# **CRETIN**

Session 7

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### **Session topics**

#### Line radiation transport

- Physics considerations
  - what is important / different about lines?
  - material coupling and convergence
  - important physical effects
- Code options
  - setting up frequency meshes
  - options for including physical effects
  - methods for achieving convergence



### What is important about lines?

- Transitions between levels in the same charge state
- Narrow frequency range → strong localized absorption / emission
- Radiation is strongly coupled to bound electrons
- Most radiation emission from multi-electron atoms is due to lines
- At low densities, line effects can dominate the kinetics

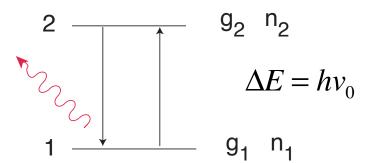
Probability (per unit time) of

- Spontaneous emission:  $A_{21}$
- Absorption:
- Stimulated emission:

Stimulated emission: 
$$B_{21}$$
  
 $g_1B_{21} = g_2B_{12}$  ,  $A_{21} = \frac{2hv_0^3}{c^2}B_{21}$ 

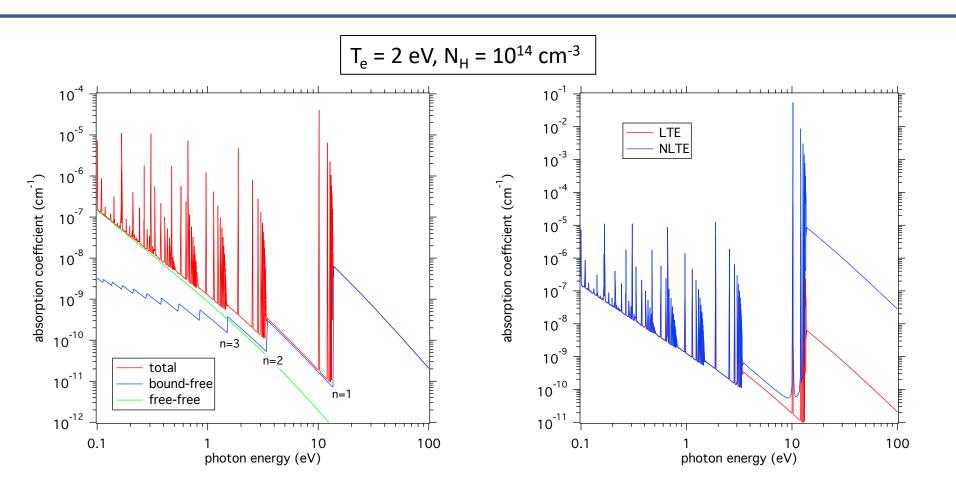
 $A_{21}$ ,  $B_{12}$ ,  $B_{21}$  are Einstein coefficients

