CRETIN

Session 9

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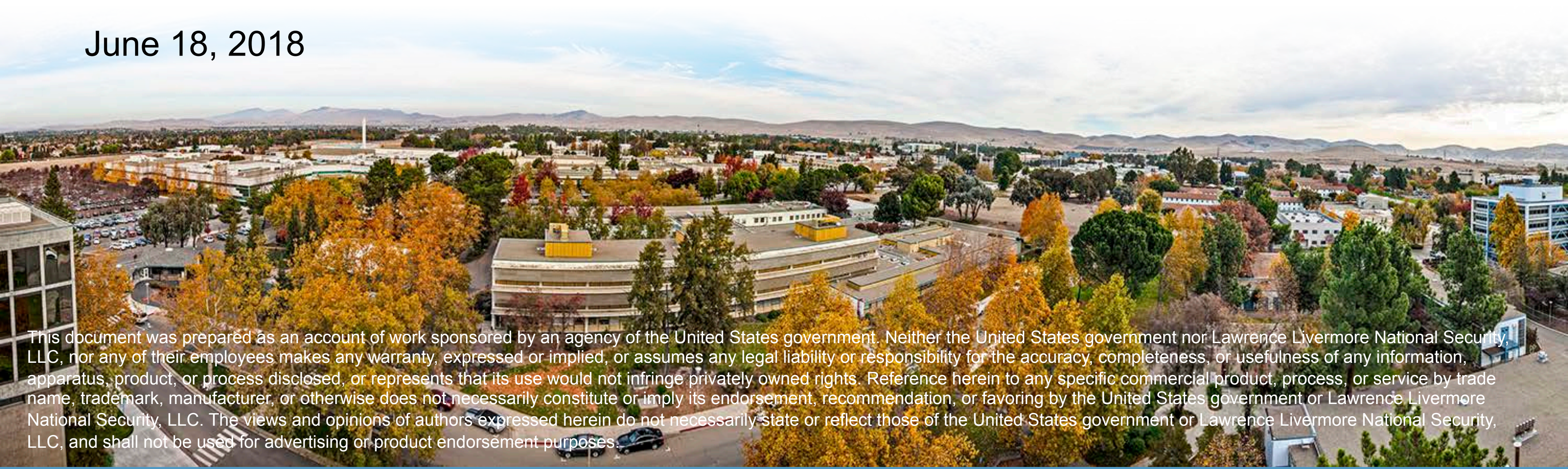

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Session topics

1. Stark lineshapes
2. Escape factors

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
- **Stark effect** (plasma microfields) - complex

Stark effect

- Splits and shifts lines → additional components + broadening
- Increases strongly with quantum number *n* (n^{6-7})
- Increases with n_e ($n_e^{2/3}$ for e^- broadening)
- Decreases with *Z* (Z^{-1} for hydrogenic → $\Delta E / E \sim Z^{-3}$)

Total is a lineshape code which runs standalone or as part of Cretin

- Stark effect from electron collisions + ion microfields + ion dynamics
- Zeeman splitting

SLS is a rewritten version of Total not completely integrated into Cretin

Total (and SLS) are located in /usr/apps/cretin/bin

Specifying transitions for Stark lineshapes

For line transport:

line *iline iz iso i1 iso i2*
linetype *total (totalb)*

For spectral calculations:

stark transition *iz iso i1 i2* - or -
stark manifold *iz iso n1 n2*

Total requires (*n,l,j*) detailed levels + transition matrix elements

- available in dca_*xx*k models
- additional switches control Total options (88, 114-117)

Example: dca_18k H-α transitions

```
data  phxs
  d   1   1   1   2   1.37957E-01  3.73646E+00  0.00000E+00  5.82580E-02
  d   1   1   1   3   1.90219E-08  3.73629E+00  0.00000E+00  2.16322E-05
  d   1   1   1   4   2.73463E-01  3.73105E+00  0.00000E+00  8.19629E-02
```

