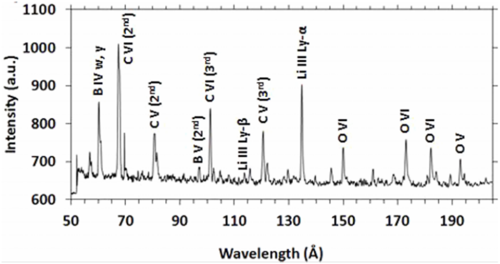
Basics of Plasma Spectroscopy

2019 Graduate Summer School at PPPL
Presented by Brian Kraus

August 14, 2019



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NSTX-U EUV spectra (Weller 2016, RSI 87, 11E324)

Plasma spectra are plentiful and rich in information

1. Plasmas emit light—here, $0.1\ \text{Å} < \lambda \lesssim 1\ \mu\text{m}$
   - Line emission
   - Continuum emission
2. Spectral features influenced by plasma properties
   - Brightness/intensity
   - Line ratios
   - Line positions and widths
3. Spectrometer design considers wavelength of interest and geometry
4. Complicated spectra + sophisticated analysis =
   wealth of plasma information
   (with Dr. Shaun Haskey)

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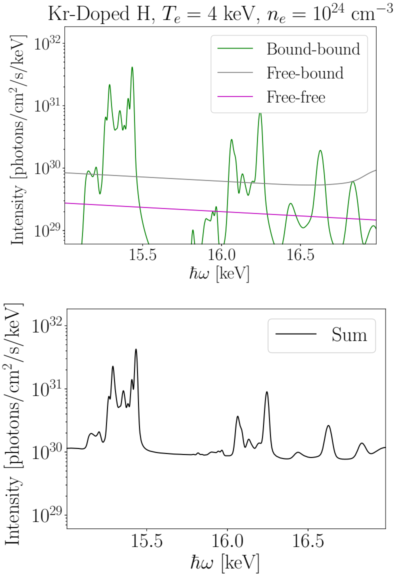
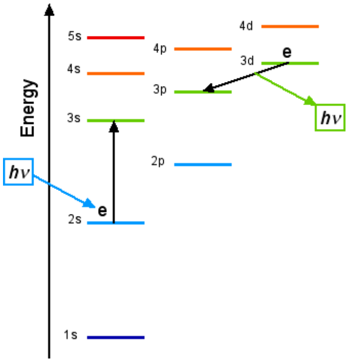
Most plasma radiation is a consequence of electron motion

Classified by electron state before and after emission:

- Bound-bound
- Free-bound
- Free-free



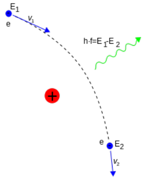
Atoms (and ions) with **bound** electrons emit **line radiation**



- Bound electrons transition between quantum states
- Transitions must conserve:
  - Energy
  - Total angular momentum $J = |\boldsymbol{L} + \boldsymbol{S}|$
- "Selection rules" establish how often transitions occur
  - $\Delta J \in \{-1, 0, 1\}$: electric dipole transitions
  - Less frequent: magnetic dipole, electric quadropole

Free electrons "brake," recombine $\rightarrow$ **continuum radiation**

Bremsstrahlung



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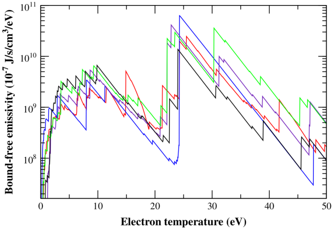
- Colliding electrons and ions behave like a time-varying dipole
- Photon energy $\hbar\omega = \Delta E$ of electron
- Intensity depends on electron distribution function $f(E)$

Free-bound

- Electrons captured according to time-dependent perturbation theory
- Photon energy $\hbar\omega = E_{\text{electron}} + E_{\text{bound state}}$
- Spectrum depends on $f(E)$ and bound state energies



