Lecture Notes on Radiation Transport for Spectroscopy

ICTP-IAEA School on Atomic Processes in Plasmas

27 February – 3 March 2017 Trieste, Italy

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LLNL-PRES-668311
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Radiation Transport

Outline

- Definitions, assumptions and terminology
  - Equilibrium limit
- Radiation transport equation
  - Characteristic form & formal solution
  - Material radiative properties
    - Absorption, emission, scattering
- Coupled systems
  - LTE / non-LTE
- Line radiation
  - Line shapes
  - Redistribution
  - Material motion
- Solution methods
  - Transport operators
  - 2-level & multi-level atoms
  - Escape factors

Basic assumptions

Classical / Semi-classical description –

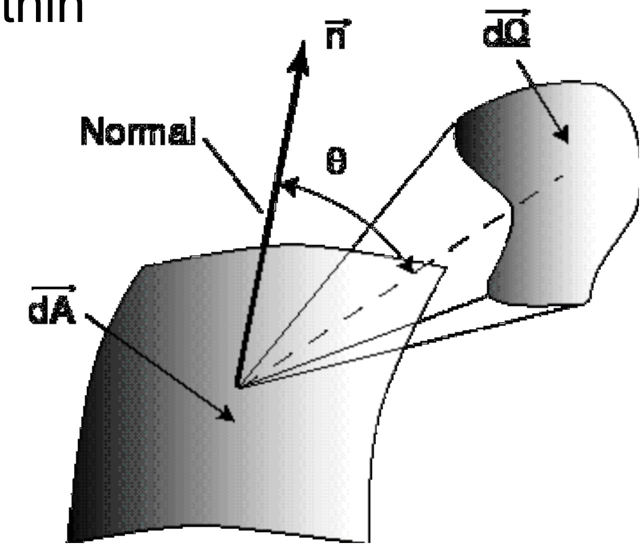
- Radiation field described by either specific intensity I_ν or the photon distribution function f_ν
- Unpolarized radiation
- Neglect index of refraction effects ($n \approx 1$, $\omega >> \omega_p$)
  - ➔ Photons travel in straight lines
- Neglect true scattering (mostly)
- Static material (for now)
  - ➔ Single reference frame

Radiation Description

Macroscopic - specific intensity I_ν

- energy per (area x solid angle x time) within the frequency range $(\nu, \nu + d\nu)$

$$dE = I_\nu\left(\vec{r}, \Omega, t\right)\left(\vec{n} \bullet \vec{\Omega}\right) dA\, d\Omega\, d\nu\, dt$$



- dE = energy crossing area dA within $(d\Omega\, d\nu\, dt)$

Microscopic - photon distribution function

$$dE = \sum_{spins}\left(h\nu\right) f_\nu\left(\vec{r}, \vec{p}, t\right)\frac{d^3\vec{x}\, d^3\vec{p}}{h^3}$$

$$I_\nu = 2\frac{h\nu^3}{c^2} f_\nu\left(\vec{r}, \vec{p}, t\right) \qquad \vec{p} = \frac{h\nu}{c}\vec{\Omega}$$

Angular Moments

0th moment $J_\nu = \frac{1}{4\pi}\int I_\nu \, d\Omega$ = energy density x *c/4π*

1st moment $\mathbf{H}_\nu = \frac{1}{4\pi}\int \mathbf{n} I_\nu \, d\Omega$ = flux x *1 /4π*

2nd moment $\mathbf{K}_\nu = \frac{1}{4\pi}\int \mathbf{n}\mathbf{n} I_\nu \, d\Omega$ = pressure tensor x *c /4π*

For isotropic radiation, K_ν is diagonal with equal elements:

$$\mathbf{K}_\nu = \frac{1}{3} J_\nu \mathbf{I} \qquad \left(P = \frac{1}{3} E\right)$$

In this case, radiation looks like an ideal gas with γ = 4/3

Thermal Equilibrium

Intensity: Planck function

$$B_\nu = 2\frac{h\nu^3}{c^2}\frac{1}{e^{h\nu/kT_r}-1}$$

Distribution function: Bose-Einstein

$$f_\nu = \frac{1}{e^{h\nu/kT_r}-1}$$

Energy density

$$E_{rad}\left(T_r\right) = \frac{4\pi}{c}\int_0^\infty B_\nu\left(T_r\right)d\nu = aT_r^{\,4}$$

For $T_e = T_r$ and $n_H = 10^{23}$ cm^{-3} : $E_{rad} = E_{matter} \Leftrightarrow T \approx 300\,eV$

LTE (Local Thermodynamic Equilibrium) -

particles have thermal distributions (T_e, T_i)

photon distribution can be arbitrary

Radiation Transport Equation

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t} + \vec{\Omega} \bullet \nabla I_\nu = -\alpha_\nu I_\nu + \eta_\nu$$

α_ν = absorption coefficient (fraction of energy absorbed per unit length)

η_ν = emissivity (energy emitted per unit time, volume, frequency, solid angle)

- Boltzmann equation for the photon distribution function:

$$\frac{1}{c}\frac{\partial f_\nu}{\partial t} + \vec{\Omega} \bullet \nabla f_\nu = \left(\frac{\partial f_\nu}{\partial t}\right)_{coll} \qquad I_\nu = 2h\nu\left(\frac{h\nu}{c}\right)^2 f_\nu$$

- The LHS describes the flow of radiation in phase space
- The RHS describes absorption and emission
  - Absorption & emission coefficients depend on atomic physics
  - Photon # is not conserved (except for scattering)
- Photon mean free path $\lambda_\nu = 1/\alpha_\nu$

Characteristic Form

Define the source function S_ν and optical depth τ_ν:

$S_\nu = \eta_\nu/\alpha_\nu$ $= B_\nu$ in LTE $\qquad\qquad d\tau_\nu = \alpha_\nu\, ds$

Along a characteristic, the radiation transport equation becomes

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \;\Rightarrow\; I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S_\nu(\tau'_\nu)\,d\tau'_\nu$$

This solution is useful when material properties are fixed, e.g. postprocessing for diagnostics

Important features:

- Explicit non-local relationship between I_ν and S_ν
- Escaping radiation comes from depth $\tau_\nu \approx 1$
- Implicit $S_\nu(I_\nu)$ dependence comes from radiation / material coupling

Self-consistently determining S_ν and I_ν is the hard part of radiation transport

Limiting Cases

Optically-thin τ_ν<<1 (viewed in emission):

$$I_\nu = \int_0^{\tau_\nu} S_\nu d\tau'_\nu = \int_0^{dx} \eta_\nu dx' \rightarrow \eta_\nu dx$$

I_ν reflects spectral characteristics of emission, independent of absorption

Optically-thick τ_ν>>1:

$$I_\nu(\tau_\nu) = \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)} S_\nu(\tau'_\nu) d\tau'_\nu \rightarrow S_\nu(\tau_\nu)$$

I_ν reflects spectral characteristics of S_ν (over ~last optical depth)

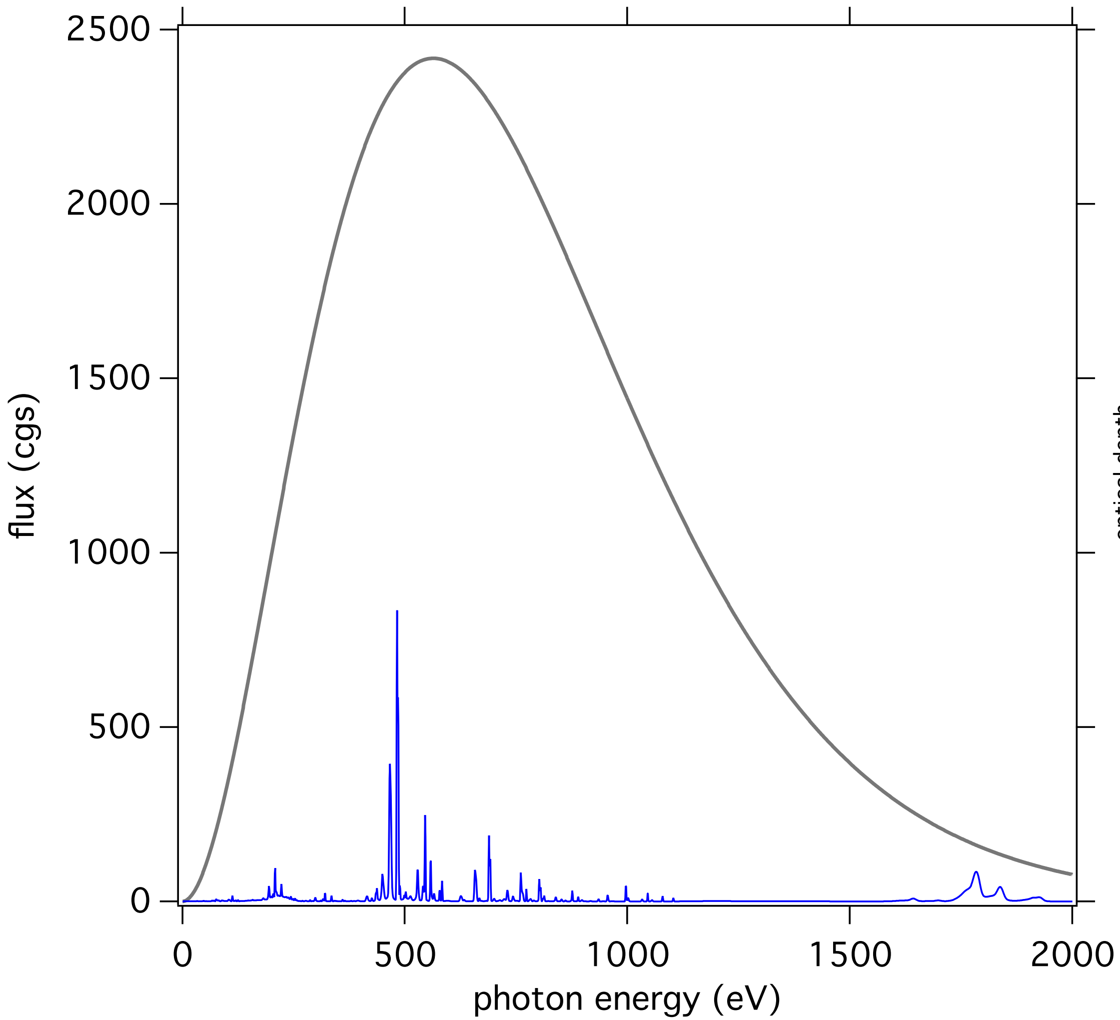
Negligible emission (viewed in absorption):

$$I_\nu(\tau_\nu) = I_\nu(0) e^{-\tau_\nu}, \; \tau_\nu = \int_0^{dx} \alpha_\nu dx' \rightarrow \alpha_\nu dx$$

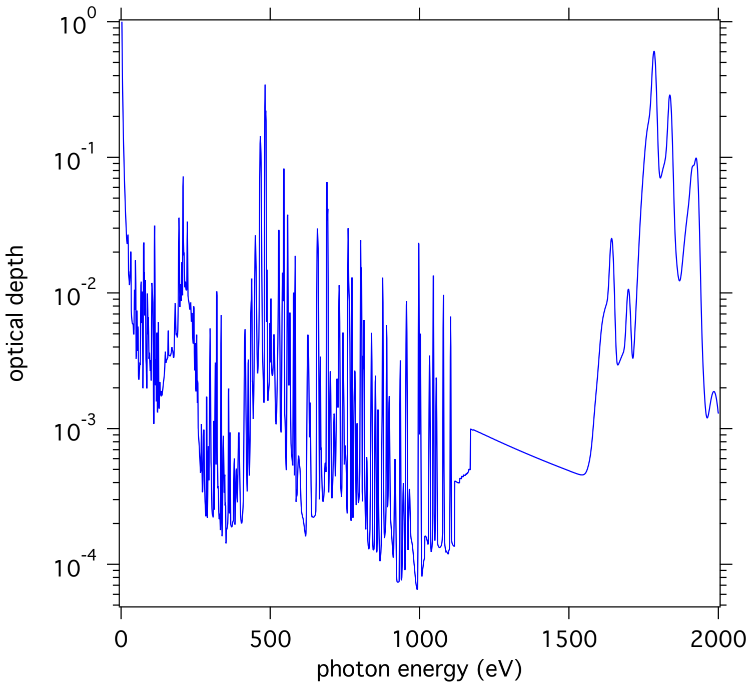
$I_\nu / I_\nu(0)$ reflects spectral characteristics of absorption

