ATOMIC PROCESSES IN LABORATORY & ASTROPHYSICAL PLASMAS

X-Ray Spectroscopy School
MSSL , March 2009

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, Nebular (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 $I_{ji} = n_j A_{ji}$
- The Einstein coefficient for spontaneous emission A_{ji} (s^{-1}) is a constant of nature, e.g., in dipole approximation $A_{ji} = (4/3\hbar)(\omega_{ij}/c)^3 |\, \langle i|\mathbf{r}_{ij}|j\rangle \,|^2$
- Diagnostics come from population of upper levels $n_j\,(T_e, n_e, \tau_{ij}, \ldots)$ and mostly from line ratios $I_{ji} / I_{lk} \propto n_j / n_l\,(T_e, n_e, \tau_{ij}, \tau_{kl}, \ldots)$
- Absolute line flux (photons s^{-1} cm^{-2}) $F_{ji} = \int I_{ji} dV / 4\pi d^2 \cong n_j A_{ji} V / 4\pi d^2$

Spectral Line Intensities (2/2)

- Recast $n_j \equiv (n_j/n_g)\,(n_g/n_Z)\,(n_Z/n_H)\,n_H$

$$= \bigcirc\!\!\!\!\!(n_j/n_g)\ f_q\ A_Z\ n_H$$

population frac. abundance elemental abundance

- Take a two-level atom in steady state, excitation rate coefficient $Q_{ij}(T_e) = \langle \sigma v \rangle$ (s^{-1} cm^3) and say (I_{ji} =) $n_j A_{ji} = n_e n_i Q_{ij}$
- Emission Measure for unresolved volume $EM \equiv \int n_e n_H dV = 4\pi d^2 F_{ji} \,/\, Q_{ij}(T_e) f_q(T_e) A_Z$
- Should *EM* be the same for different lines?
- Generally, Emission Measure Distribution $EMD(T) = dEM \,/\, dT$

Survey of Atomic Processes

- Basically, all permutations on reactions of ions, electrons, and photons
- Two body reactions and threesomes
- 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

Continuum Processes

- Bremsstrahlung (braking radiation)
  $X^{+q} + e^{-*} \Rightarrow X^{+q} + e^{-} + h\nu$
- Bremsstrahlung spectrum (erg s^{-1} cm^{-3} Hz^{-1})
  $\varepsilon_\nu^{ff} \propto 6.8\times10^{-38} \, (n_e n_q q^2 \, / \, T_{e[K]}^{1/2}) \, e^{-h\nu/kTe} \, g_{ff}$
  - becomes increasingly important with density, with charge, and maximal for $\lambda_{max}{}^{*}\ T = 7\times10^{7}$ Å K ($g_{ff} \sim 1$)
- Inversely, Bremsstrahlung absorption
- Absorption coefficient
  $\alpha_\nu \propto 3.7\times10^{8} \, (n_e n_q q^2 \, / \, \nu^3 \, T_e^{1/2})(1-e^{-h\nu/kTe}) \, g_{ff}$ 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 ~ n_e^2, hence unimportant for vast majority of astrophysical plasma

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, $X^{+q**} \Rightarrow X^{+(q+1)} + e^-$
  e.g. $1s\ 2l\ n'l' \Rightarrow 1s^2 + e^-$
- Inversely, di-electronic capture
  $X^{+(q+1)} + e^- \Rightarrow X^{+q**}$ $(1s^2 + e^- \Rightarrow 1s\ 2l\ n'l')$
  - ion absorbs excess energy
  - radiationless resonant process - well defined $E(e^-)$

Continuum Processes (4/4)

- Di-electronic recombination - 2 step process
  $X^{+(q+1)} + e^- \Rightarrow X^{+q**} \Rightarrow X^{+q*} + h\nu_{df}$
  e.g. $1s^2\ (i) + e^-_{id} \Rightarrow 1s\ 2l\ n'l'\ (d) \Rightarrow 1s^2\ 2l\ (f) + h\nu_{fd}$
- Same initial and final states as RR
- Quantum interference? $\alpha \propto |\langle f|\ T^{RR} + T^{DR}|i\rangle|^2$
- Excitation-Autoionization - also 2 step process
  $X^{+q} + h\nu_{fd} \Rightarrow X^{+q**} \Rightarrow X^{+(q+1)} + e^-$
  or (resonant) electron impact
  $X^{+q} + e^{-*} \Rightarrow X^{+q**} + e^- \Rightarrow X^{+(q+1)} + 2e^-$
- Important only with energetic photons/electrons

Bound-Bound Transitions

- Spontaneous photon (line) emission
  $X^{+q*} \Rightarrow X^{+q} + h\nu_{ij}$
- Inversely, photo-excitation (~ resonant scattering)
  $X^{+q} + h\nu_{ij} \Rightarrow X^{+q*}$
- Induced photon emission
  $X^{+q*} + h\nu_{ij} \Rightarrow X^{+q} + 2h\nu_{ij}$
- Electron impact (collisional) excitation
  $X^{+q} + e^{-*} \Rightarrow X^{+q*} + e^{-}$
- Inversely, electron impact de-excitation
  $X^{+q*} + e^{-} \Rightarrow X^{+q} + e^{-*}$
- Resonant excitation via di-electronic capture
  $X^{+(q+1)} + e^{-*} \Rightarrow X^{+q**} \Rightarrow X^{+(q+1)*} + e^{-}$ (interference?)