Fontes 2009, HEDP 5, 15

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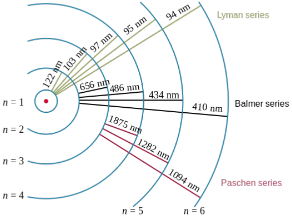
Line **intensity** proportional to radiative rate

For a transition $n_u \to n_l + \hbar\omega$, emissivity $\varepsilon \left[\frac{\text{photons}}{\text{cm}^3\ \text{s}}\right] = n_u A_r$

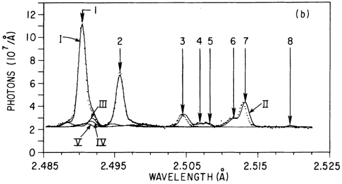
$A_r\ [\text{s}^{-1}]$ = Radiative rate

As in $\partial_t n_u = -A_r n_u$

- Depends drastically on
  - Nuclear charge
  - Number of bound electrons
- Neutral H Balmer series:
  - 656 nm, $A_r^{-1} = 45$ ns
- Ti^{20+} $n = 2 \to 1$:
  - 2.61 Å, $A_r^{-1} = 4.2$ fs



Bohr model of H (Creative Commons)



Ti^{20+} spectrum from PLT (Bitter 1984, PRA 29, 661)

Line **intensity** proportional to excited population density

For a transition $n_u \to n_l + \hbar\omega$, emissivity $\varepsilon \left[\frac{\text{photons}}{\text{cm}^3\ \text{s}}\right] = n_u A_r$

$n_u\ [\text{cm}^{-3}]$ = Density of upper state X^*

Depends on many atomic kinetic processes:

- Collisional excitation

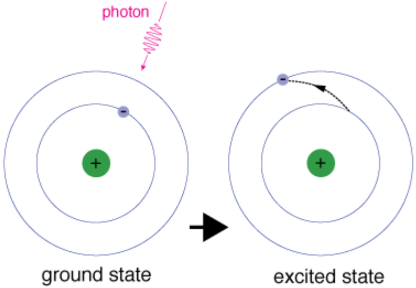
$$X + e^- \to X^* + e^-$$

- Collisional recombination

$$X^+ + e^- \to X^*$$

- Photoexcitation

$$X + \hbar\omega \to X^*$$



NASA

Upper state might be **deexcited** without emitting a photon:

- Auger effect
- Collisional deexcitation

How bright is a line? Varies with **atomic** and **plasma** physics

(more frequent transitions $\rightarrow$ more photons)

Atomic physics

- What are the properties of different quantum states?
- Solve Schrödinger equation for atomic wavefunction
- Eigenvalues $\rightarrow$ energies $\rightarrow$ wavelengths

$$i\hbar \frac{\partial}{\partial t} |\Psi(\boldsymbol{r}, t)\rangle = \hat{H} |\Psi(\boldsymbol{r}, t)\rangle$$

- LS- and JJ-coupling approximate transition rates
- Calculated with Flexible Atomic Code, Cowan's Atomic Structure code...

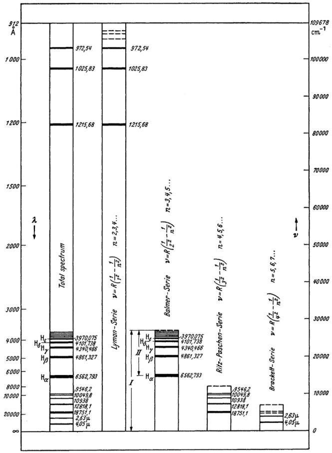


Fig. 3. The spectral lines of the hydrogen spectrum (the height of a line is proportional to its frequency, the number written next to a line is its wave length in Ångström units).