Example – Flux from a uniform sphere

Kr @ T = 200 eV, ρ = 0.01 g/cc, LTE



Δr = 0.001 cm



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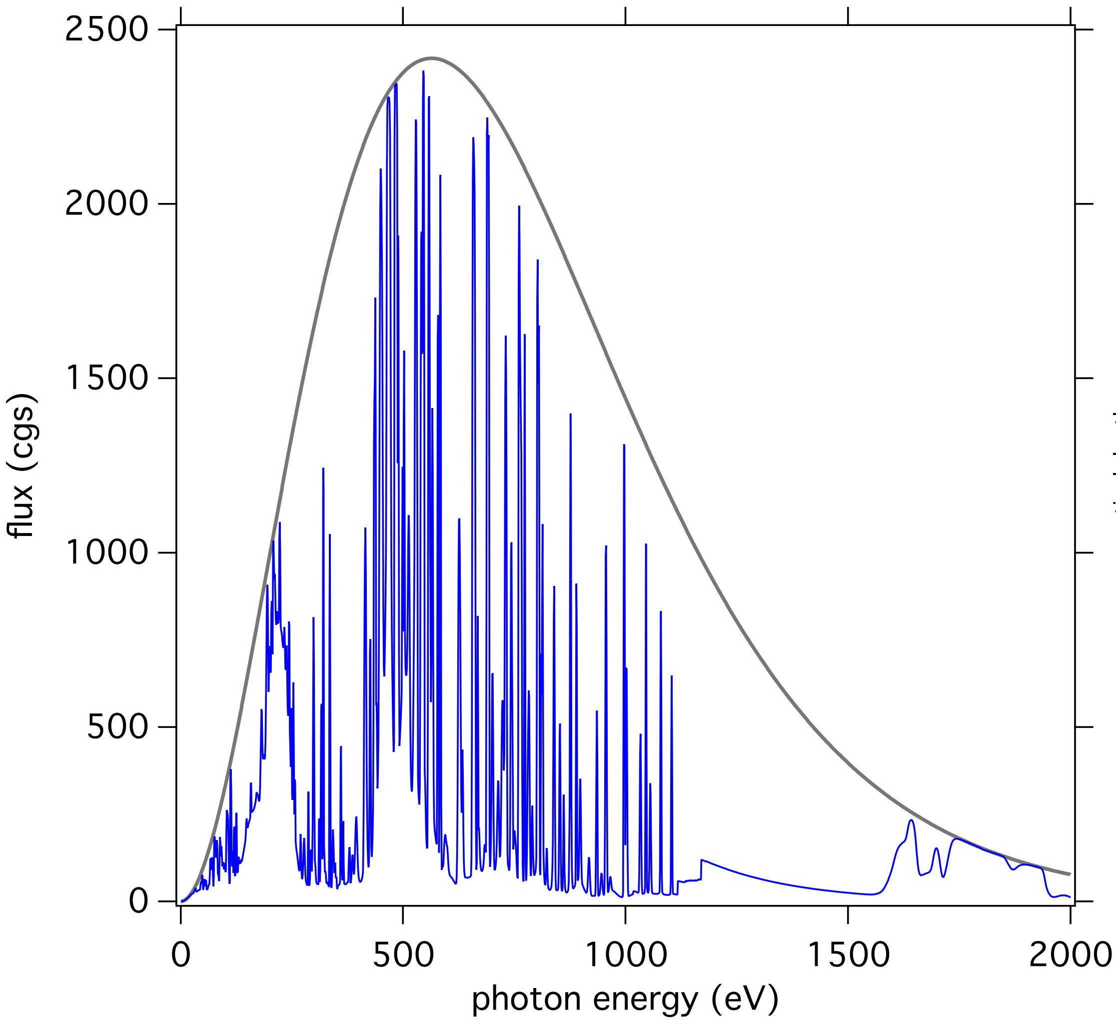

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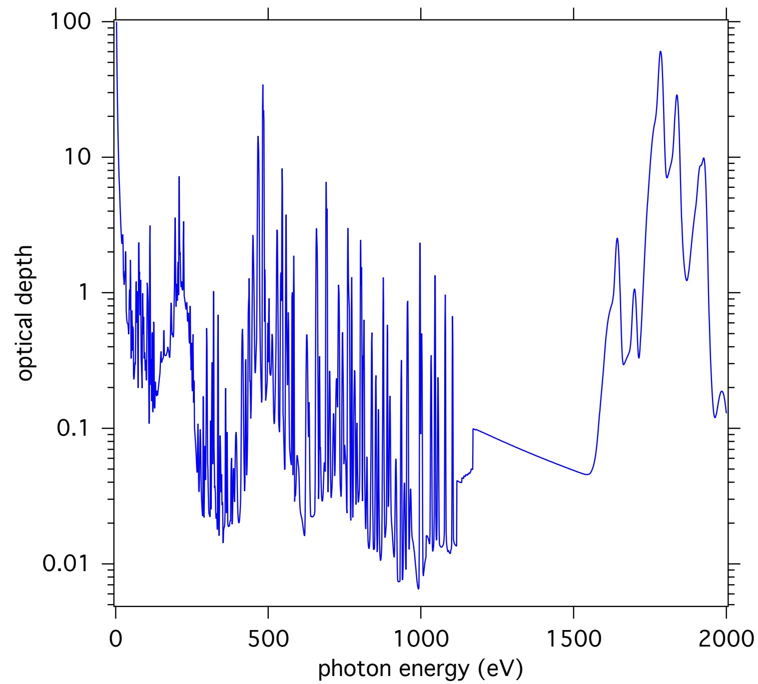

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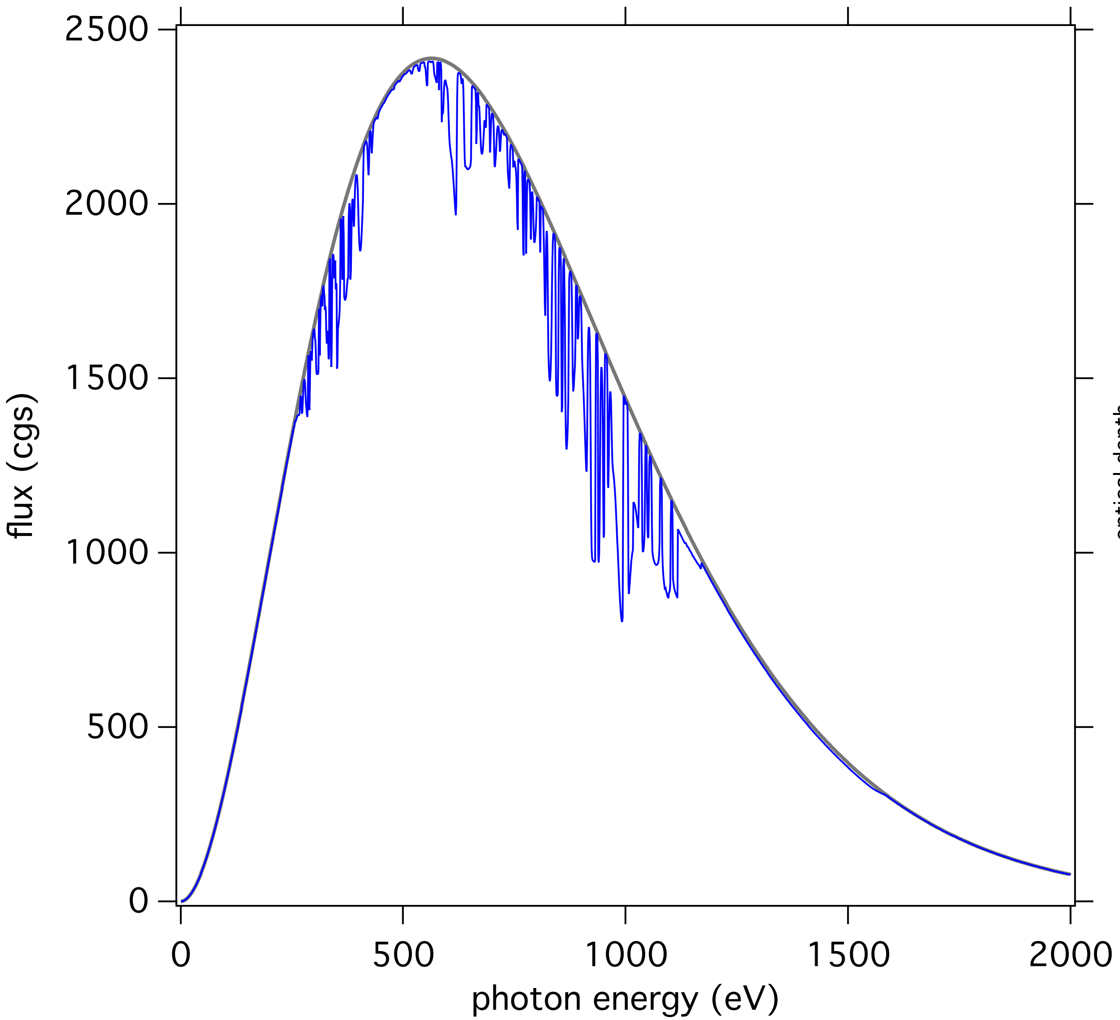
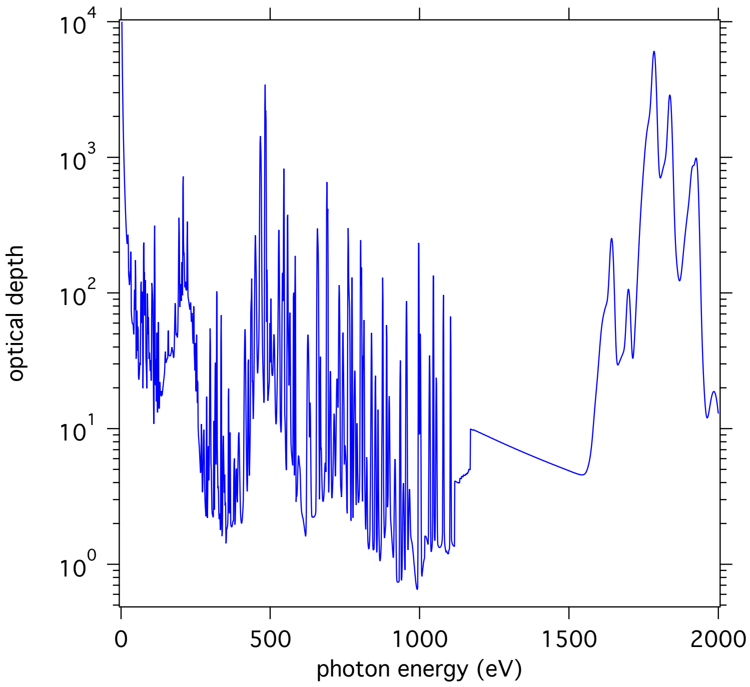