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 ($Q \propto v$)
- Charge exchange collisions with neutrals could be important in interfaces of ionized and neutral gas
- Common in bulk motion scenarios (solar wind, SNRs), 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 determined by statistical physics and the 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

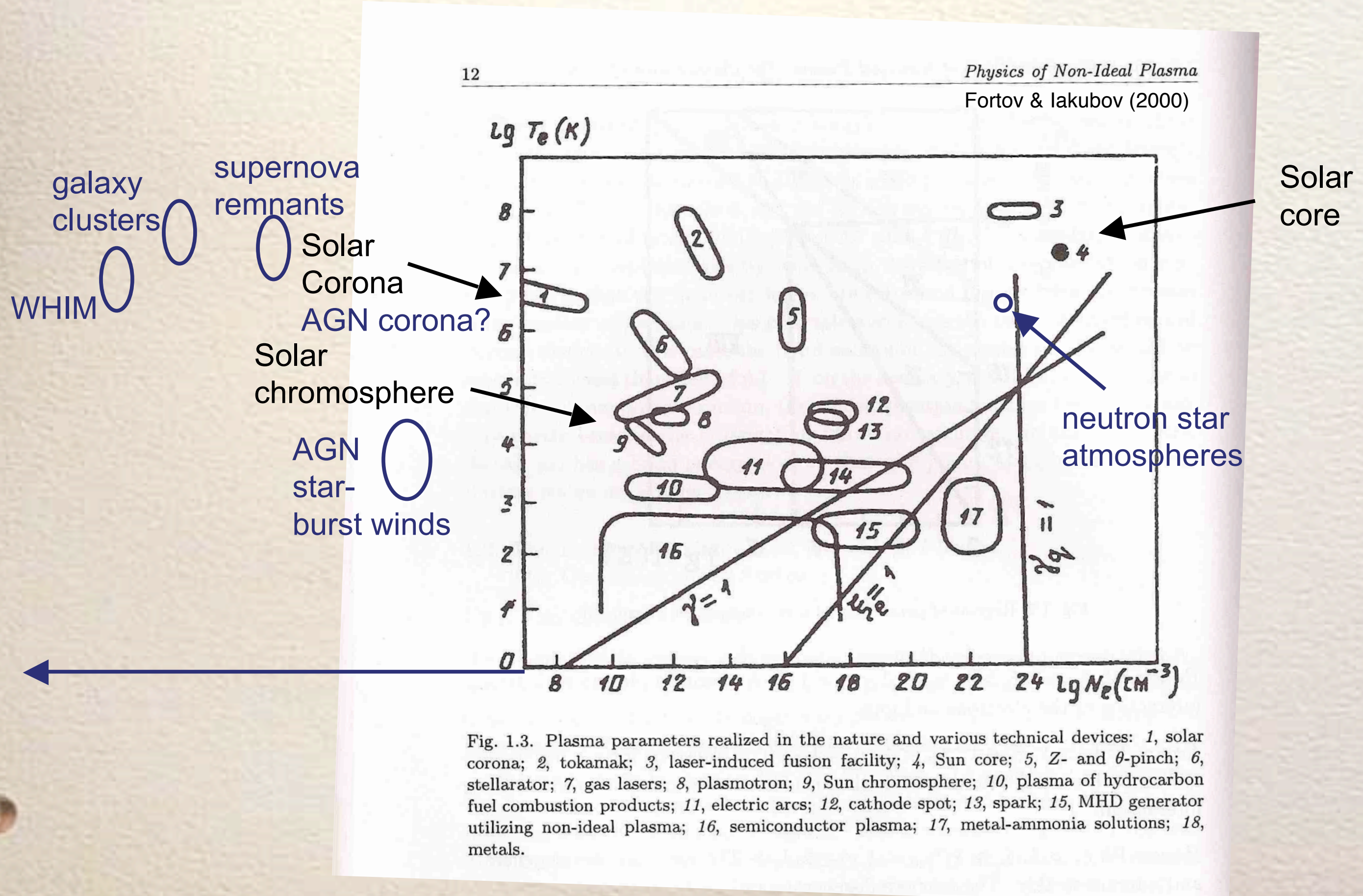
Detailed Balance: Example

- Auto-ionization and di-electronic capture (level *d*) $X^{+q**} <=> X^{+(q+1)} + e^-$ (level *i*)
- In TE the rates ($cm^{-3}\ s^{-1}$) are balanced locally $n_d A^a_{di} = n_e n_i \beta^{DC}_{id}(T)$
- But in TE also, the populations are given by the Saha + Boltzmann equations
  $n_d/n_e n_i = (g_d/2g_i)(2\pi\hbar^2/mkT)^{3/2} e^{(-Edi/kT)}$
  $=> \quad \beta^{DC}_{id}(T) = (g_d/2g_i)(2\pi\hbar^2/mkT)^{3/2} e^{(-Edi/kT)} A^a_{di}$
- Since this is a relation between atomic quantities it is general and valid in *any* plasma

Detailed Balance: Example (2/2)