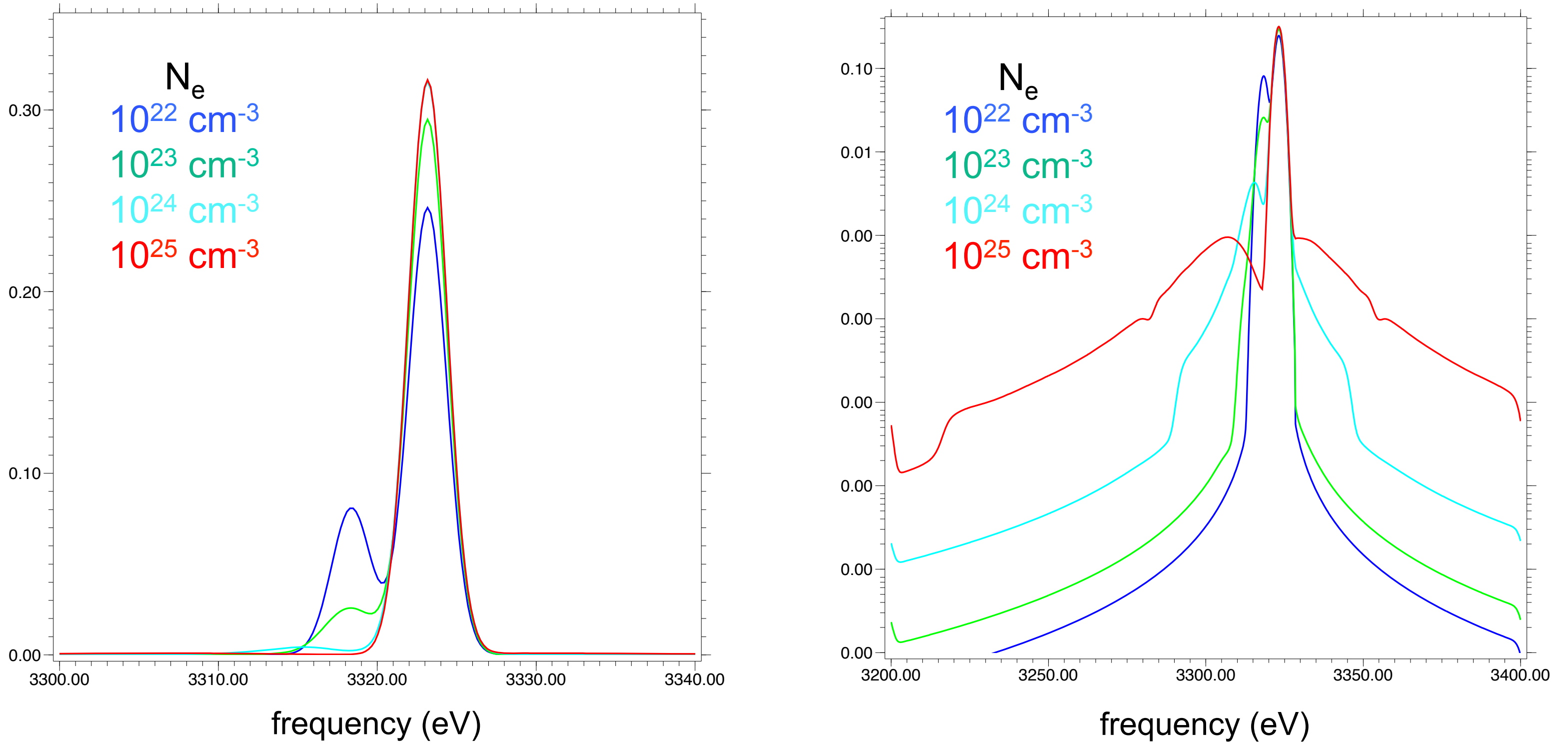
For transitions not treated with Total:

- broadening can be added if switch(52) < 0
- formulas provided by Hans Griem (aimed at dense plasmas)
- both Doppler core and Lorentzian wing are affected if switch(52) = -1

Ar H-α Stark profile

- Doppler widths dominate at low density
- Larger ($J=3/2$) component has no linear Stark broadening
- Wings fall off as $(\Delta\nu)^{-5/2}$ for frequencies $\Delta\nu$ > collision frequency