Two energy level system



### Line radiation is critical to non-LTE physics

### A simple example – low density H

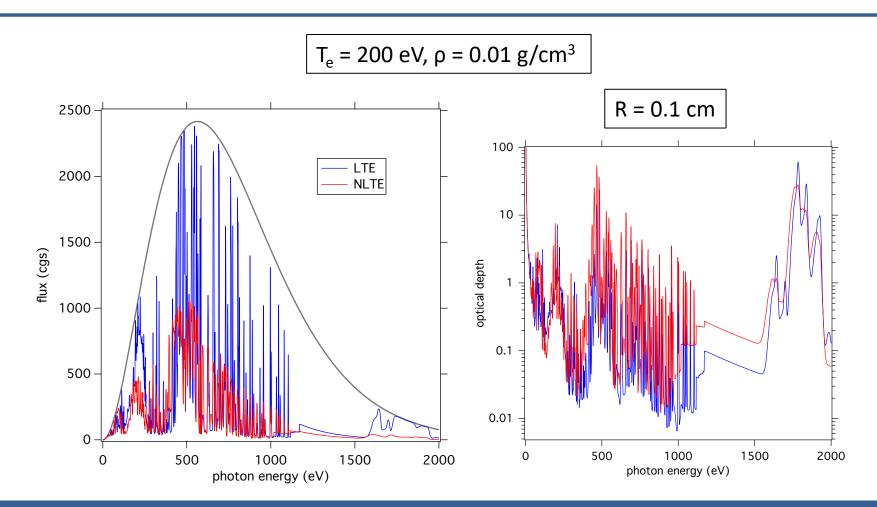


### Lines become optically thick before the continuum





### A mid-Z example – Kr sphere

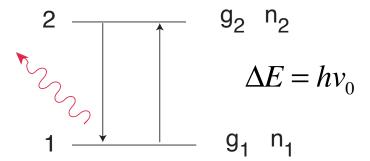


### Line radiation dominates the escaping flux

### **Coupling to material – effective scattering**

- Line radiation couples directly to just the two levels involved
- Line radiation "scatters" by resonant absorption / emission
- Upper level decays
  - Radiatively with rate  $A_{21}$
  - Collisionally with rate  $n_e C_{21}$
- The fraction  $\varepsilon \approx n_e C_{21} / A_{21}$ of photons are destroyed / thermalized
- The fraction  $(1-\varepsilon)$  of photons are "scattered"
  - > energy changes only slightly (mostly Doppler shifts)
  - → undergo many "scatterings" before being thermalized
- Convergence by lambda iteration takes  $\sim \tau^2$  iterations

Two energy level system



 $\varepsilon \ll 1$  is the condition for a strongly non-LTE transition and is easily satisfied for low density or high  $\Delta E$ !

### Line profiles

Bound-bound absorption cross section:

$$\sigma(v) = \frac{hv_0}{4\pi} B_{21} \phi(v) = \frac{\pi e^2}{mc} f_{12} \phi(v)$$
  $\frac{\pi e^2}{mc} = 0.02654 \text{ cm}^2/\text{s}$ 

- Oscillator strength  $f_{12}$  relates the quantum mechanical result to the classical treatment of a harmonic oscillator
  - Strong transitions have  $f^{\sim}1$

$$\int_0^\infty \phi(v) \, dv = 1$$

The line profile  $\phi(v)$  describes the frequency dependence of the absorption coefficient

$$\alpha_{v} = n_{1} \frac{\pi e^{2}}{mc^{2}} f_{12} \phi(v) \left[ 1 - \frac{g_{1} n_{2}}{g_{2} n_{1}} \right]$$

$$\eta_{v} = \left(\frac{2hv^{3}}{c^{2}}\right) n_{2} \frac{\pi e^{2}}{mc^{2}} f_{12} \phi(v)$$

- $\alpha_v = n_1 \frac{\pi e^2}{mc^2} f_{12} \phi(v) \left| 1 \frac{g_1 n_2}{g_2 n_1} \right|$  This assumes absorption and emission profiles are the same profiles are the same
  - If line width is small ( $\Delta v \ll v_0$ ), can replace v by  $v_0$

# Cretin line transport assumes $\Delta v \ll v_0$



### **Line profiles**

Line profiles are determined by multiple effects:

• Natural broadening  $(A_{12})$ 

- Lorentzian
- Collisional broadening  $(n_e, T_e)$
- Lorentzian

• Doppler broadening  $(T_i)$ 

- Gaussian

 $\Gamma$  = destruction rate

 $\phi(v) = \frac{\Gamma/4\pi^2}{(v-v_0)^2 + (\Gamma/4\pi)^2}$ 

Stark effect (plasma microfields) - complex

The convolution of Gaussian and Lorentzian shapes gives the Voigt profile:

- Gaussian core
- Lorentzian wings

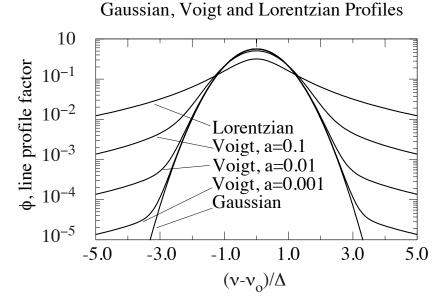
$$\phi(v) = \frac{1}{\Delta v_D \sqrt{\pi}} H(a, x) , H(a, x) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(x - y)^2 + a^2} dy$$

$$a = \frac{\Gamma}{4\pi\Delta v_D} , \Delta v_D = \frac{v_0}{c} \sqrt{\frac{2kT_i}{m_i}}$$

$$\frac{\partial v_D}{\partial v_D} = \frac{v_0}{c} \sqrt{\frac{2kT_i}{m_i}}$$

$$\frac{\partial v_D}{\partial v_D} = \frac{v_0}{c} \sqrt{\frac{2kT_i}{m_i}}$$

a = Voigt parameter



# Configuration "broadening"

For multi-electron ions, multiple atomic states are combined into "levels" representing