- If one is bothered by the temperature, and one should, detailed balance is valid just the same for the cross section or rates per dE interval
- DC being a resonant process
  $\sigma^{DC}_{id}(E) = R^{DC}_{id}\delta(E-E_{di})$, where
  $R^{DC}_{id} \equiv \int \sigma^{DC}_{id}(E)dE$ is the resonance strength
- Since $\beta^{DC}_{id} = \int \sigma^{DC}_{id}(E) v f(E,T) dE$, it is easy to show
  $R^{DC}_{id} = (g_d/2g_i)(\pi^2\hbar^3/mE_{di})\, A^a_{di}$
  with truly exclusive atomic quantities that obviously cannot depend on the plasma

Laboratory and Astrophysical Plasma Regimes



12 *Physics of Non-Ideal Plasma*

Fortov & Iakubov (2000)

galaxy clusters

supernova remnants

WHIM

Solar Corona

AGN corona?

Solar chromosphere

AGN star-burst winds

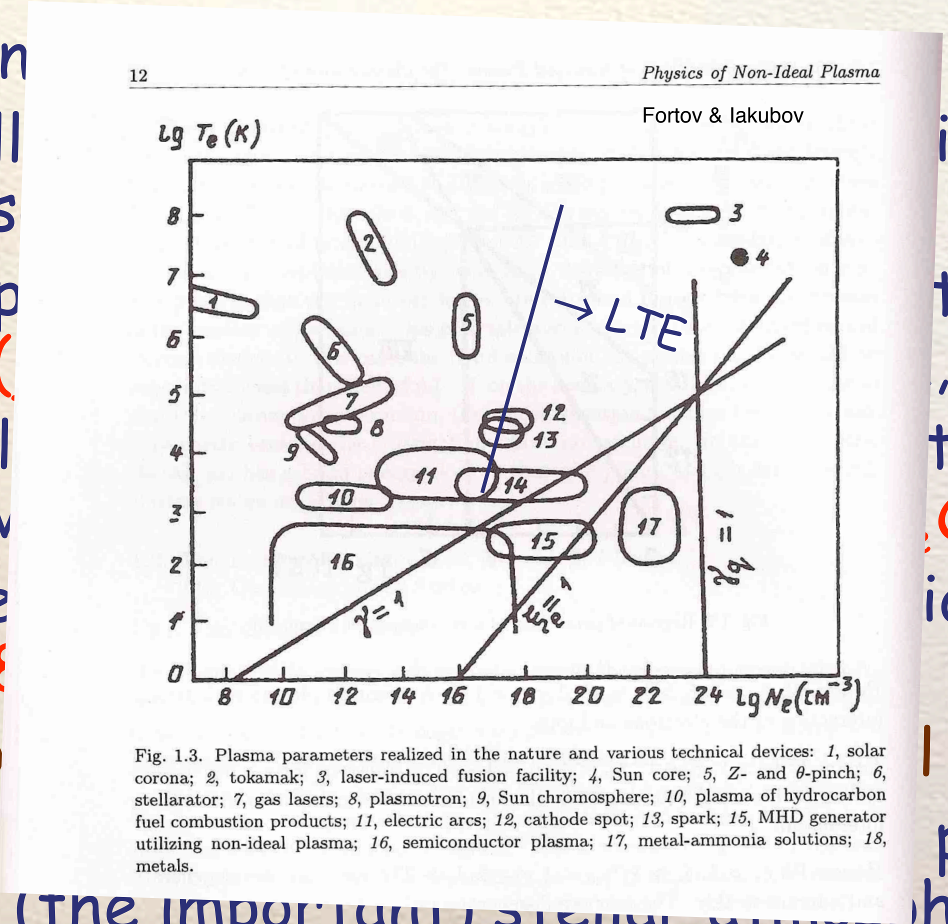
Solar core

neutron star atmospheres

Fig. 1.3. Plasma parameters realized in the nature and various technical devices: *1*, solar corona; *2*, tokamak; *3*, laser-induced fusion facility; *4*, Sun core; *5*, Z- and θ-pinch; *6*, stellarator; *7*, gas lasers; *8*, plasmotron; *9*, Sun chromosphere; *10*, plasma of hydrocarbon fuel combustion products; *11*, electric arcs; *12*, cathode spot; *13*, spark; *15*, MHD generator utilizing non-ideal plasma; *16*, semiconductor plasma; *17*, metal-ammonia solutions; *18*, metals.

Local Thermodynamic Equilibrium

- Collision
- Not full ional process
- TE prop trum, E.g., n_j/n_i = (, Kirchoff)
- For coll te over radiativ $Q_{ji} >> A_{ji}$
- Require ion $n_e >> 4.8$
- How do l j ?
- Clearly plasmas except (the important) stellar atmospheres