$T_e = T_i = 5$ keV



Escape factors

An approximate treatment of trapped radiation which (usually) assumes:
uniform spatial conditions (+ line profile remains the same)
2-level atom treatment is sufficient (with negligible upper-level population)
isotropic emission with complete redistribution

Definitions:

monochromatic escape probability $p_e(\nu) = e^{-\tau_\nu}\ ,\ \tau_\nu = \int \alpha_\nu^0(r)\phi_\nu\, dr$

escape probability $\langle p_e \rangle = \int \phi_\nu p_e(\nu)\, d\nu$

escape factor $P_e = \frac{1}{4\pi}\oint \langle p_e \rangle\, d\Omega$

averaged escape factor $\bar{P}_e = \int P_e\, dV \Big/ \int dV$

- Escape probabilities require knowledge of the line profile
- Escape factors also require knowledge of the complete problem geometry, but are applied locally

Applying escape factors

Two-level atom (steady-state) rate equation:

$$n_1(B_{12}\bar{J}_{12} + C_{12}) = n_2(A_{21} + B_{21}\bar{J}_{12} + C_{21}) \qquad \bar{J}_{12} = \int_0^\infty J_\nu \phi(\nu)\, d\nu$$

The escape factor replaces radiative terms with <u>decreased</u> spontaneous emission:

$$n_2(A_{21} + B_{21}\bar{J}_{12}) - n_1 B_{12}\bar{J}_{12} \rightarrow n_2 A_{21} P_e \qquad \Rightarrow \qquad n_1 C_{12} = n_2(P_e A_{21} + C_{21})$$

Comments:

- Iron's theorem says this is correct on average (emissivity-weighted spatial)
- This substitution happens for all transitions treated with escape factors

  $$A_{ij} \rightarrow P_e^{ij} A_{ij}$$

- Since P_e depends on populations, this adds non-linearity to the rate equations
- P_e incorporates global information through the optical depth

- Escape factors are used to calculate populations (absorption, emission)
  Radiation transport is used to calculate intensities along a given path

$$I_\nu = \int_0^s e^{-\alpha_\nu s} \eta_\nu\, ds$$

Choosing the appropriate escape factor

- Escape factors depend on line shape and geometry
- Analytic approximations to P_e are available for
  - Doppler, Lorentzian, Voigt profiles + Stark (in wings)
  - planar, cylindrical, spherical geometry (central location)

What about Doppler shifts?

- Sobolev approximation accounts for a constant velocity gradient dV/ds
  - photons shift frequency w.r.t. local frame by $\frac{\Delta\nu}{\nu} = \frac{\Delta s}{c}\frac{dV}{ds}$
  - in the Sobolev limit of large dV/ds

$$\langle p_e \rangle \to \frac{1-e^{-\tau_S}}{\tau_S} \qquad \tau_S = \frac{\Delta\nu_D}{dV/ds}$$ ← escape probability

Other issues –

- Overlapping lines / continuum opacity
- Continuum opacity
- Non-central locations in non-planar geometry
- Doppler shifts <u>not</u> in Sobolev limit
- Other radiation fields

Escape factors in 0D simulations

In a 0D simulation, the goal is (usually) to calculate the <u>average</u> emissivity

- Calculate averaged escape factors $\bar{P}_e$ by evaluating P_e for optical depth

  $\tau_\nu = \alpha_\nu \langle R \rangle \,,\; \langle R \rangle = 4V/S$ ← mean chord

- Evaluate escaping intensity for desired line-of-sight

Ref: G.J. Phillips, J.S. Wark, F.M. Kerr, S.J. Rose, R.W. Lee, HEDP **4**, 18-25 (2008)

Important points:

- This can give the correct <u>average</u> emission for a single transition
- Averaging transitions does <u>not</u> produce average plasma properties
  → may not give the correct emission for multiple transitions
- Averaging spreads out the radiative boundary layer over the whole plasma
  → does not produce boundary layer effects