Δr = 10.0 cm



Absorption / emission coefficients

<u>Macroscopic</u> description – energy changes

- Energy removed from radiation passing through material of area dA, depth ds, over time dt

$$dE = -\alpha_\nu I_\nu \, dA\, ds\, d\Omega\, d\nu\, dt$$

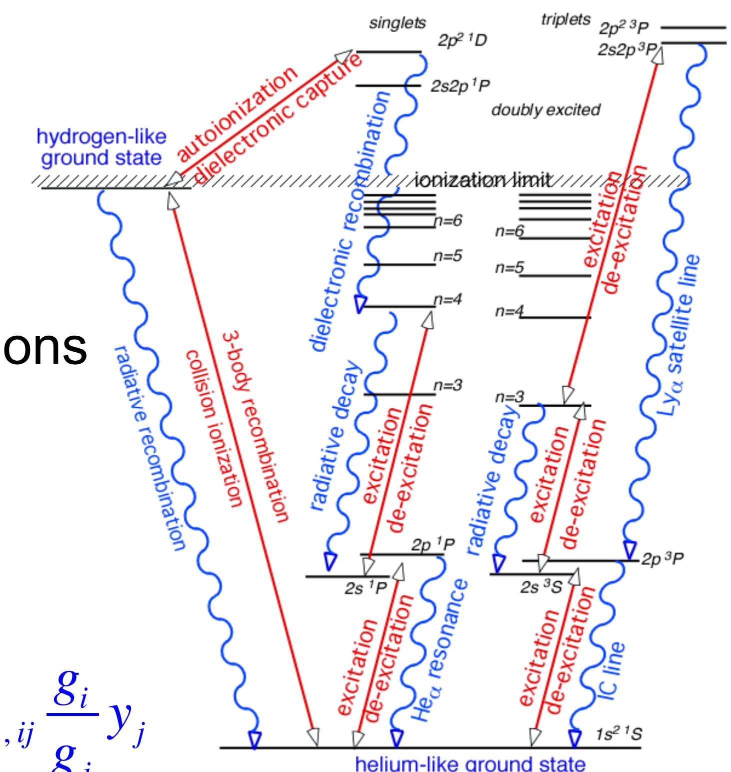
- Energy emitted by material

$$dE = \eta_\nu \, dA\, ds\, d\Omega\, d\nu\, dt$$

<u>Microscopic</u> description – radiative transitions

- Absorption and emission coefficients are constructed from atomic populations y_i and cross sections σ_{ij}:

$$\alpha_\nu = \sum_{i<j} \sigma_{\nu,ij}\left(y_i - \frac{g_i}{g_j} y_j\right) \;,\; \eta_\nu = \frac{2h\nu^3}{c^2} \sum_{i<j} \sigma_{\nu,ij} \frac{g_i}{g_j} y_j$$



from T. Mehlhorn

Bound-bound Transitions

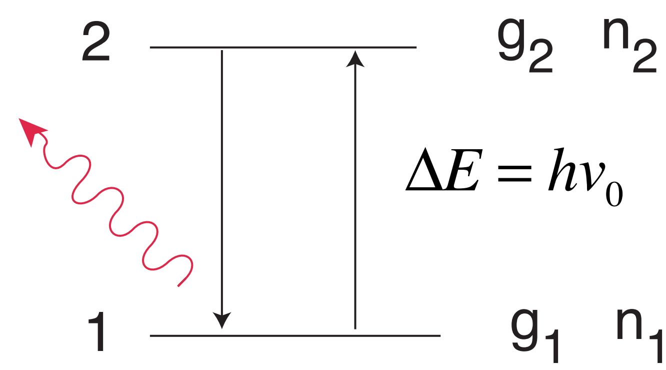
Probability (per unit time) of

- Spontaneous emission: A_{21}
- Absorption: $B_{12}\,\bar{J}$
- Stimulated emission: $B_{21}\,\bar{J}$

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

$$g_1 B_{21} = g_2 B_{12} \quad , \quad A_{21} = \frac{2h\nu_0^{\,3}}{c^2} B_{21}$$

Two energy level system



Line profile $\phi(\nu)$ measures probability of absorption

$$\int_0^\infty \phi(\nu)\,d\nu = 1$$

Transition rate from level 1 to level 2

$$R_{12} = B_{12}\bar{J} \;,\; \bar{J} = \int_0^\infty J_\nu \phi(\nu)\,d\nu$$

(assuming that the linewidth << ΔE)

Cross section for absorption

$$\sigma(\nu)=\frac{h\nu_o}{4\pi}B_{21}\phi(\nu)=\frac{\pi e^2}{mc}f_{12}\phi(\nu)$$

f_{12} = oscillator strength

$$\frac{\pi e^2}{mc}=0.02654\ \mathrm{cm^2/s}$$

Oscillator strength f_{12} relates the quantum mechanical result to the classical treatment of a harmonic oscillator

- Strong transitions have $f \sim 1$
- Sum rule $\sum_j f_{ij}=Z$ (# of bound electrons)

Absorption and emission coefficients:

$$\alpha_\nu=n_1\frac{\pi e^2}{mc}f_{12}\phi(\nu)\left[1-\frac{g_1 n_2}{g_2 n_1}\right]$$

absorption − stimulated emission

$$\eta_\nu=\left(\frac{2h\nu^3}{c^2}\right)n_2\frac{\pi e^2}{mc}f_{12}\phi(\nu)$$

spontaneous emission

For now we are assuming that absorption and emission have the same line profile

Bound-free absorption

Absorption cross section from state of principal quantum number n and charge Z

$$\sigma_{bf} = 7.91 \cdot 10^{-18} n g_{bf} \left(\frac{\nu_0}{\nu} \right)^3 \left(1 - e^{-h\nu / kT_e} \right) \mathrm{cm}^2$$

Gaunt factor

$h\nu_0 =$ threshold energy

Free-free absorption

Absorption cross section per ion of charge Z

$$\sigma_{ff} = 3.69 \cdot 10^{8} \frac{Z^2}{\nu^3 \sqrt{T_e}} g_{ff} n_e \left(1 - e^{-h\nu / kT_e} \right) \mathrm{cm}^2$$

Gaunt factor

The term $1 - e^{-h\nu / kT_e}$ accounts for stimulated emission

Scattering

Interaction in which the photon energy is (mostly) conserved (i.e. not converted to kinetic energy)

Examples:

Scattering by bound electrons – Rayleigh scattering

- important in atmospheric radiation transport

Scattering by free electrons – Thomson / Compton scattering

$$\sigma_T = \frac{8\pi}{3}\left(\frac{e^2}{m_e c^2}\right)^2 = 6.65 \times 10^{-25}\,\mathrm{cm}^2 \quad h\nu \ll m_e c^2$$

Note: frequency shift from scattering is $\sim h\nu / m_e c^2$

Doppler shift from electron velocity is $\sim \sqrt{2kT / m_e c^2}$

For most laboratory plasmas, these types of scattering are negligible

Note: X-ray Thomson scattering (off ion acoustic waves and plasma oscillations) can be a powerful diagnostic for multiple plasma parameters (T_e, T_i, n_e)

Radiation transport equation with scattering (and frequency changes):

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t}+\vec{\Omega}\bullet\nabla I_\nu=-\alpha_\nu I_\nu+\eta_\nu+$$

$$\sigma_\nu\int_0^\infty d\nu'\int\frac{d\Omega'}{4\pi}\left[-R(\nu',\Omega';\nu,\Omega)\frac{\nu}{\nu'}I_\nu(1+f'_\nu)+R(\nu,\Omega;\nu',\Omega')I_{\nu'}(1+f_\nu)\right]$$

stimulated scattering

The redistribution function R describes the scattering of photons (ν,Ω) ➔ (ν',Ω')

Neglecting frequency changes, this simplifies to

$$\frac{1}{c}\frac{\partial I_\nu}{\partial t}+\vec{\Omega}\bullet\nabla I_\nu=-(\alpha_\nu+\sigma_\nu)I_\nu+\eta_\nu+\sigma_\nu\int\frac{d\Omega'}{4\pi}I_\nu(\vec{\Omega}')g\left(\vec{\Omega}\bullet\vec{\Omega}'\right)$$

$$\rightarrow-(\alpha_\nu+\sigma_\nu)I_\nu+\eta_\nu+\sigma_\nu J_\nu$$ for isotropic scattering

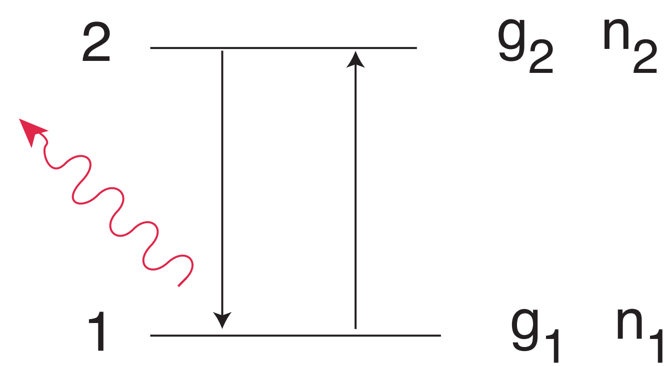
Scattering contributes to both absorption and emission terms (and may be denoted separately or included in α_ν and η_ν)

Effective scattering

Photons also "scatter" by e.g. resonant absorption / emission

Upper level 2 can decay
  a) radiatively A_{21}
  b) collisionally $n_e C_{21}$

Two energy level system



The fraction $\varepsilon \approx n_e C_{21} / A_{21}$
of photons are destroyed / thermalized

The fraction $(1\text{-}\varepsilon)$ of photons are "scattered"

➔ energy changes only slightly (mostly Doppler shifts)

➔ undergo many "scatterings" before being thermalized

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

Population distribution

LTE: Saha-Boltzmann equation

- Excited states follow a Boltzmann distribution $\dfrac{y_i}{y_j} = \dfrac{g_i}{g_j} e^{-(\varepsilon_i - \varepsilon_j)/T_e}$ $\varepsilon_i = \text{energy of state } i$, $T_e = \text{electron temperature}$
- Ionization stages obey the Saha equation

$$\frac{N_q}{N_{q+1}} = \frac{1}{2} n_e \frac{U_q}{U_{q+1}} \left(\frac{h^2}{2\pi m_e T_e} \right)^{3/2} e^{-(\varepsilon_0^{q+1} - \varepsilon_0^q)/T_e}$$

$$N_q = \sum_{i \in q} y_i e^{-(\varepsilon_i - \varepsilon_0^q)/T_e} \quad \text{number density of charge state } q$$

$$U_q = \sum_{i \in q} g_i e^{-(\varepsilon_i - \varepsilon_0^q)/T_e} \quad \text{partition function of charge state } q$$

NLTE: Collisional-radiative model

- Calculate populations by integrating rate equations

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}\mathbf{y} \quad A_{ij} = C_{ij} + R_{ij} + (other)_{ij} \qquad C_{ij} = n_e \int \mathrm{v}\,\sigma_{ij}(\mathrm{v}) f(\mathrm{v})\, d\mathrm{v}$$

$$R_{ij} = \int \sigma_{ij}(\nu) J(\nu) \frac{d\nu}{h\nu}, \quad R_{ji} = \int \sigma_{ij}(\nu) \left[J(\nu) + \frac{2h\nu^3}{c^2} \right] e^{-h\nu/kT} \frac{d\nu}{h\nu}$$

Summary of absorption / emission coefficients

- Summed over populations and radiative transitions:

$$\alpha_\nu = \sum_{ij} y_i \left\{ \frac{\pi e^2}{mc^2} f_{ij} \phi_{ij}(\nu) \left(1 - \frac{g_i y_j}{g_j y_i} \right) + \left[\sigma_{ij}^{bf}(\nu) + n_e \bar{\sigma}_{ij}^{ff}(\nu) \right] (1 - e^{-h\nu/kT_e}) \right\}$$

$$\eta_\nu = \frac{2h\nu^3}{c^2} \sum_{ij} y_j \left\{ \frac{\pi e^2}{mc^2} \frac{g_i}{g_j} f_{ij} \phi_{ij}(\nu) + \left[\sigma_{ij}^{bf}(\nu) + n_e \bar{\sigma}_{ij}^{ff}(\nu) \right] e^{-h\nu/kT_e} \right\}$$