12 Physics of Non-Ideal Plasma

Fortov & Iakubov

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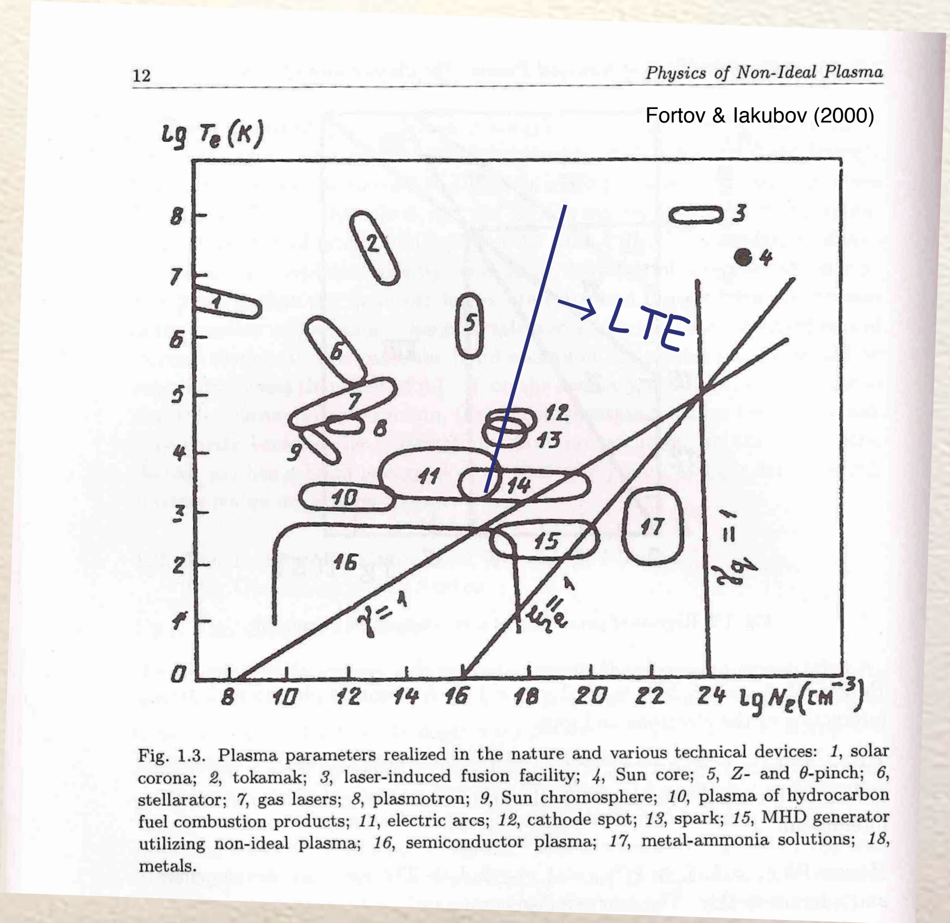
Local Thermodynamic Equilibrium

- Collisionally dominated plasma
- Not full TE: Equilibrium between collisional processes only, but not radiation field
- TE properties hold except Planck spectrum, E.g., $n_j/n_i = (g_j/g_i) e^{(-E_{ij}/kT)}$ (& Maxwell, Saha, Kirchoff)
- For collisional de-excitation to dominate over radiative decay for excited level (*j*) $n_e Q_{ji} \gg A_{ji}$
- Requires high density => Wilson criterion $n_e \gg 4.8 \times 10^{18} q^6 (kT/1\mathrm{keV})^{1/2}\ \mathrm{cm}^{-3}$
- How does this depend on specific level *j* ?
- Clearly, invalid for most astrophysical plasmas except (the important) stellar atmospheres

LTE Regime



12 *Physics of Non-Ideal Plasma*

Fortov & Iakubov (2000)

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Atomic Level-Population Kinetic Equations

- Non-LTE brute-force: Include all processes in transition-rate matrix
- For each level i (1 … N) dn_i/dt = + (populating) - (depleting) rates
- J_ν may require proper radiative transfer
- Need to solve set of N linear equations
- For N levels, how many independent equations?

$$\frac{d}{dt}\begin{pmatrix} n_0 \\ . \\ . \\ . \\ n_N \end{pmatrix} = \begin{pmatrix} \\ \hat{T}(n_e, T_e, J_\nu) \\ \\ \end{pmatrix} \begin{pmatrix} n_0 \\ . \\ . \\ . \\ n_N \end{pmatrix} \overset{?}{=} 0$$

Coronal Approximation

- High-*T* low-*n* Optically-Thin Plasmas ($J_\nu = 0$)
- Rates (n_e^2) << Rates (n_e) << 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: Collis. 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 (2/5)