Escape factors in Cretin

<u>0-dimensional</u>

- uses $\bar{P}_e$ for each transition
- special spectral edits for integrated quantities (*isp_0d, esp_0d, tausp_0d, trsp_0d*)

<u>1-dimensional</u>

- applies P_e at each position averaged over +/- directions
- τ in each direction calculated with scaled integrated column density of charge state
- assumes constant line profile, fractional lower state population

<u>2- / 3-dimensional</u>

- applies P_e at each position averaged over +/- directions along 1 or more axes
- option to specify directions for averaging is partially complete

Escape factors are also applied to extant radiation fields

Escape factors in Cretin

Main controls

switch 33: use escape factors for lines only if <0, all photoexcitations if >0

±1: static ±2: Sobolev ±3: interpolation between static & Sobolev

±4: generalized escape factor ← **recommended**

includes continuum, velocity gradients, arbitrary profile & geometry

param 54: minimum optical depth for calculating escape factors

Additional controls (mostly for 0D applications)

switch 78: choose line profile (Voigt, Doppler, Lorentzian)

switch 79: include continuum opacity?

switch 80: specify problem geometry

switch 81: single- or double-sided

switch 82: use integrated density, local density, or param(53)

switch 154: choose axes for integrations in 2D/3D

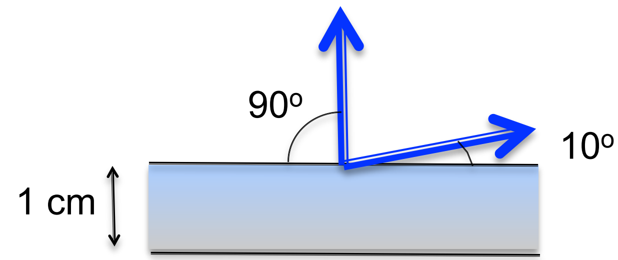
param 53: Δr or $\Delta(nr)$ to use for escape factors (average chord)

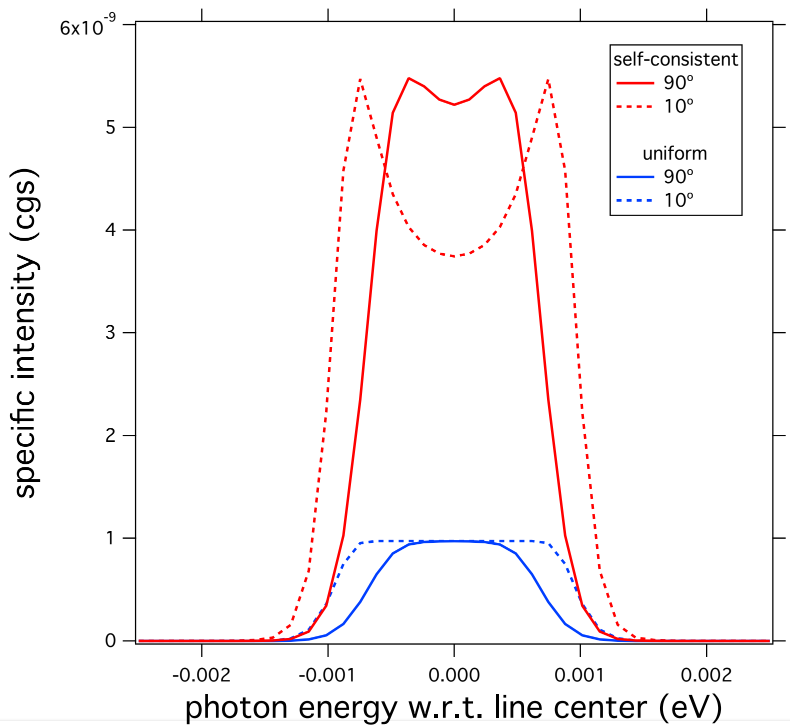
param 139: Δr or $\Delta(nr)$ to use for escape factor edits (LOS distance)