Bethe and Salpeter, Quantum Mechanics of One- and Two-Electron Atoms

How bright is a line? Varies with **atomic** and **plasma** physics

Plasma physics, or collisional-radiative (CR) modeling

- Based on plasma parameters like n_i, n_e and T_e, evaluate:
  - Each ion's **charge state distribution**
  - Cross sections at electron energies across $f(E)$
  - Potential depression, or continuum lowering
- To find these values, must solve high-dimensional rate equation:

$$\frac{dn_i}{dt} = \sum_{j \neq i} R_{ji} n_j - \left(\sum_{j \neq i} R_{ij} \right) n_i, \text{ or}$$

$$\frac{d\boldsymbol{n}}{dt} = R\boldsymbol{N} \qquad \boldsymbol{n} = [n_1, n_2, ..., n_s] \qquad R = \{R_{ij}\}, \quad i, j \in [1, s],$$

- where R_{ij} are based on atomic codes!

In low-density ($\nu_{\text{coll}} \ll A_r$), use simplified **coronal model**

- No collisional deexcitation or three-body recombination
- Ionization distribution from balance of collisional ionization and radiative recombination:

$$e^- + X^{n+} \to 2e^- + X^{(n+1)+}; \qquad e^- + X^{(n+1)+} \to X^{n+} + \hbar\omega$$

- Line emission balances collisional excitation and **spontaneous emission only:**

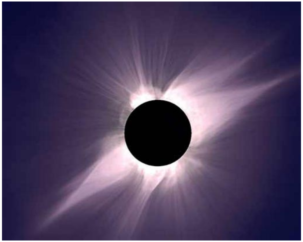
$$e^- + X \to e^- + X^*; \qquad X^* \to X + \hbar\omega$$

Named for conditions in solar corona:

$$n_e \sim 10^9 \text{ cm}^{-3} \implies \nu_{ei} \sim 60 \text{ s}^{-1}$$

vs. decay of Fe^{13+} ("coronium") lines,

$$A_r \sim 10^7\text{–}10^{11} \text{ s}^{-1}$$



If the full CR problem seems intractable, you may have a point:

Assume a single one-electron ion with nuclear charge Z

$$E_n = Z^2 \left(1 - \frac{1}{n^2}\right) \times 13.6057 \text{ eV}$$

Each Rydberg level n has many degenerate states with multiplicities g_n

$$g_n = 2n^2$$

If a plasma in **local thermodynamic equilibrum** has a finite temperature T, each energy level is populated with Boltzmann statistics

$$X_n = g_n \exp\left(-\frac{E_n}{T}\right)$$

But this system **diverges** at high n:

$$\lim_{n\to\infty} X_n \quad \sim \quad \lim_{n\to\infty} n^2 \times \exp\left[\frac{(13.6 \text{ eV}) \times Z^2}{T}\right] = \infty$$

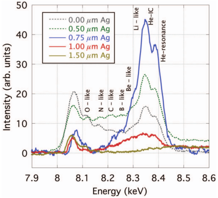
S. B. Hansen, Ch. 2 in Modern Methods in Collisional-Radiative Modeling of Plasmas (2016)

Codes solve this problem by sacrificing **completeness** or **detail**

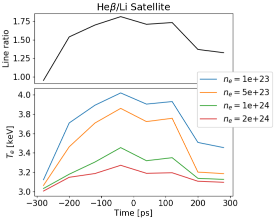
- Reduce completeness by ignoring some permutations of N electrons in all n-shell orbitals
  - Define state space that is reliably accurate and relevant to plasma parameters, or
  - Allow dynamic state space to evolve as calculation proceeds
- Reduce detail by averaging transitions that are nearby in energy
  - **Relativistic term based**: 1^1S_0, 2^1S_0, 2^1P_0, $2^3P_{0,1,2}$, ...
  - **Configurations**: $1s^2$, $1s2s$, $1s2p$
  - **Superconfigurations**: $(1)^2$, $(1)^1(2)^1$, $(2)^2$
- This difficult task is attempted by many collisional-radiative codes: FLYCHK, SCRAM, ATOMIC...