- Leads to very simple expressions
- Steady state excitation

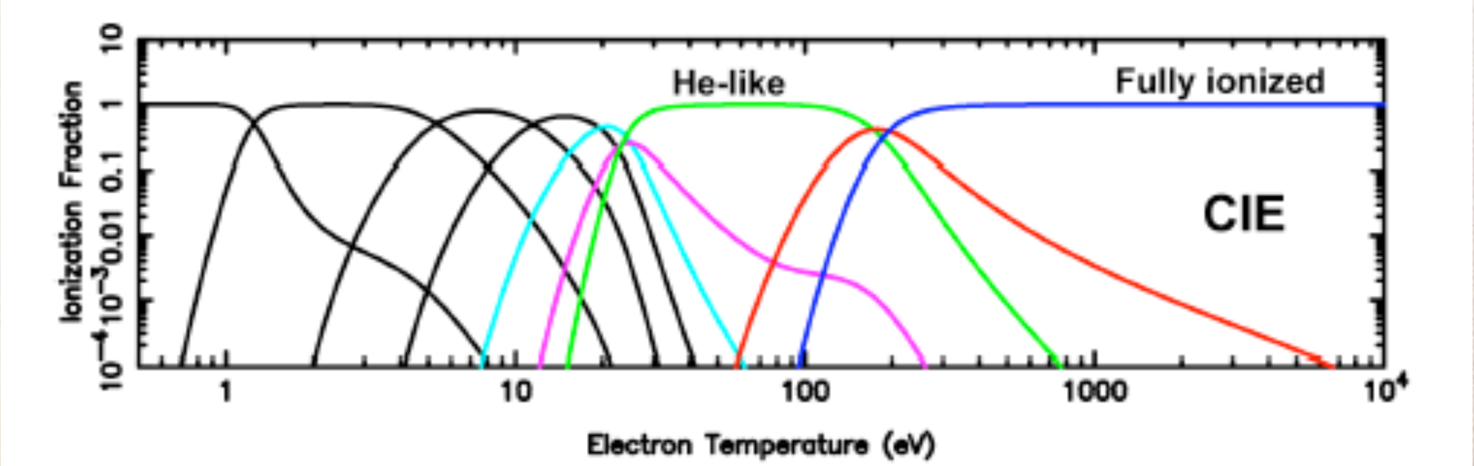
  $n_e n_i Q_{ij}(T) = n_j \Sigma A_{jx} \Rightarrow n_j / n_i = n_e Q_{ij}(T) / \Sigma A_{jx}$
- Unlike LTE (Boltzmann), depends on rates & n_e
- Line ratios independent of density
- Steady state ionization balance

  $n_{q-1} S_{q-1\rightarrow q}(T) + n_{q+1} \alpha_{q+1\rightarrow q}(T) = n_q S_{q\rightarrow q+1}(T) + n_q \alpha_{q\rightarrow q-1}(T)$
- Since for q=0 $n_0 S_{0\rightarrow 1}(T) = n_1 \alpha_{1\rightarrow 0}(T)$
- The general solution is:

  $n_{q+1} / n_q = S_{q\rightarrow q+1}(T) / \alpha_{q+1\rightarrow q}(T)$

Coronal Approximation (3/5)

- Ionization balance depends on atomic rates (and *T*), but not on n_e, opposite from LTE (Saha)
- Exponentially narrow formation region for each ion
- Ion emission typical of same temperature always => Best plasma thermometers, even with *EMD*



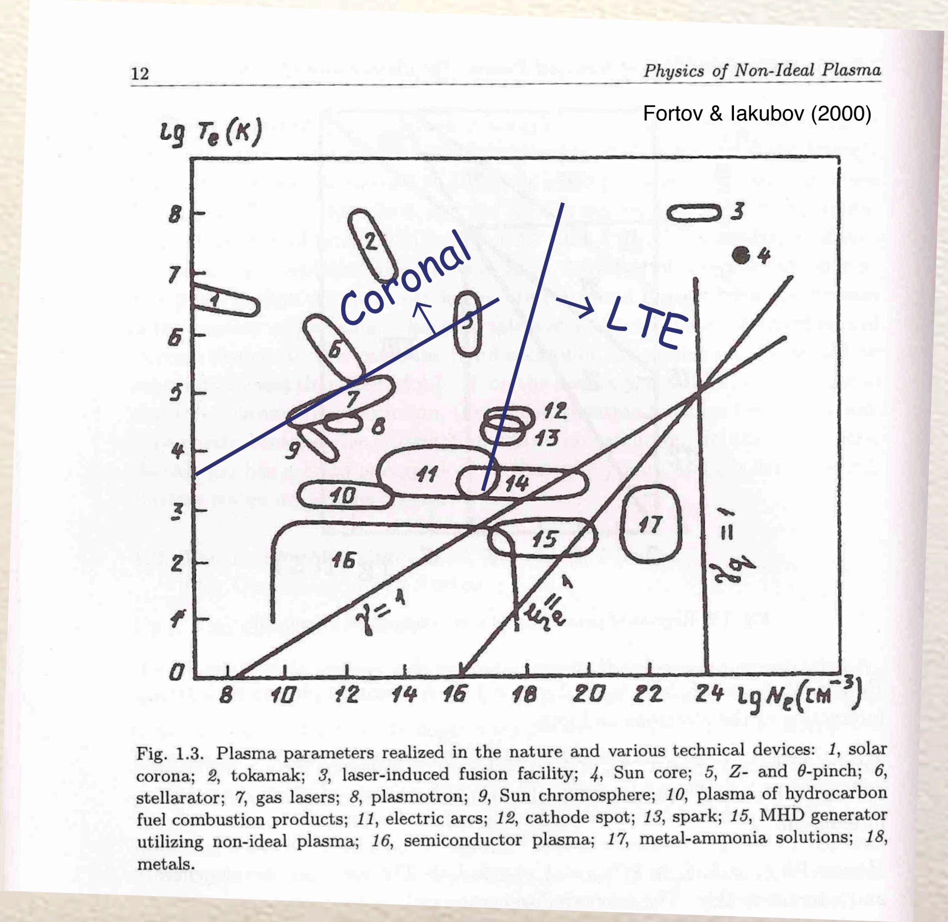
Coronal Approximation (4/5)

- Approximation breaks down for
  - Meta-stable levels (forbidden decay)
  - Close (high) lying levels $Q_{jk} \propto E_{jk}^{-1}$; $S_{j\infty} \propto E_I^{-2}$
- Effect of "continuum lowering" to "thermal limit" where high-lying levels => 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 used to determine validity of approximation, say $S^{\text{thermal}} \ll S$
- Results in another Wilson criterion
  $n_e < 4\text{x}10^{21}\, q^{-1} (kT/1\text{keV})^4\ \text{cm}^{-3}$
- Intermediate densities (laboratory plasmas) hardest to model
- How do populations & ionizations compare with LTE? Are they higher? lower?