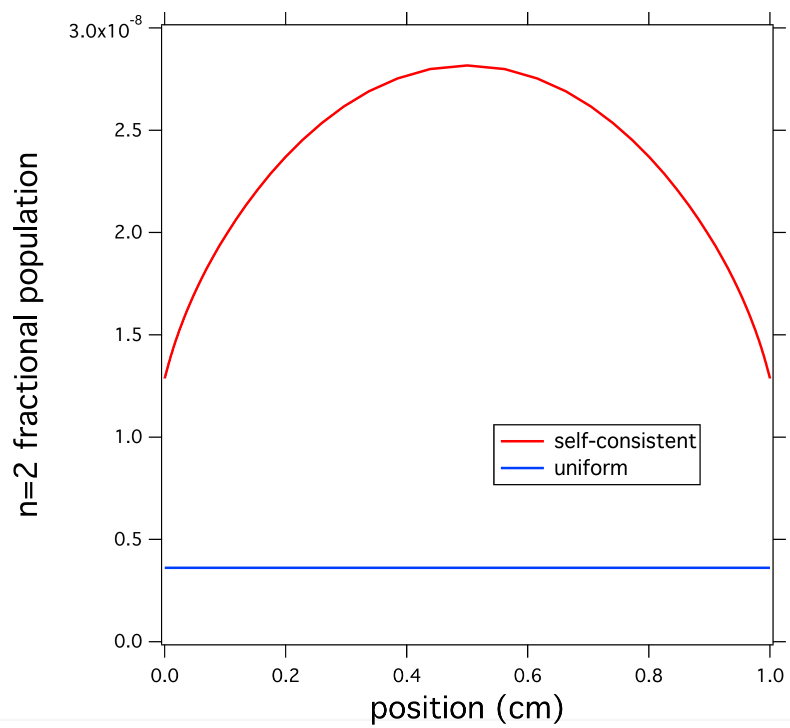
combinations of switch(79) + switch(80) can also choose specific analytic or tabulated escape factor formulations