- In NLTE, the source function has a complex dependence on plasma parameters and on the radiation spectrum:

$$S_\nu = S_\nu(n_e, T_e; y_i(J_\nu))$$

- In LTE, absorption and emission spectra are complex but the source function obeys Kirchoff's law:

$$S_\nu = B_\nu(T_e)$$

Opacity & mean opacities

opacity = absorption coefficient / mass density $\kappa_\nu = \alpha_\nu / \rho$

Rosseland mean opacity:

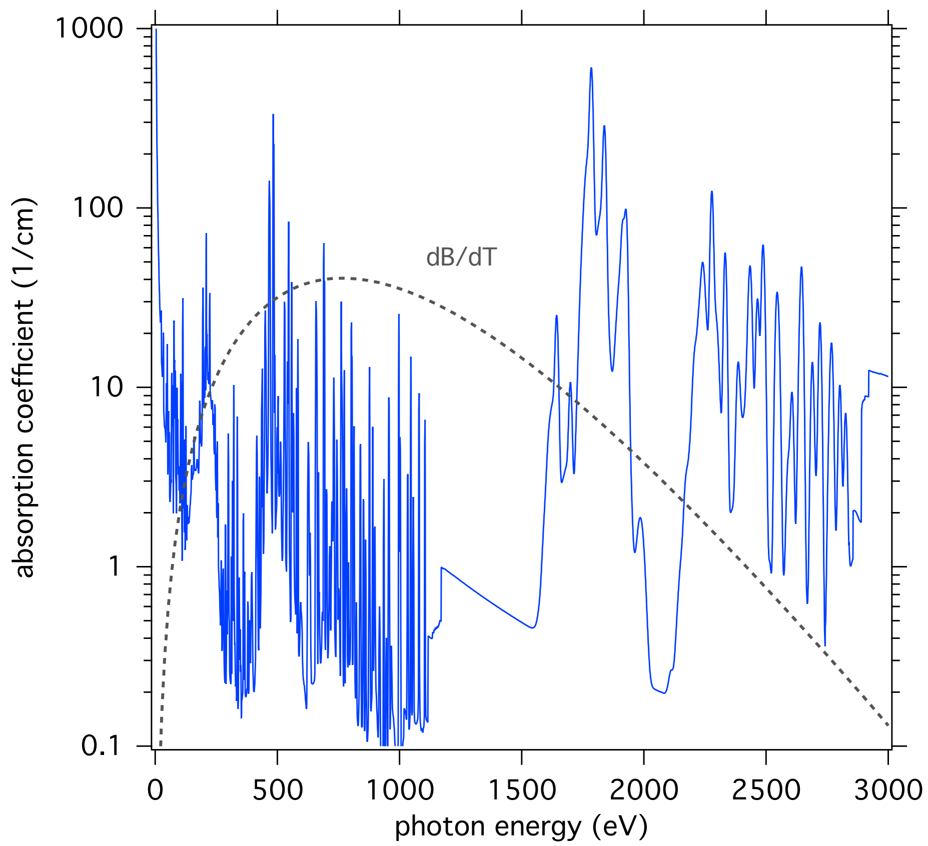
- emphasizes transmission
- includes scattering
- appropriate for average flux

Planck mean opacity:

- emphasizes absorption
- no scattering
- appropriate for energy exchange

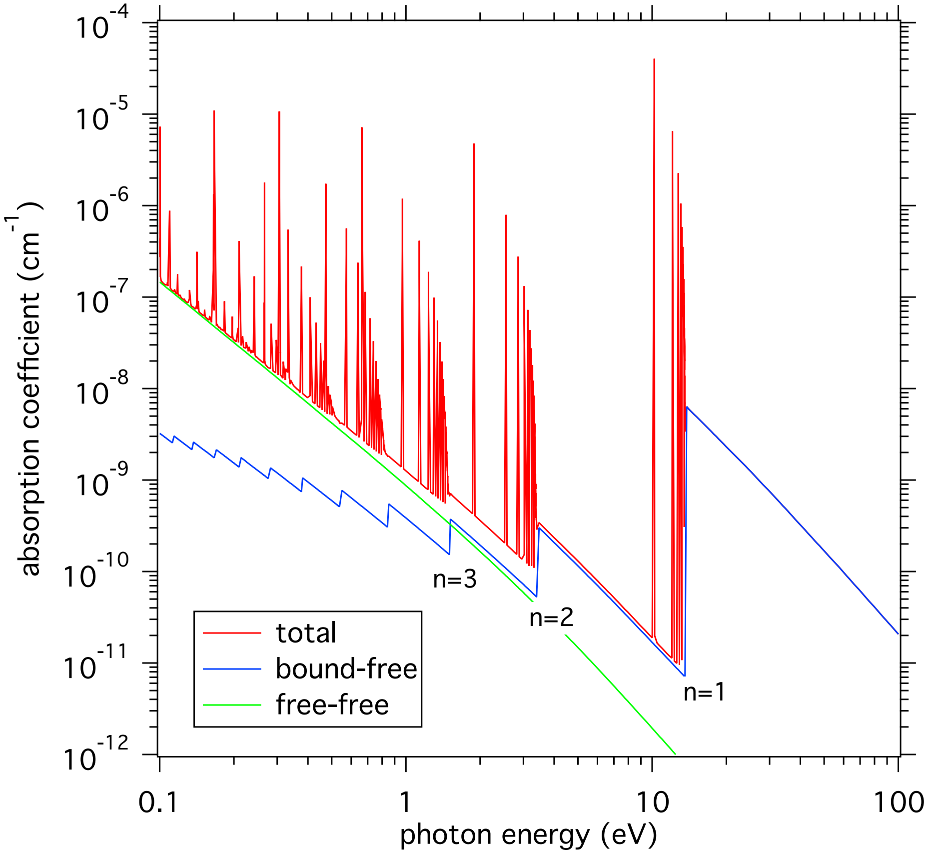
$$\frac{1}{\kappa_R} = \frac{\int_0^\infty d\nu \frac{1}{\kappa_\nu}\frac{dB_\nu}{dT}}{\int_0^\infty d\nu \frac{dB_\nu}{dT}} \qquad \kappa_P = \frac{\int_0^\infty d\nu\, \kappa_\nu B_\nu}{\int_0^\infty d\nu\, B_\nu}$$

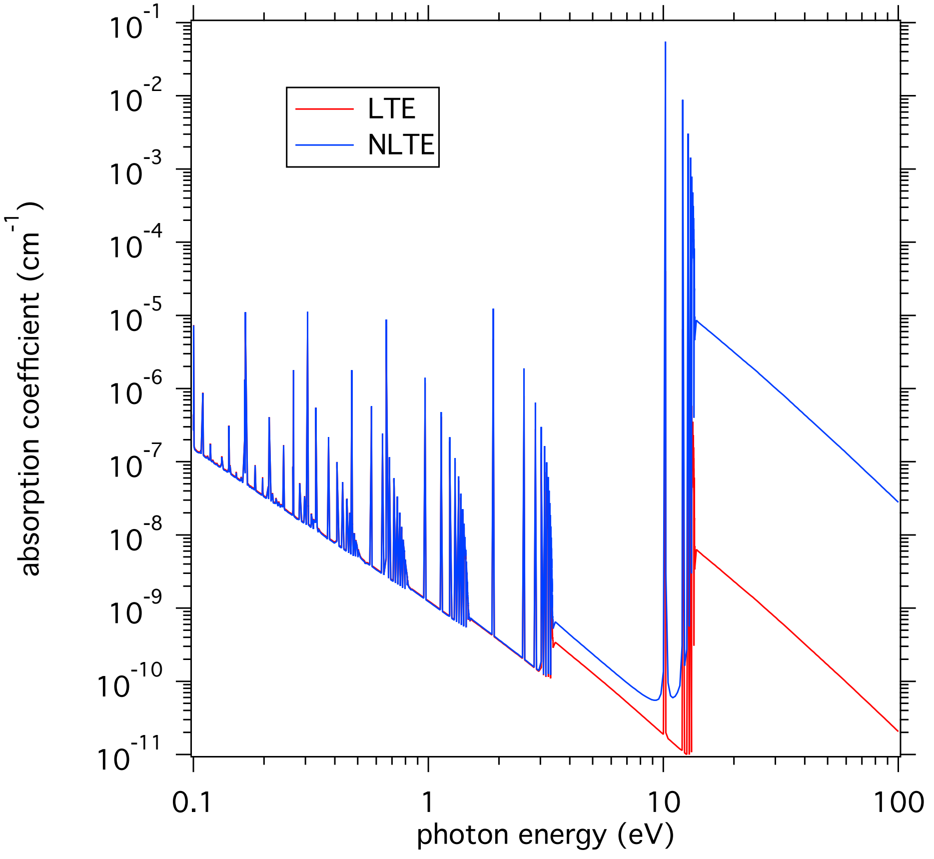
Kr @ T = 200 eV, ρ = 0.01 g/cc, LTE



Example – Hydrogen (T_e= 2 eV, n_e=10^{14} cm^{-3})