Coronal Regime



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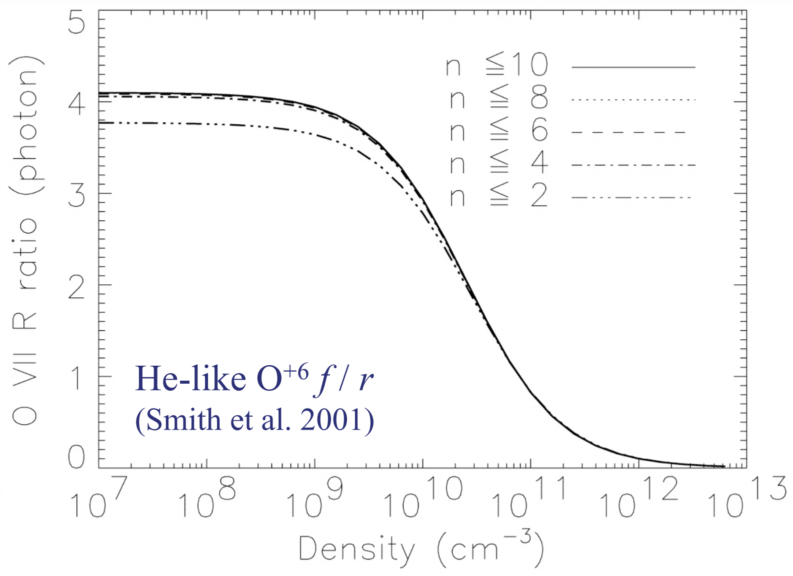
Collisional-Radiative Model

- Intermediate density, but optically thin
- Includes cascades and collisional transitions to/from excited levels
  $\Sigma n_x A_{xj} \approx n_e n_j \Sigma Q_{jy}(T)$
  $\approx n_j \Sigma A_{jz}$
- Need to solve transition matrix (for ionization?)
- Normalize and assume no particle losses (laboratory)

$$\frac{d}{dt}\begin{pmatrix} n_0 \\ . \\ . \\ . \\ n_N \end{pmatrix} = \begin{pmatrix} \\ \hat{T}(n_e, T_e) \\ \\ \end{pmatrix} \begin{pmatrix} n_0 \\ . \\ . \\ . \\ n_N \end{pmatrix} = 0$$

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?



He-like O^{+6} f / r
(Smith et al. 2001)

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: $n_j A_{ji} T_{ij}$
  $0 < T_{ij} = \exp[-N(\pi e^2/mc) f_{ij} \phi(\nu)] < 1$
- $N = \int n dl$ column density, f_{ij} - oscillator strength, and $\phi(\nu)$ - profile, generally Voigt profile, but dominated by Doppler broadening
- Think of geometrical effects in extended sources

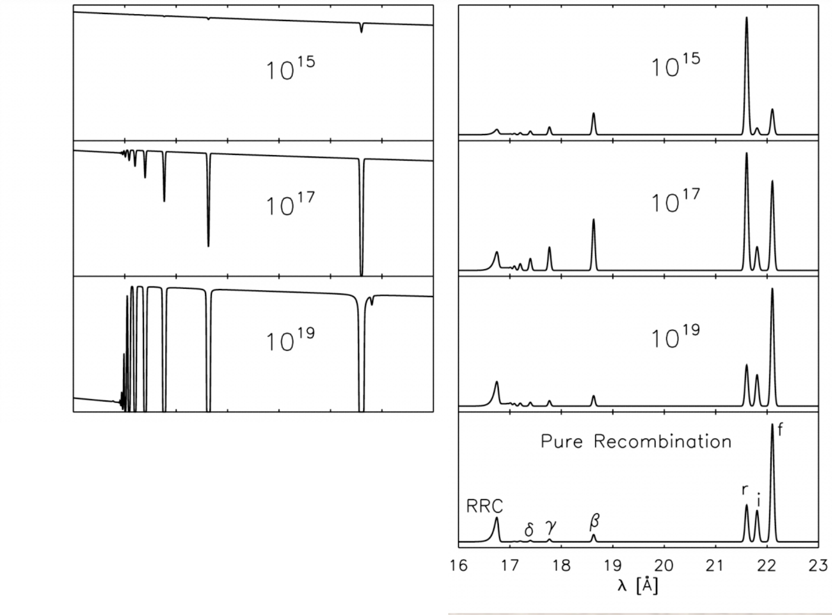
Nebular Approximation

- 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 (~F_E spectrum) and recombination (n_e):