Example – Hydrogen Ly-α

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

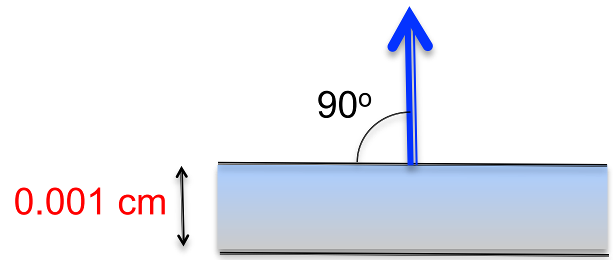


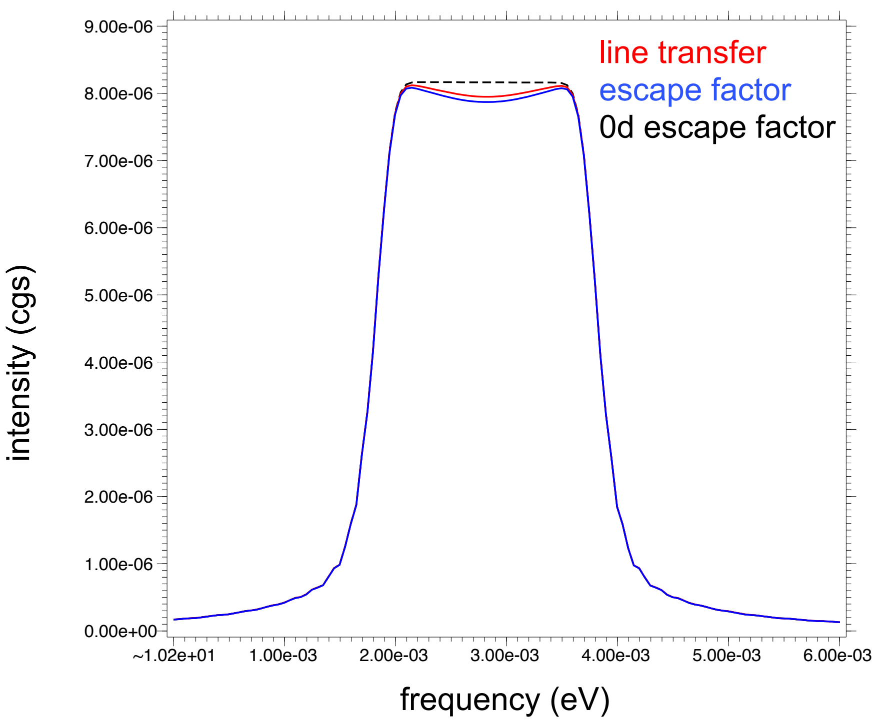


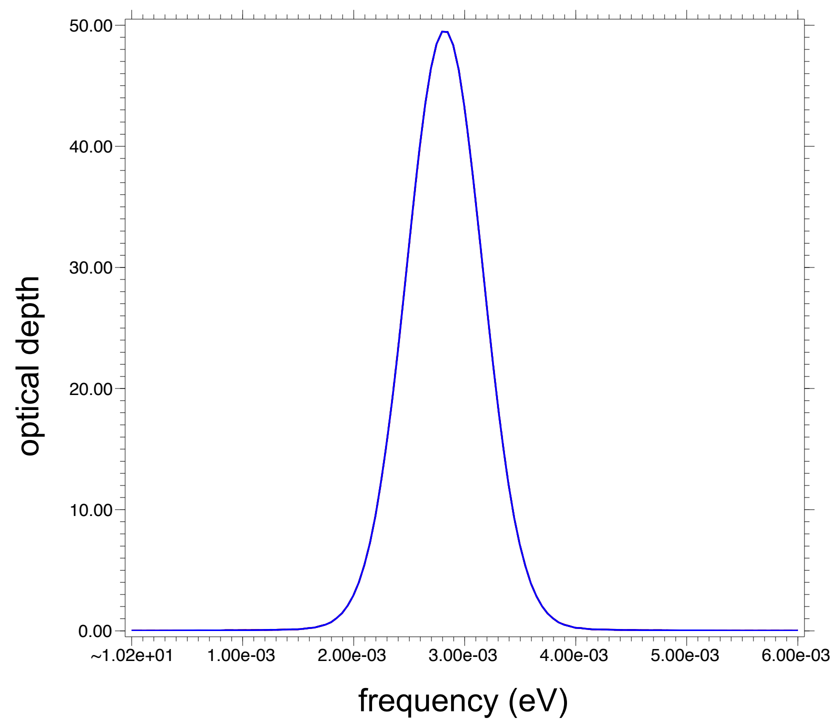


Hydrogen Ly-α with escape factor – easy case

- Uniform conditions: T_e = 1 eV