S. B. Hansen, Ch. 2 in Modern Methods in Collisional-Radiative Modeling of Plasmas (2016)

Collisional-radiative calculations enable plasma diagnosis



Multiple charge states of Cu
(Chen 2009, PoP 16, 062701)



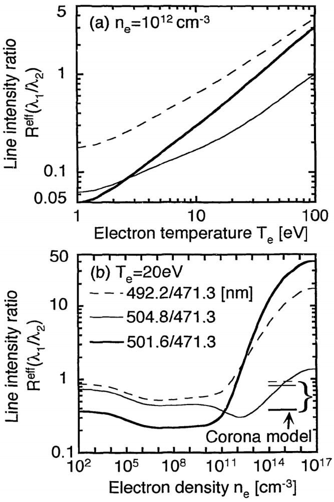
Line ratios changing in NIF

- Intensity $\rightarrow$ density of a given population
  - Relative line strength approximates relative densities of upper states
  - Absolutely calibrated signals ($I = \frac{\text{photons}}{\text{keV s sr}}$) can be compared directly to codes
- Line ratios $\rightarrow$ density or temperature

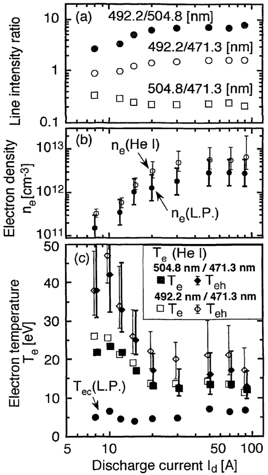
$$\frac{I_a}{I_b} = \frac{\int_a I(E)dE}{\int_b I(E)dE} = \text{ function of } n_e, T_e$$

  - Change $n_e \rightarrow$ change electron-ion collision frequency vs. A_r
  - Change $T_e \rightarrow$ change charge state distribution $\rightarrow$ change line ratios

Ex. He line ratios diagnose n_e, T_e in edge of linear device



Model results including fast electron excitation



Inferred plasma parameters, corroborated with other diagnostics

Sasaki 1995, National Institute for Fusion Science 346

Broadening mechanisms fill **line widths** with information

Lorentzian, width γ

- Natural line width from Heisenberg uncertainty

$$\Delta E\ \Delta t \geq \hbar/2$$

$$A_r^{-1} = 2.2 \text{ fs} \rightarrow \Delta E \geq 0.15 \text{ eV}$$

- Stark broadening from time-varying electric fields
  - Collisions effectively alter A_r
  - Very dense plasmas widen natural broadening

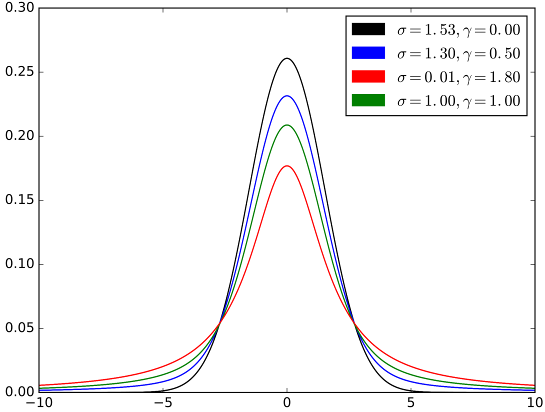
Gaussian / Doppler, width σ

- Plasma flow $\rightarrow$ Doppler shift

$$\Delta\omega = \omega\left(1 + \frac{v}{c}\right)$$

- Thermal broadening: Doppler shift from all E in $f(E)$
- Instrumental broadening: spectrometers introduce error

Convolve all broadening: Gaussian $*$ Lorentzian = Voigt



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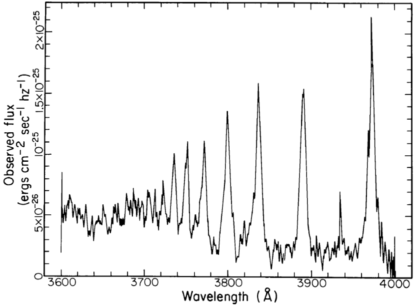
In practice, separating all contributions to line widths requires high-resolution spectrometers and careful planning