  $n_q \int F_E \sigma^{PI}(E) dE = n_{q+1} n_e \alpha(T_e)$
- Ionization $n_{q+1}/n_q \propto F/n_e \propto L/n_e r^2 \equiv \xi$
- Unlike coronal approximation, does depend on density. Where else does ionization depend on *n*?
- With no additional energy source, *T* not independent parameter, depends on photo-heating and cooling

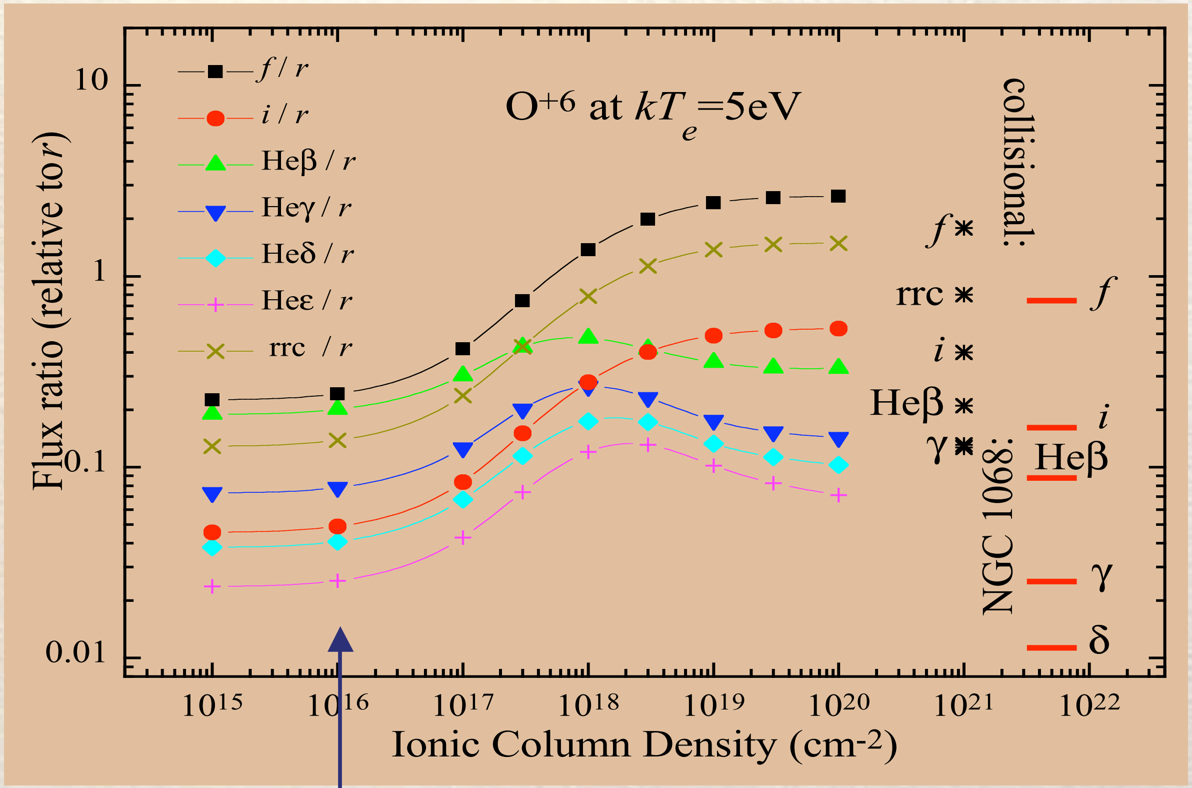
Nebular Approximation (2/3)

- T_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?



Absorption **Emission**

Nebular Approximation (3/3)



resonance
line saturates

Transient Plasma

- What are the important X-ray plasma time scales?
- Use Coulomb collision theory (Spitzer 1956) - neglecting collective plasma effects
- Individual-species temperature acquisition times through self collisions T_e , T_{ion}
- In velocity-driven excitation (shock) $T_e \ll T_{ion}$
- Much longer equilibration time for $T_e = T_{ion}$
- Ionization times $\sim 1 / n_e S_{q \rightarrow q+1}$
- Usually used within coronal approximation (low n)

Transient Plasma (2/6)

- Temporal Hierarchy

$$t_{c,e} = 10.4 \left(\frac{k_B T_e}{1\mathrm{keV}}\right)^{3/2} \left(\frac{1\mathrm{cm}^{-3}}{n_e}\right) \mathrm{yrs}$$

$$t_{c,ion} = 530 \left(\frac{k_B T_{ion}}{1\mathrm{keV}}\right)^{3/2} \left(\frac{1\mathrm{cm}^{-3}}{n_{ion}}\right) \frac{A_{ion}^{\frac{1}{2}}}{Z^4} \mathrm{yrs}$$

$$t_{eq} = 23,000 \left(\frac{k_B T_e}{1\mathrm{keV}}\right)^{3/2} \left(\frac{1\mathrm{cm}^{-3}}{n_{ion}}\right) \left(\frac{A_{ion}}{Z_{ion}^2}\right) \mathrm{yrs}$$

$$t_{ionization} = \frac{1}{n_e \alpha^R(T_e)} \simeq 100,000 \left(\frac{1\mathrm{cm}^{-3}}{n_e}\right) \mathrm{yrs}$$