• LSJ-configurations  $1s^22p^6 3s^2 3p_{3/2}$ 

LS-configurations
 1s<sup>2</sup>2p<sup>6</sup> 3s<sup>2</sup> 3p

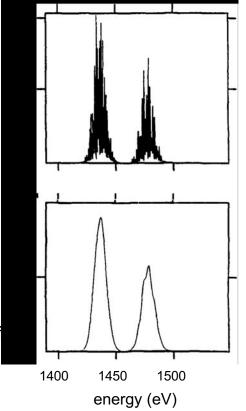
Superconfigurations (1)<sup>2</sup>(2)<sup>6</sup>(3)<sup>3</sup>

A single transition between levels represents many transitions between states

UTA – unresolved transition array

The screened-hydrogenic models dca\_xx use superconfigurations for levels + multiple UTAs between levels for transitions

Tm (Z=69) 3d-4f C. Smith (1995)

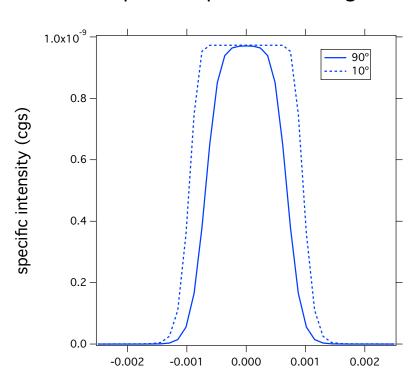


### Configuration broadening often dominates high-Z spectra

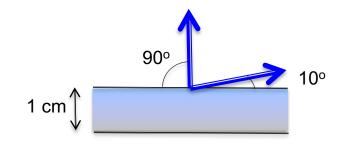


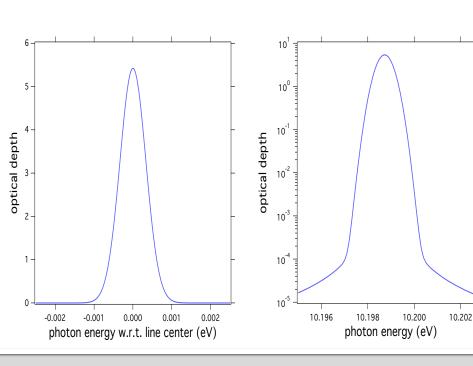
# Example – Hydrogen Ly-α

- Uniform conditions:  $T_e = 1 \text{ eV}$ ,  $n_e = 10^{14} \text{ cm}^{-3}$
- Moderate optical depth  $\tau \sim 5$
- Viewing angles 90° and 10° show optical depth broadening



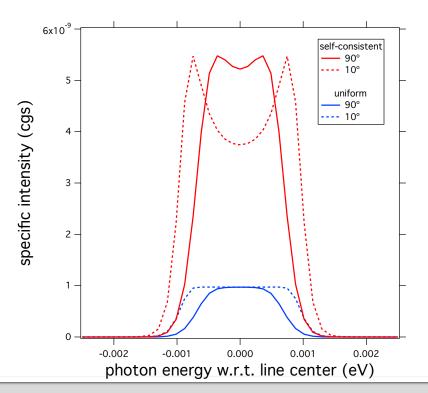
photon energy w.r.t. line center (eV)