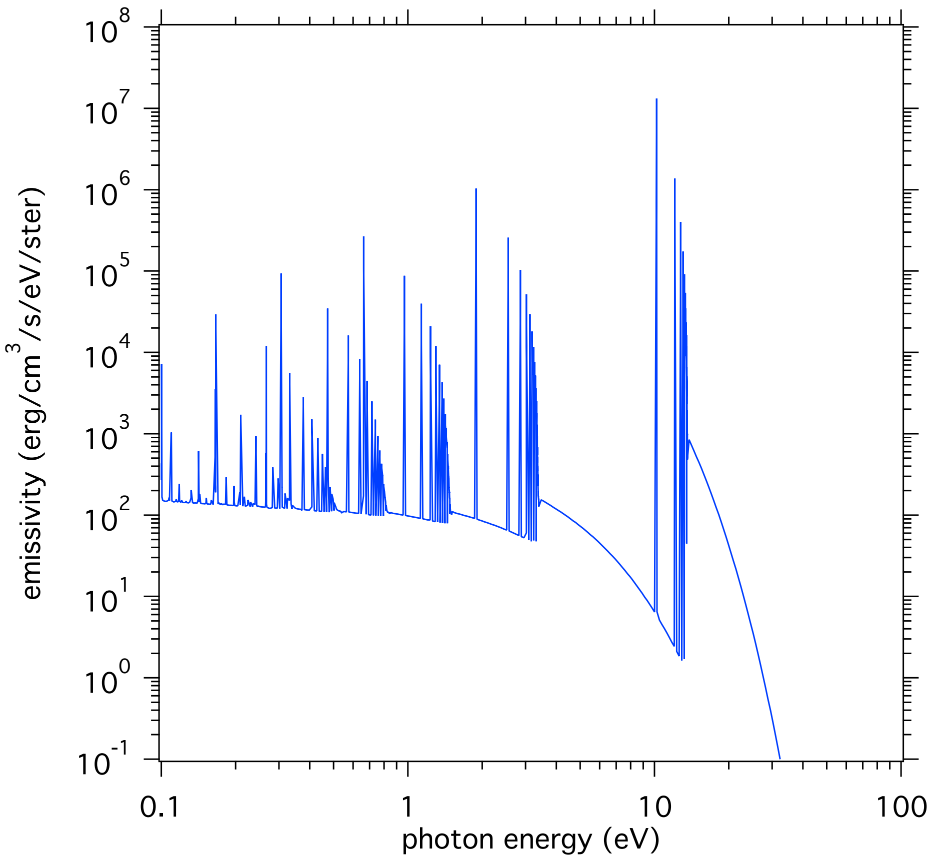
absorption coefficient



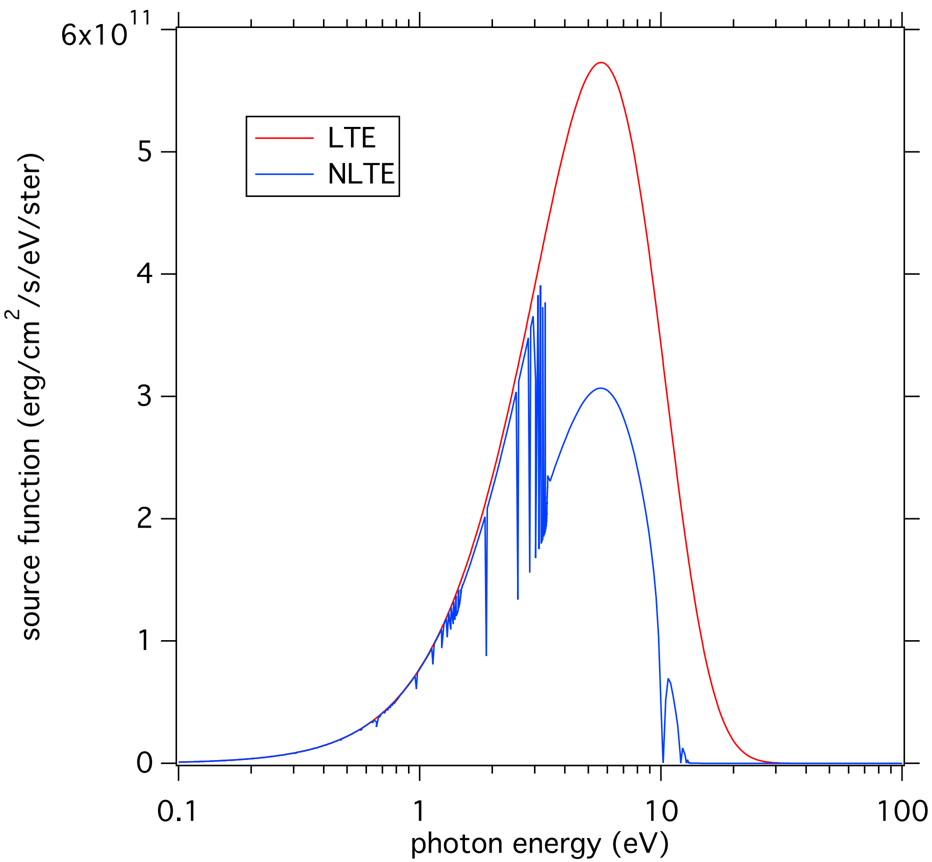


Hydrogen, again (T_e= 2 eV, n_e=10^{14} cm^{-3})