Transient Plasma (3/6)

- Transition matrix of electron impact ionization and recombination rates
- In coronal approximation depends on T_e and $\propto n_e$
- If rates (T) constant, analytical solution possible by recasting T with similar diagonal matrix $T = S^{-1}DS$ (eigenvalues λ_i in diagonal)
- How to normalize?

$$\frac{d}{dt}\begin{pmatrix} n_0 \\ . \\ . \\ . \\ n_Z \end{pmatrix} = n_e \left(\hat{T}(T_e) \right) \begin{pmatrix} n_0 \\ . \\ . \\ . \\ n_Z \end{pmatrix}$$

Transient Plasma (4/6)

- Set of independent differential equations (for ***Sn***)

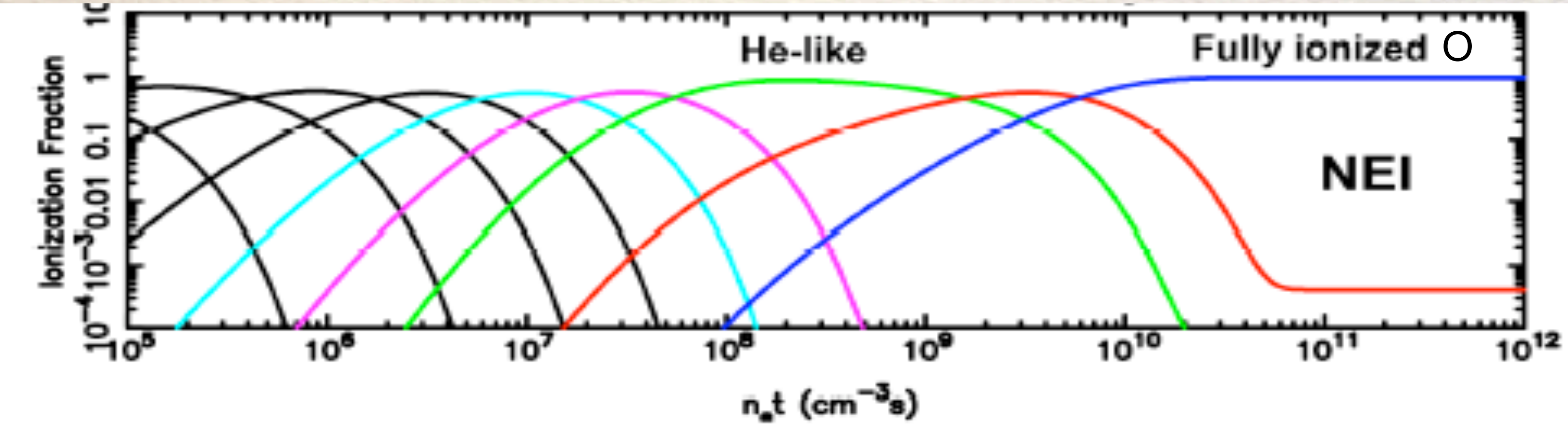
$$\frac{d}{dt}\left(\hat{S}\right)\begin{pmatrix} \mathrm{n}_0 \\ . \\ . \\ . \\ \mathrm{n}_Z \end{pmatrix} = n_e \begin{pmatrix} \lambda_1 & & & \\ & . & & \\ & & \hat{D} & \\ & & & . \\ & & & & \lambda_N \end{pmatrix}\left(\hat{S}\right)\begin{pmatrix} \mathrm{n}_0 \\ . \\ . \\ . \\ \mathrm{n}_Z \end{pmatrix}$$

$$\left(\hat{S}\right)\begin{pmatrix} \mathrm{n}_0 \\ . \\ . \\ . \\ \mathrm{n}_Z \end{pmatrix} = \begin{pmatrix} e^{\lambda_1 n_e t} \\ . \\ . \\ . \\ e^{\lambda_N n_e t} \end{pmatrix} \longrightarrow \begin{pmatrix} \mathrm{n}_0(t) \\ . \\ . \\ . \\ \mathrm{n}_Z(t) \end{pmatrix} = \left(\hat{S}^{-1}\right)\begin{pmatrix} e^{\lambda_1 n_e t} \\ . \\ . \\ . \\ e^{\lambda_N n_e t} \end{pmatrix}$$

- 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 $n_e t$
- 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_q and n_{q-1} (= $1 - n_q$)
- The rate equation then is simply

  $dn_q/dt = n_e\,(n_{q-1}S_{q-1\rightarrow q} - n_q\alpha_{q\rightarrow q-1})$

  whose solution is

  $n_s = S/(S + \alpha)\ \ (1 - e^{-ne(S + \alpha)t})$
- 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 are considerably shorter $<10^{-8}$ s, don't affect transient ionization/recombin.

Recap: Models & Diagnostics

- Coronal model:
  - Temperature (*EMD*) from charge states - independent of *n* (and less from inter-ion lines and from bremsstrahlung)
  - 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
  - Column density from absorption & *emission*
- Transient plasma
  - Ionization time, but temperature?
  - Density and time from emission measure

Acknowledgments

- I am greatly indebted to
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THANK YOU
FOR YOUR ATTENTION