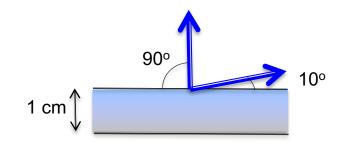


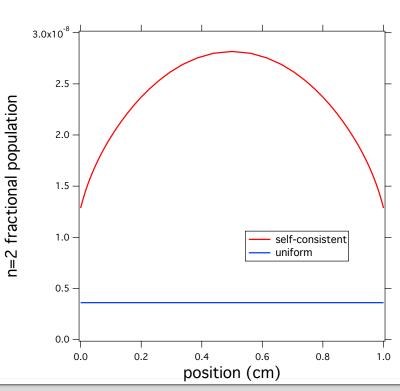


## Example – Hydrogen Ly-α

- Uniform conditions:  $T_e = 1 \text{ eV}$ ,  $n_e = 10^{14} \text{ cm}^{-3}$
- Self-consistent solution displays effects of
  - Radiation trapping / pumping
  - Non-uniformity due to boundaries







#### Redistribution

- The emission profile  $\psi_{\nu}$  is determined by multiple effects:
  - coherent scattering, elastic scattering, Doppler broadening
- It is related to the absorption profile through the redistribution function

$$\int_{0}^{\infty} R(v,v') dv = \phi(v') , \quad \psi(v) = \int_{0}^{\infty} R(v,v')J(v') dv' / \int_{0}^{\infty} \phi(v')J(v') dv'$$

- Complete redistribution (CRD):  $\psi_v = \phi_v$
- Doppler broadening is only slightly different from CRD, while coherent scattering gives  $R(v,v') = \phi(v)\delta(v-v')$
- A good approximation for partial redistribution (PRD) is often

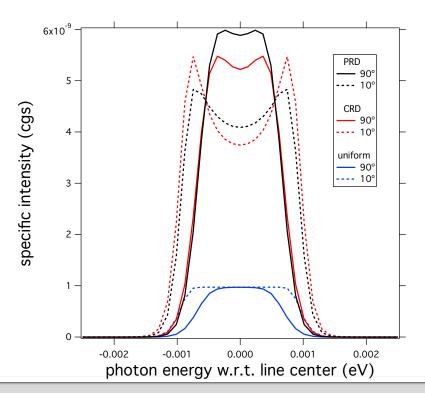
$$R(v,v') = (1-f)\phi(v')\phi(v) + f R_{II}(v,v')$$

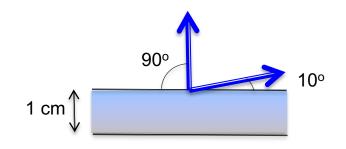
• where f (<<1 for X-rays) is the ratio of elastic scattering and de-excitation rates,  $R_{II}$  includes coherent scattering and Doppler broadening

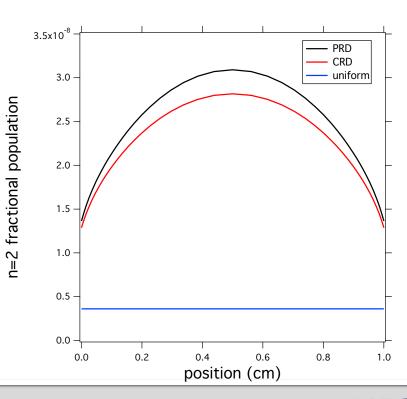
### PRD effects become stronger with increasing optical depth

### Example – Hydrogen Ly-α with Partial Redistribution

- Uniform conditions:  $T_e = 1 \text{ eV}$ ,  $n_e = 10^{14} \text{ cm}^{-3}$
- Optical depth τ ~ 5
- Voigt parameter a ~ 0.0003







### Radiation transport for 2-level atom

Rate equation for two levels in steady state:

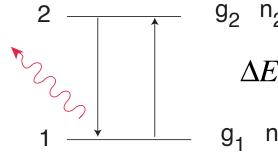
$$n_1(B_{12}\overline{J}_{12} + C_{12}) = n_2(A_{21} + B_{21}\overline{J}_{12} + C_{21})$$

$$\overline{J}_{12} = \int_0^\infty J_v \phi_{12}(v) dv$$
,  $C_{12} = \frac{g_2}{g_1} e^{-hv_0/kT} C_{21}$ 

Absorption / Emission:

$$\alpha_{v} = \frac{hv}{4\pi} (n_{1}B_{12} - n_{2}B_{21})\phi_{12}(v) , \eta_{v} = \frac{hv}{4\pi} n_{2}A_{21}\phi_{12}(v)$$

Two energy level system



Source function:

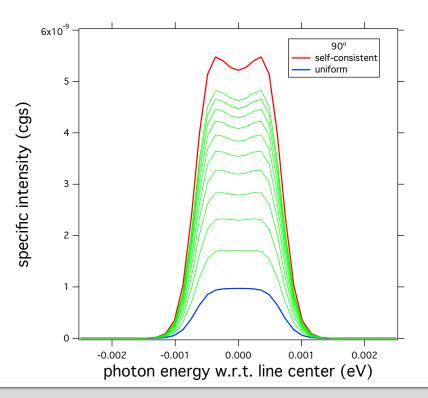
$$S_{v} = \frac{n_{2}A_{21}}{n_{1}B_{12} - n_{2}B_{21}} = (1 - \varepsilon)\overline{J}_{12} + \varepsilon B_{v} , \frac{\varepsilon}{1 - \varepsilon} = \frac{C_{21}}{A_{21}} \left(1 - e^{-hv_{0}/kT}\right)$$

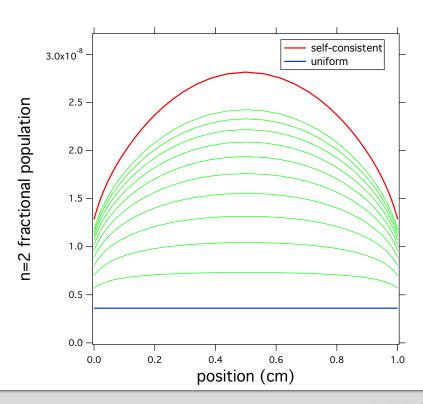
Including multiple transitions and separate emission profiles is straightforward

#### Calculating $\overline{J}$ is the focus of line radiation transport

# Example – Hydrogen Ly-α

- Source iteration (green curves) approaches self-consistent solution slowly
- Linearization achieves convergence in 1 iteration since the source function is a linear function of  $\overline{J}$   $S_{ij} = a + b \overline{J}_{ij}, \overline{J}_{ij} = \int J_{\nu} \phi_{\nu} \, d\nu$

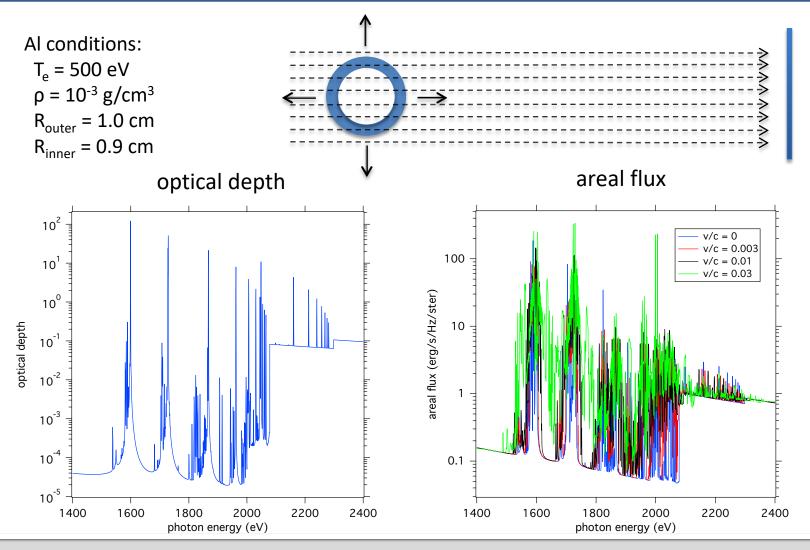




### **Velocity gradients**

- Absorption / emission is (usually) isotropic in the fluid frame
- Doppler shifts make these anisotropic in the laboratory frame
- This effect becomes significant when  $v/c \sim dE / E_0$
- For thermal velocities:  $\frac{\mathrm{v}}{\mathrm{c}} \sim \sqrt{\frac{2kT_i}{m_ic^2}} \sim 0.0015\sqrt{\frac{T_i}{A_i}}$   $T_i$  in keV
- For Doppler-broadening lines, sound speed bulk velocities become important

### Uniformly expanding spherical annulus



### Uniformly expanding spherical annulus