- **High** density: $n_i = 10^{18}$ cm^{-3}

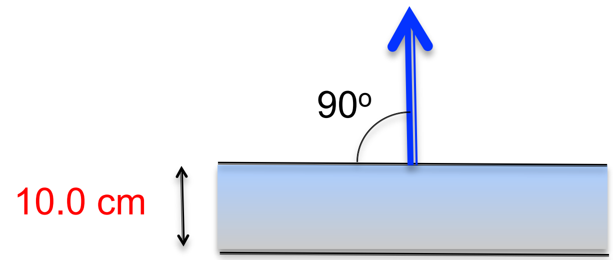


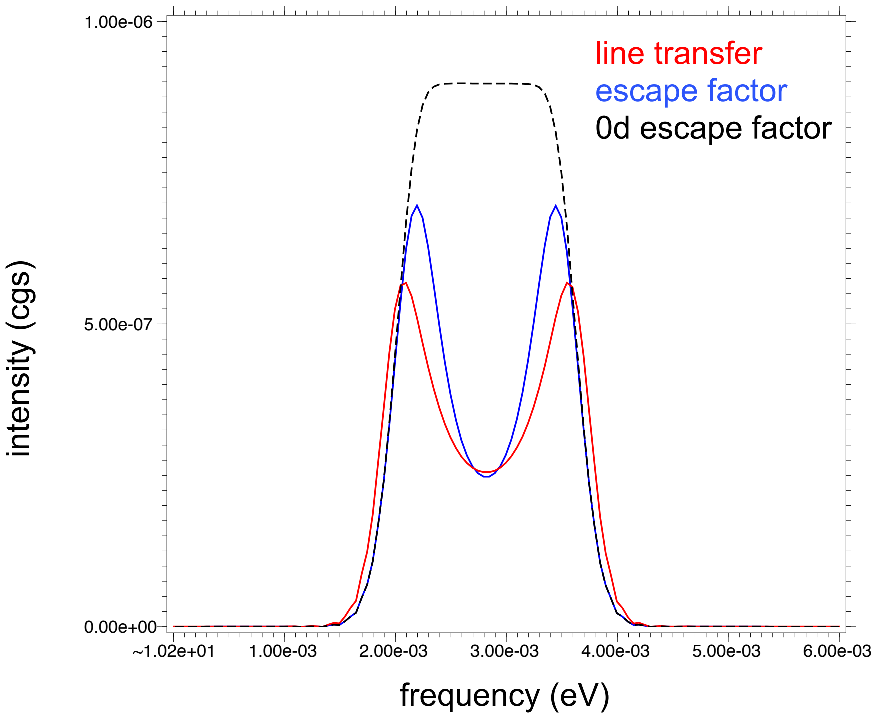


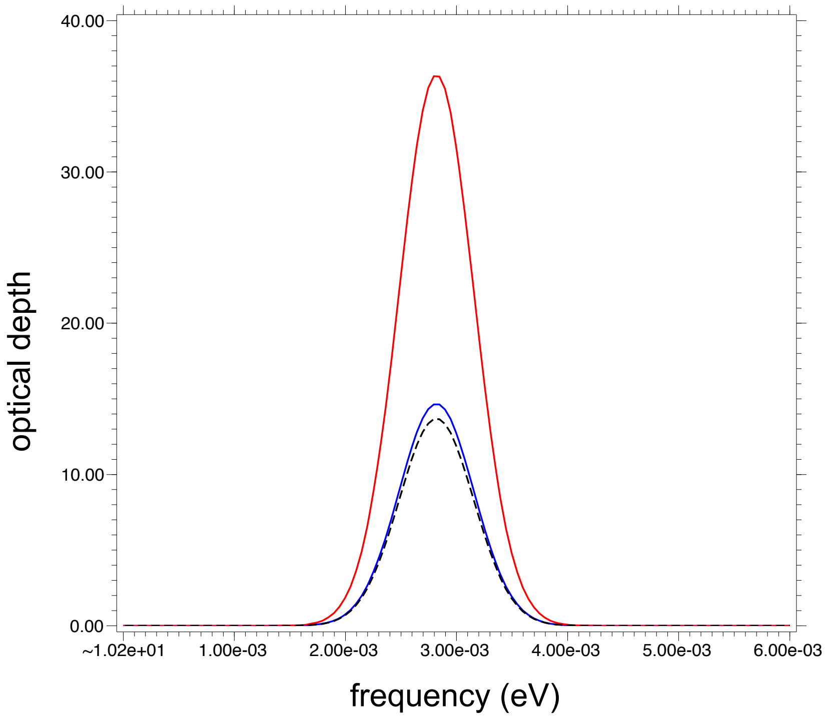


Hydrogen Ly-α with escape factor – hard case

- Uniform conditions: T_e = 1 eV
- **Low** density: $n_i = 10^{14}\ \mathrm{cm}^{-3}$

