and from bremsstrahlung)
  - Elemental abundances
- Collisional-radiative:
  - Cascades, density (and temp) from forbidden lines
  - Optical depth (and position) from line quenching
- Nebular:
  - Temperature from RRC width
  - Combination of [density + position] from charge states
- Transient plasma:
  - Ionization time, but temperature?
  - Density and time from emission measure

Thank you for your attention