emissivity

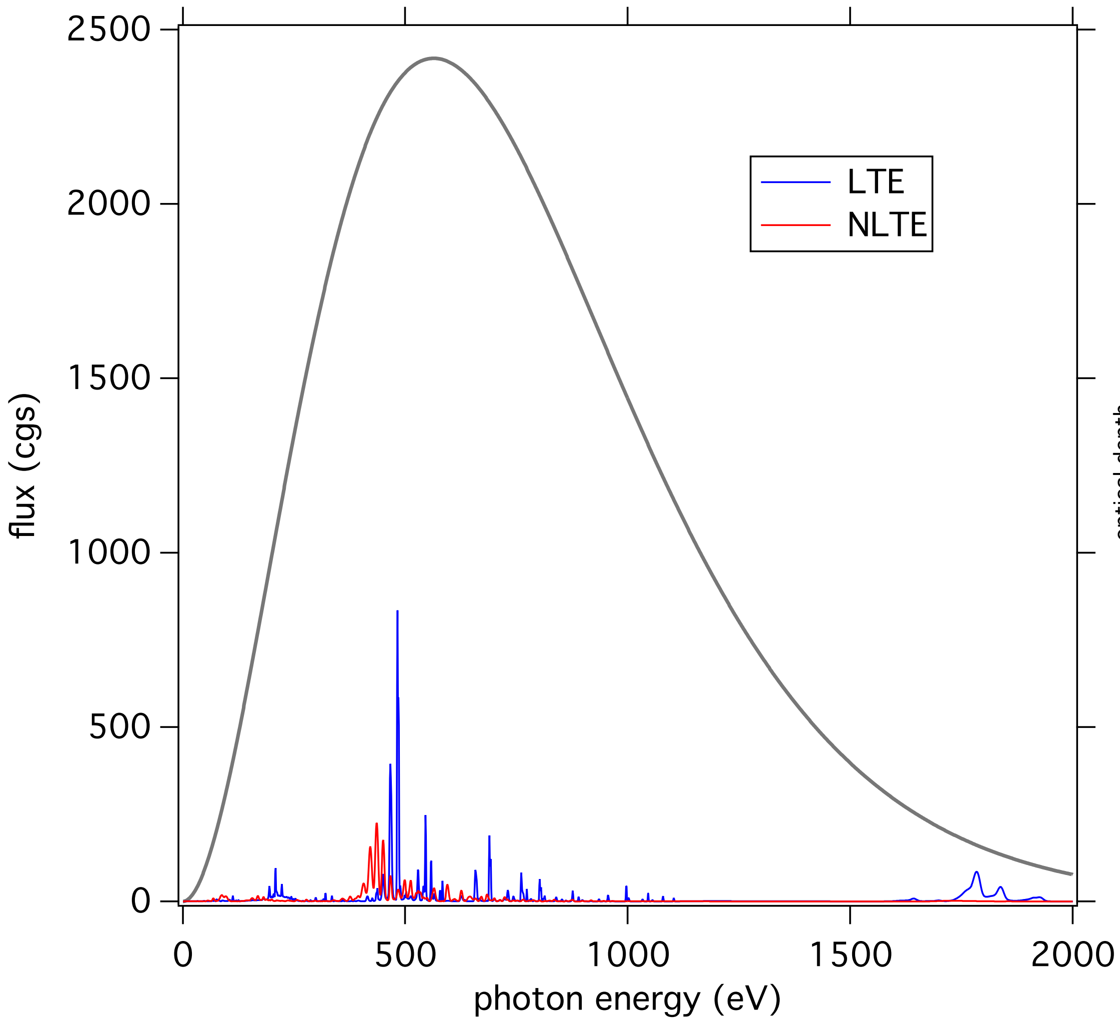


source function

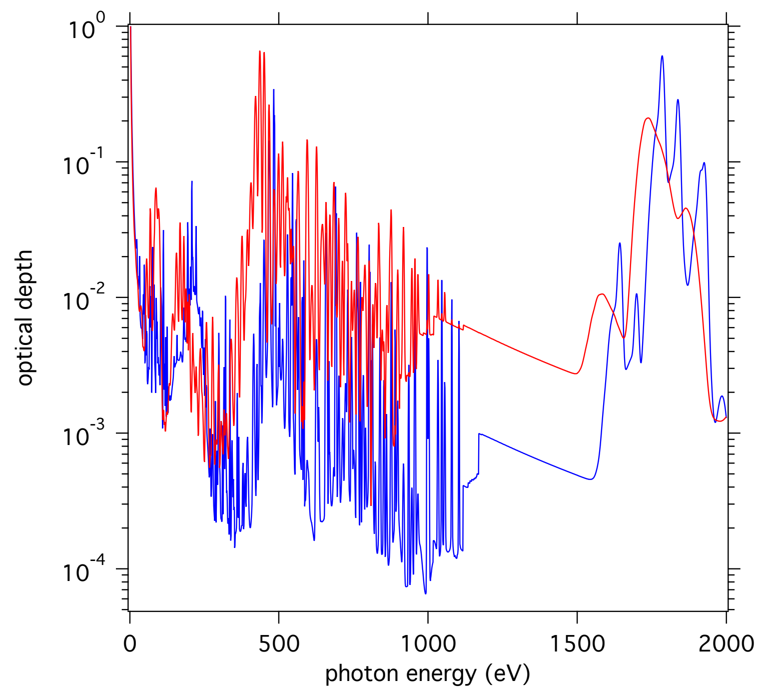


Flux from a uniform sphere revisited

Kr @ T = 200 eV, ρ = 0.01 g/cc, LTE / NLTE

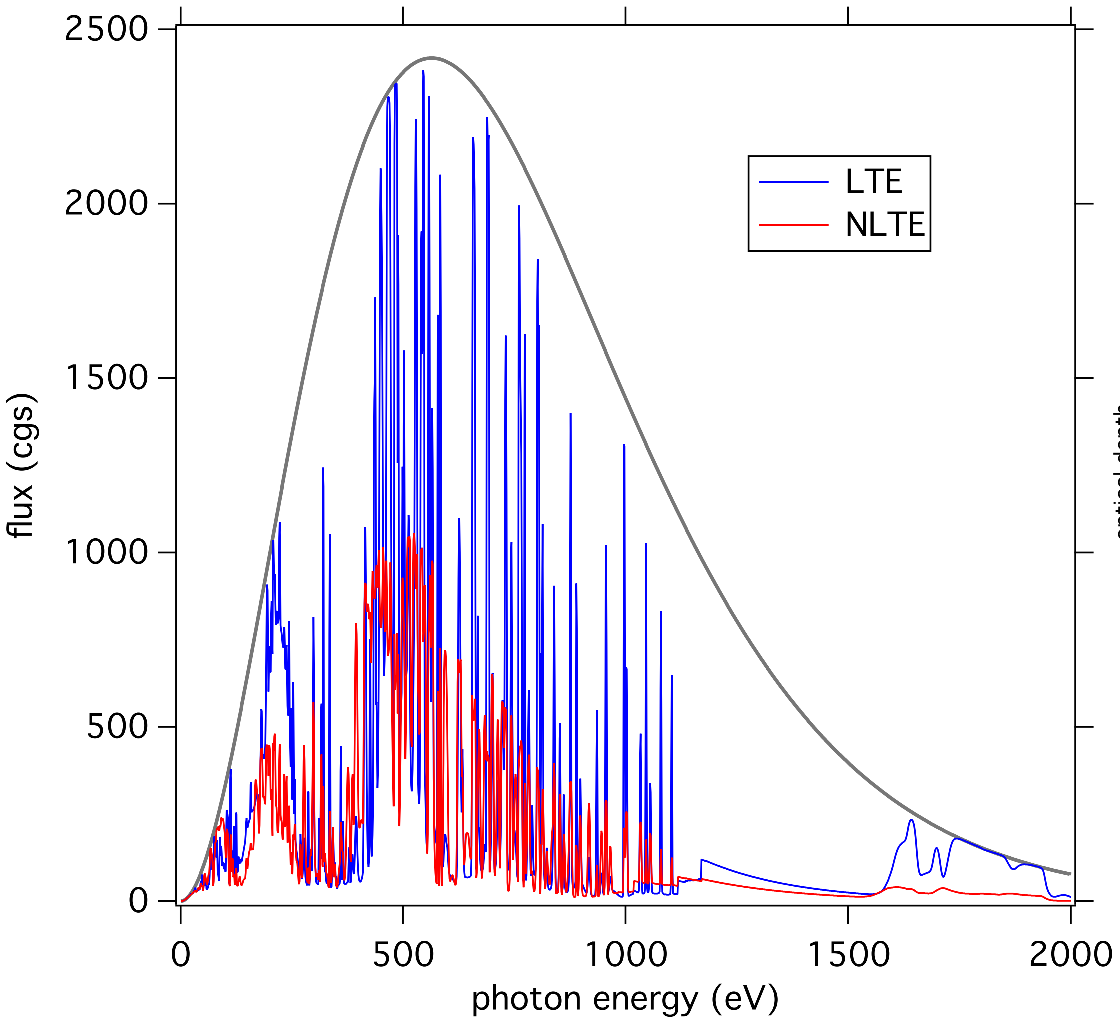


Δr = 0.001 cm

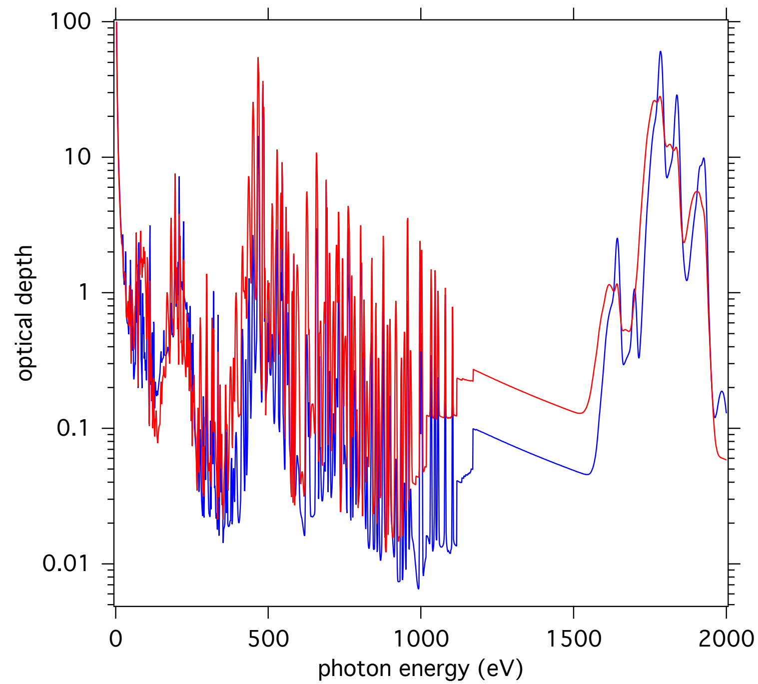


Flux from a uniform sphere revisited

Kr @ T = 200 eV, ρ = 0.01 g/cc, LTE / NLTE



Δr = 0.1 cm



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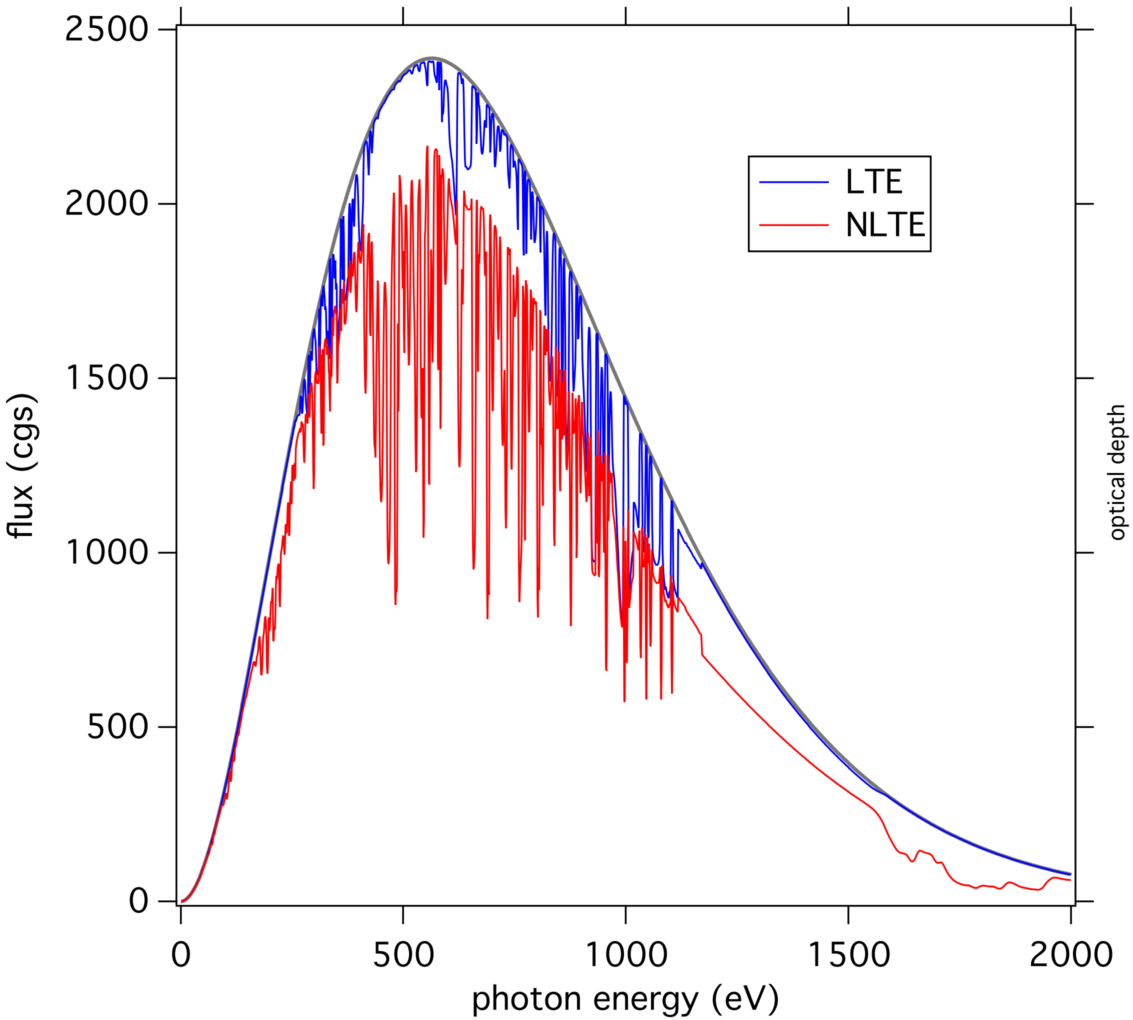
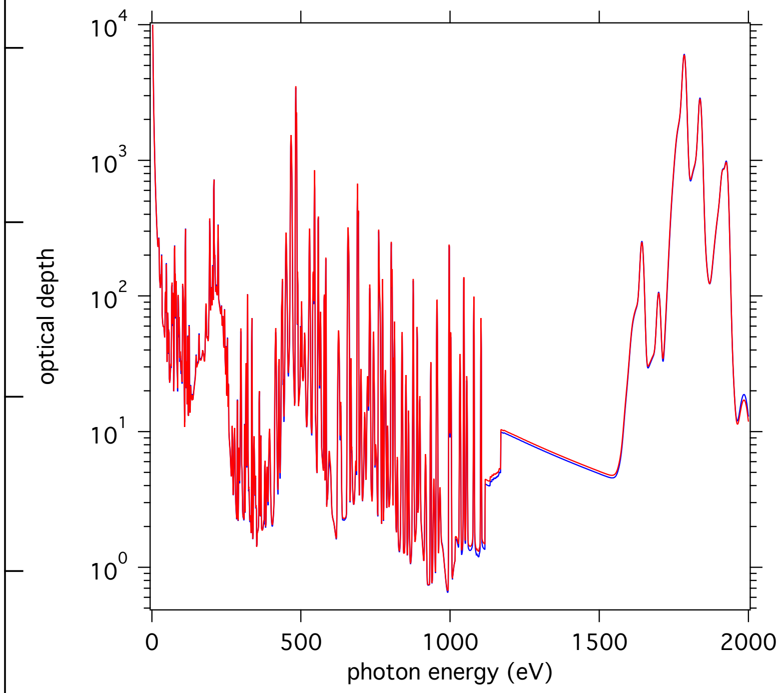
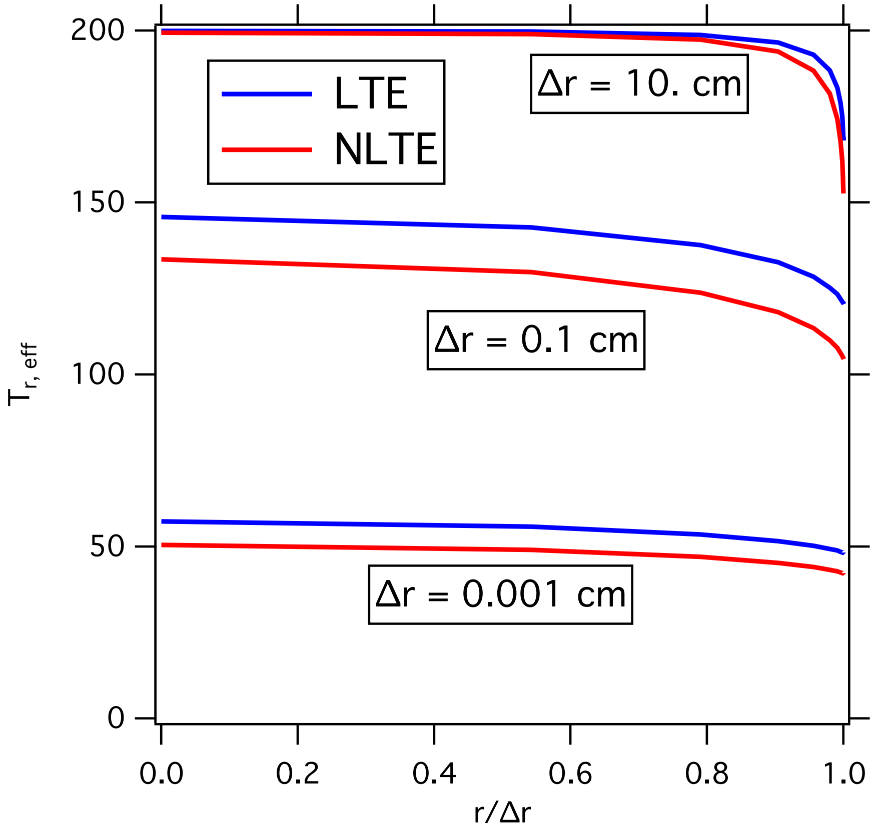


Δr = 10.0 cm



Flux from a uniform sphere - Summary

- “Black-body” emission requires <u>large</u> optical depths
- Large optical depths ➔ high radiation fields ➔ LTE conditions
- Boundaries introduce non-uniformities through radiation fields
- The radiation field will also change the material temperature

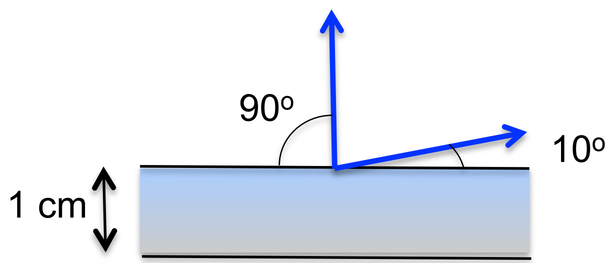


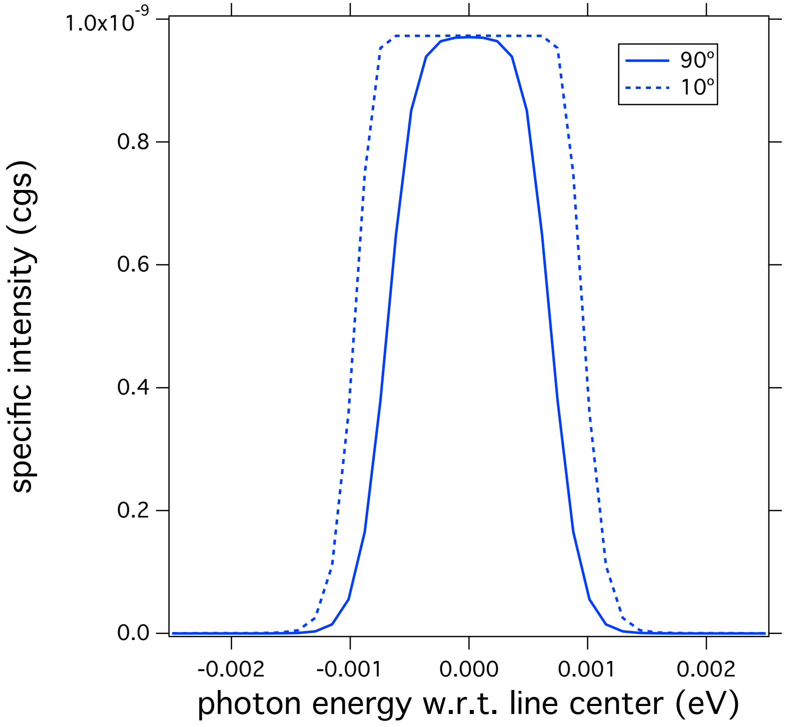
Conditions do not remain uniform in the presence of radiation transport and boundaries