Stark or pressure broadening measures n_e via net electric fields

- Stark effect: $\boldsymbol{E}$ shifts lines
- Stark **broadening**: Microfield perturbations distort lines
- In high density plasmas like NIF, Stark broadening begins at $n_e \gtrsim 10^{24}$ cm^{-3}
- In astrophysical plasmas: Inglis-Teller effect

$$\log n_e = 22.0 - 7.0 \log n_{\max}$$

- High-n lines "broadened" into continuum



Temperature changes in a stellar flare (Zarro 1985, Astronomy and Astrophysics 148, 240)

$$n_{\max} = 16 \implies n_e \approx 3.7{\times}10^{13} \text{ cm}^{-3}$$

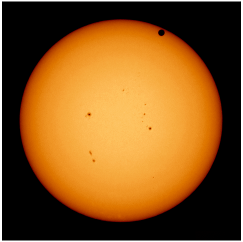
One enormous problem: plasmas are not homogeneous

- General spectra are line-integrated along varied n and T
- The emergent intensity is the solution of a radiative transfer equation

$$\frac{dI(\omega)}{d\ell} = -\kappa(\omega)I(\omega) + \varepsilon(\omega),$$

where κ = opacity $[\mathrm{m}^{-1}]$ and ε = volumetric emissivity

- κ^{-1} = photon mean-free-path



Brocken Inaglory, Creative Commons

Limb darkening in stars:

- Only see a distance $1/\kappa$
- For stars, $\kappa L \gg 1 \rightarrow$ **optically thick**
- Stellar edge emission indicates colder plasma

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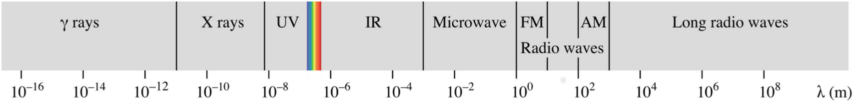
Wavelength of interest defines relevant diffraction gratings



General law of diffraction: $n\lambda = d \sin\theta$

- Visible light, $d \approx \lambda \approx 500$ nm
  - Ridges can be ruled with diamond tool, or
  - Produced with photolithography like other nanomaterials
- UV or EUV, $d \approx 10$–100 nm
  - Photolithography or multi-layered mirrors
- X-rays, $d \approx 0.1$–100 Å
  - Low energy: organic crystals, quasicrystals
  - Higher energy: "perfect" crystals (quartz, Ge, Si...)

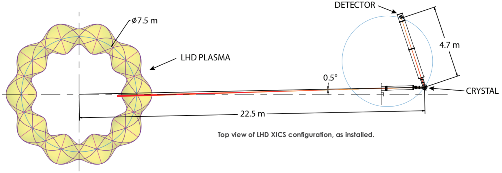
Geometric factors define spectral resolution, focusing

Generalized flat grating: no focusing

Spherical "mirror" for dispersive imaging

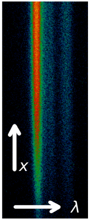
- Best resolution on Rowland circle

Pablant 2012, RSI 83, 083506



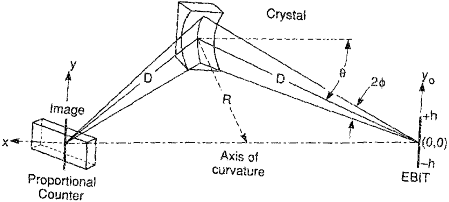
Top view of LHD XICS configuration, as installed.

$$R_{\text{Rowland}} = R_{\text{crystal}}/2$$



Cylindrical focusing for point- or line-sources

Beiersdorfer 1990, RSI 61, 2338



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