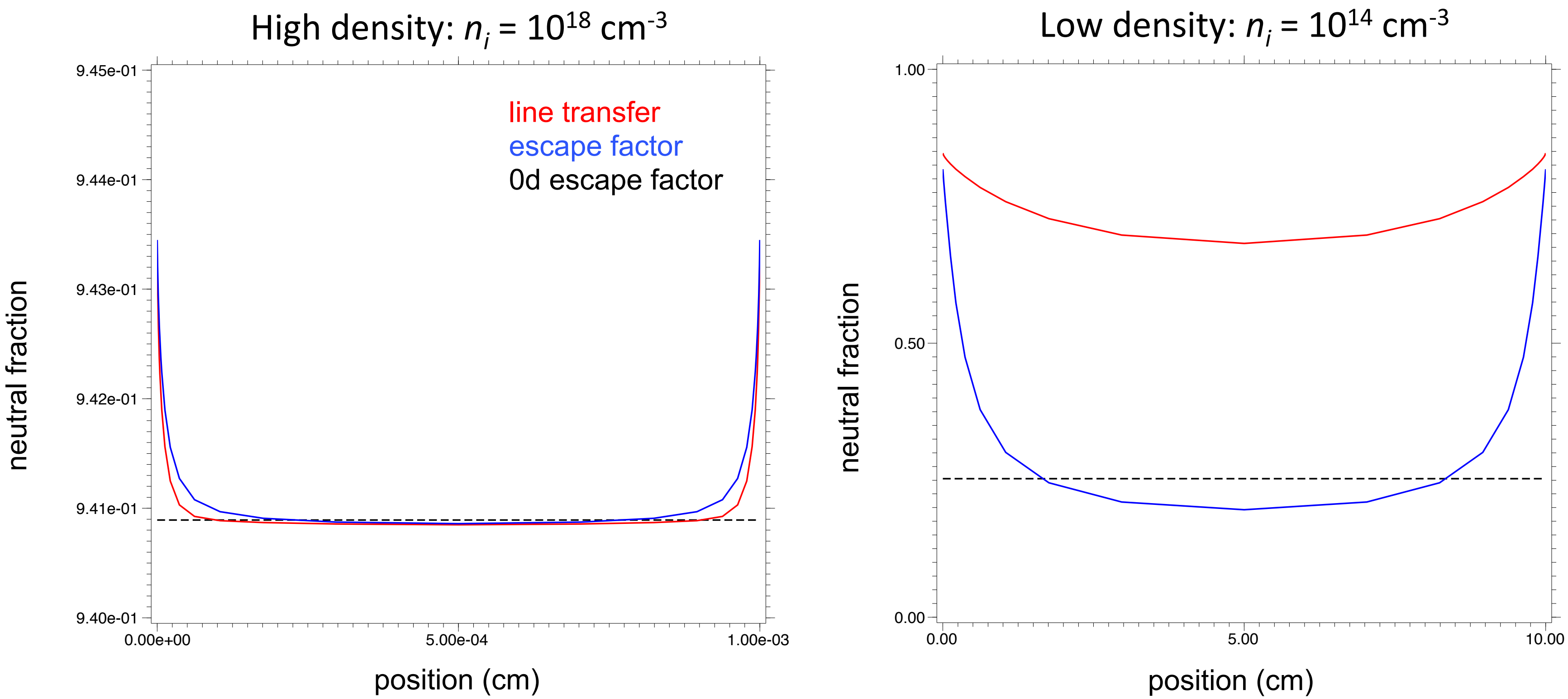






Hydrogen Ly-α with escape factor

- Ionization is dominated by collisions at high density, radiation at low density
- Position-dependent escape factors mimic boundary layer, but not ionization
- 0d escape factor assumes average conditions with no boundary layer
- Line transfer allows photons to escape by changing frequency



Advantages / disadvantages of escape factors

Advantages:

- Much faster than line transfer, can be applied to all photoexcitations
- Good results for isolated lines (with the right escape factor) under most conditions
- Escape factors give an approximation to radiation transfer

Disadvantages:

- Choosing or calculating the right escape factor can be difficult
- Applying escape factors in 0D for multiple transitions can be problematic
  - average rates for each transition ≠ rates for average conditions
- Calculating escape factors in non-uniform plasmas requires spatial information similar to that of radiation transfer (i.e. ray tracing)
- Escape factors give an approximation to radiation transfer which cannot be iteratively improved

Other notes:

- Many other variations exist in a large literature
- "Escape factors" for photoionizations appear in the literature (and some codes)
  - may or may not be better than nothing