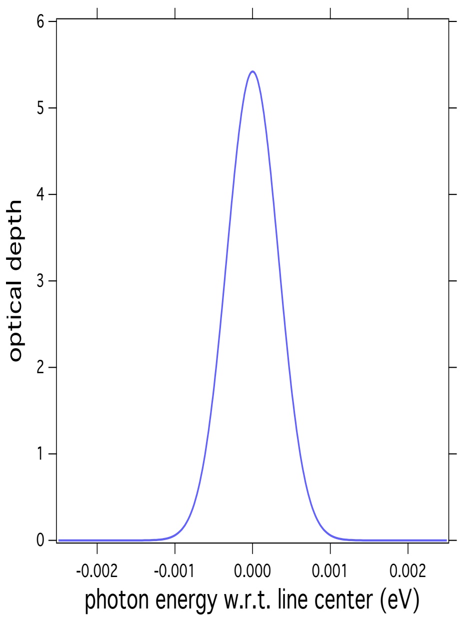
Example – Hydrogen Ly-α

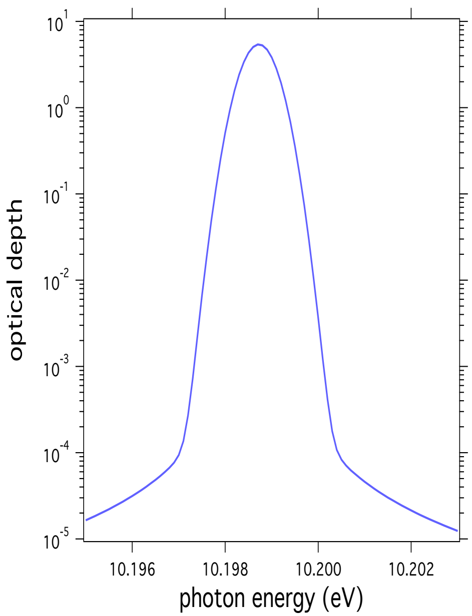
Ly-α emission from a uniform plasma

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





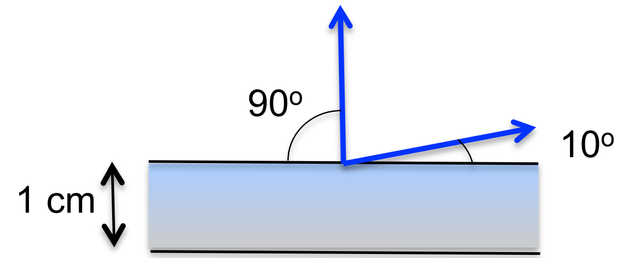


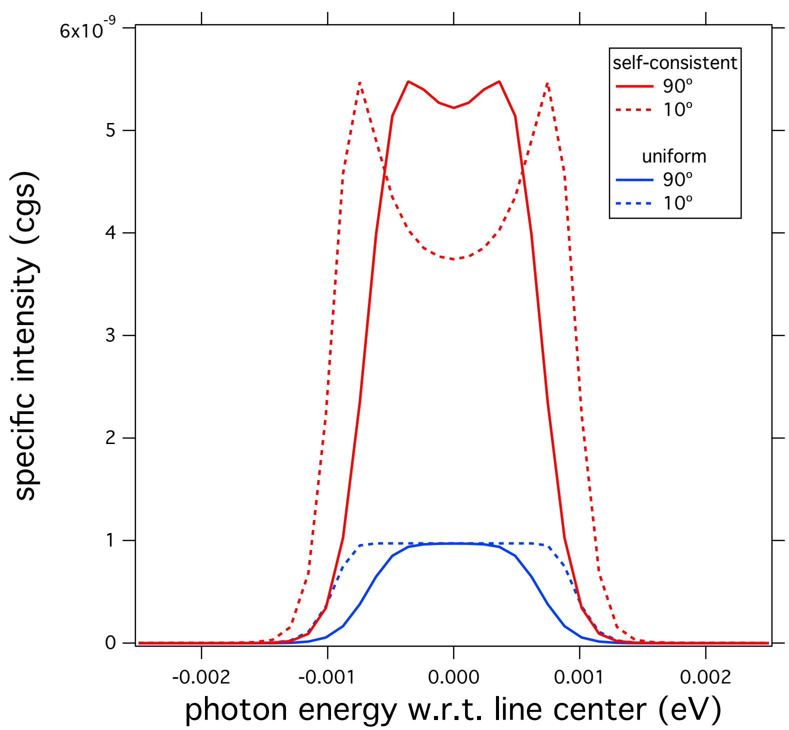


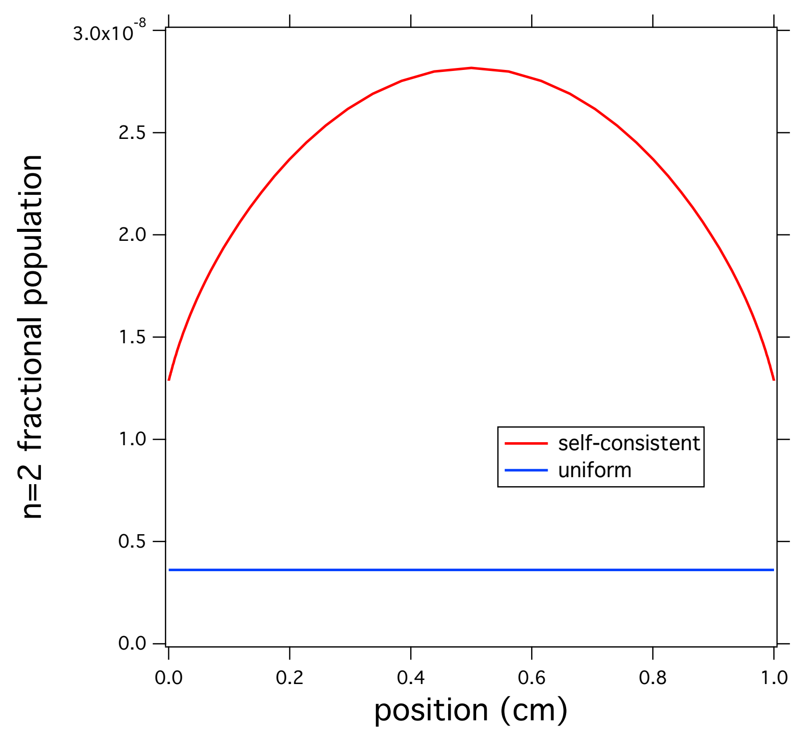
Example – Hydrogen Ly-α

Ly-α emission from a plasma with uniform temperature and density

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







Coupled systems – or – What does "Radiation Transport" mean?

The system of equations and emphasis varies with the application

For laboratory plasmas, these two sets are most useful -

LTE / energy transport :

- Coupled to energy balance

$$\frac{dE_m}{dt} = 4\pi \int \alpha_\nu (J_\nu - S_\nu)\, d\nu$$

$$\alpha_\nu = \alpha_\nu(T_e)\ ,\ S_\nu = B_\nu(T_e)$$

- Indirect radiation-material coupling through energy/temperature
- Collisions couple all frequencies locally, independent of J_ν
- Solution methods concentrate on non-local aspects

NLTE / spectroscopy :

- Coupled to rate equations

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}\mathbf{y}\ ,\ \mathbf{A}_{ij} = \mathbf{A}_{ij}(T_e, J_\nu)$$

$$S_\nu = \tfrac{2h\nu^3}{c^2} S_{ij}\ ,\ S_{ij} \approx a + b\bar{J}_{ij}$$

- Direct coupling of radiation to material
- Collisions couple frequencies over narrow band (line profiles)
- Solution methods concentrate on local material-radiation coupling
- Non-local aspects are less critical

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

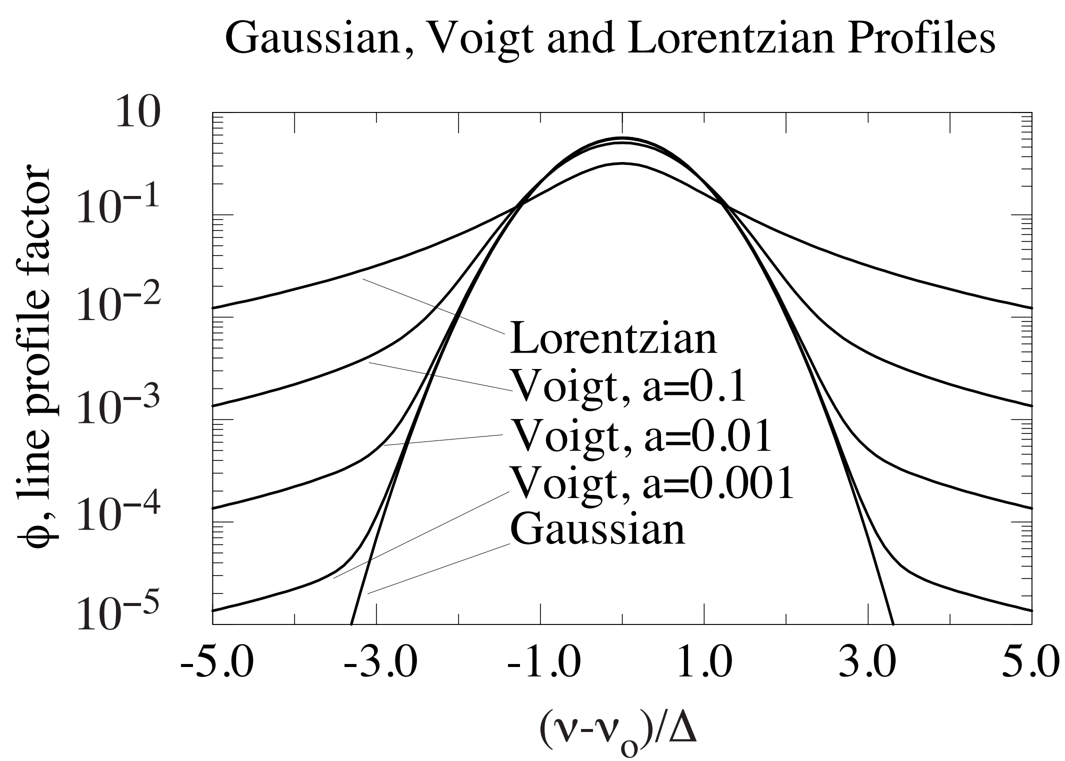
$$\phi(\nu) = \frac{\Gamma/4\pi^2}{(\nu-\nu_0)^2 + (\Gamma/4\pi)^2}$$

Γ = destruction rate

$$\phi(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} H(a,x)$$

$$a = \Gamma \big/ 4\pi\Delta\nu_D \qquad \Delta\nu_D = \frac{\nu_0}{c}\sqrt{\frac{2kT_i}{m_i}}$$

$$H(a,x) = \frac{a}{\pi}\int_{-\infty}^{\infty} \frac{e^{-y^2}}{(x-y)^2 + a^2}\, dy$$



Redistribution

The emission profile ψ_ν is determined by multiple effects:

- collisional excitation ➔ natural line profile (Lorentzian)
- photo excitation + coherent scattering
- photo excitation + elastic scattering ➔ ~absorption profile
- Doppler broadening

This is described by the redistribution function $R(\nu,\nu')$

$$\int_0^\infty R(\nu,\nu')\,d\nu = \phi(\nu') \quad , \quad \psi(\nu) = \int_0^\infty R(\nu,\nu')J(\nu')\,d\nu' \Big/ \int_0^\infty \phi(\nu')J(\nu')\,d\nu'$$

Complete redistribution (CRD): $\psi_\nu = \phi_\nu$

Doppler broadening is only slightly different from CRD, while coherent scattering gives $R(\nu,\nu') = \phi(\nu)\delta(\nu-\nu')$

A good approximation for partial redistribution (PRD) is often

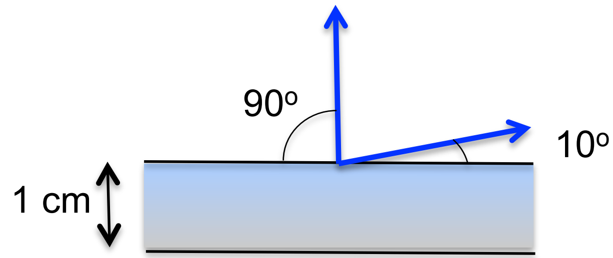
$$R(\nu,\nu') = (1-f)\phi(\nu')\phi(\nu) + f\,R_{II}(\nu,\nu')$$

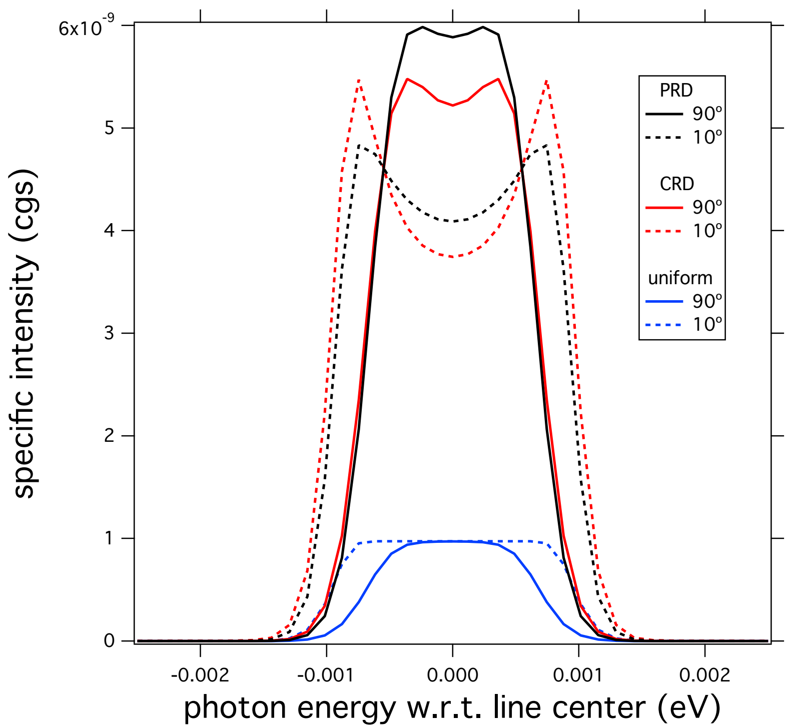
where f (<<1 for X-rays) is the ratio of elastic scattering and de-excitation rates, R_{II} includes coherent scattering and Doppler broadening

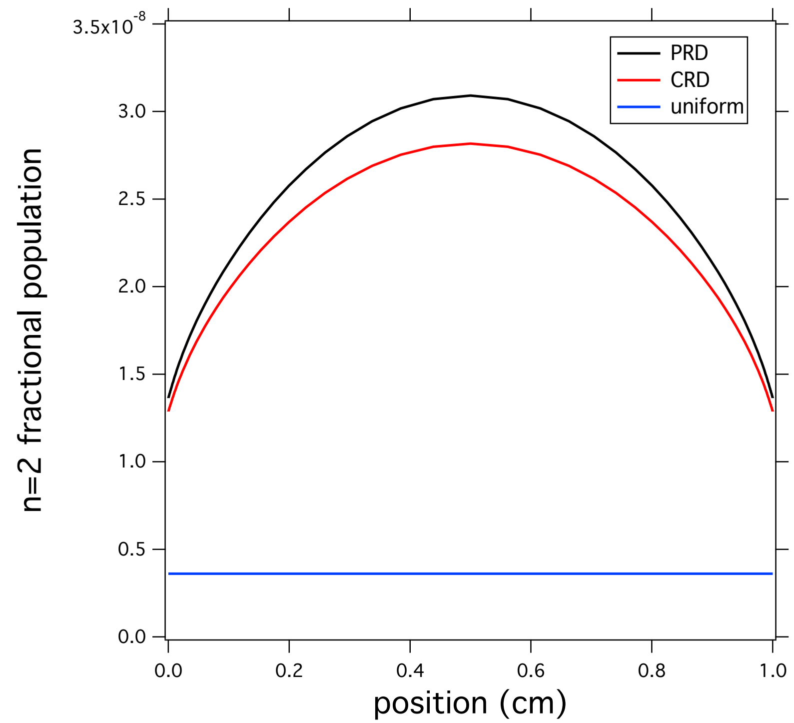
Hydrogen Ly-α w/ Partial Redistribution

Ly-α emission from a plasma with uniform temperature and density

- T_e = 1 eV, n_e = 10^{14} cm^{-3}
- Optical depth τ ~ 5
- Voigt parameter a ~ 0.0003







Material Velocity

The discussion so far applies in the reference frame of the material

Doppler shifts matter for line radiation when $v/c \sim \Delta E/E$

If velocity gradients are present, either

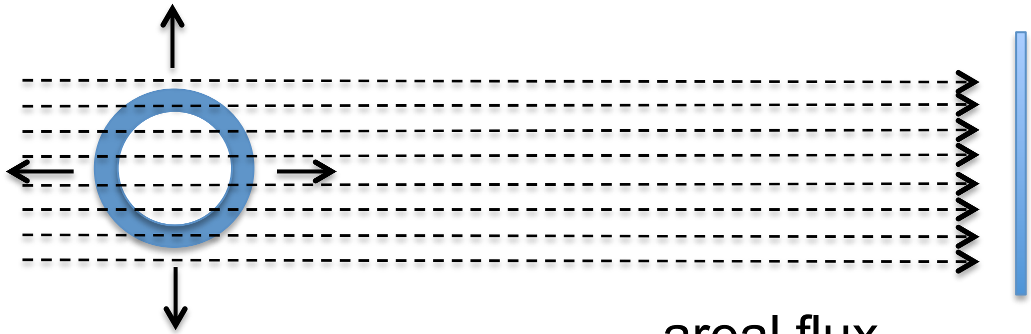
a) Transform the RTE into the co-moving frame - or –
b) Transform material properties into the laboratory frame

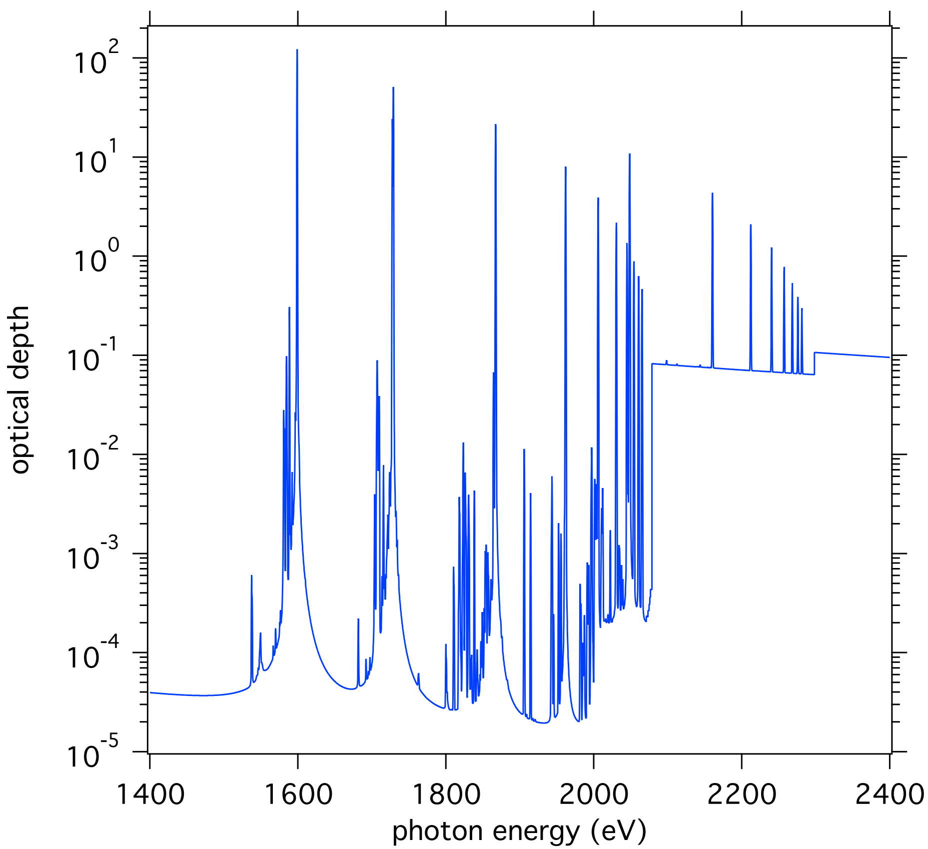
Option (a) is complicated (particularly when $v/c \rightarrow 1$)
 - see the references by Castor and Mihalas for discussions

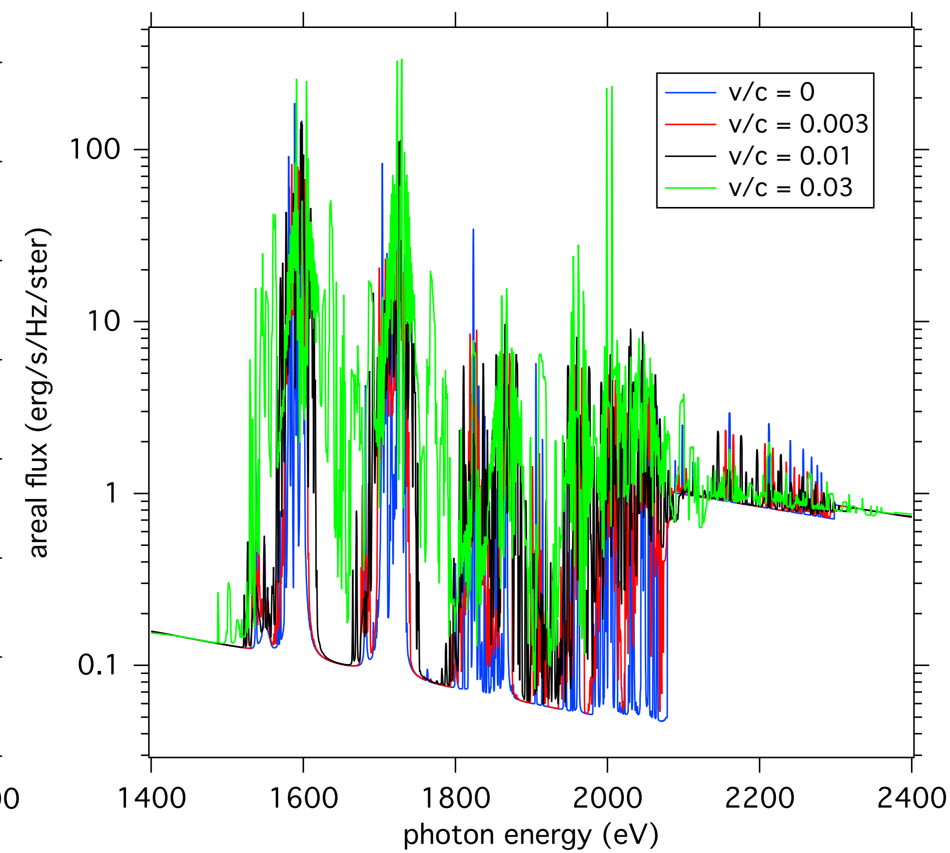
Option (b) is relatively simple, but makes the absorption and emission coefficients direction-dependent

Al sphere w/ uniform expansion velocity

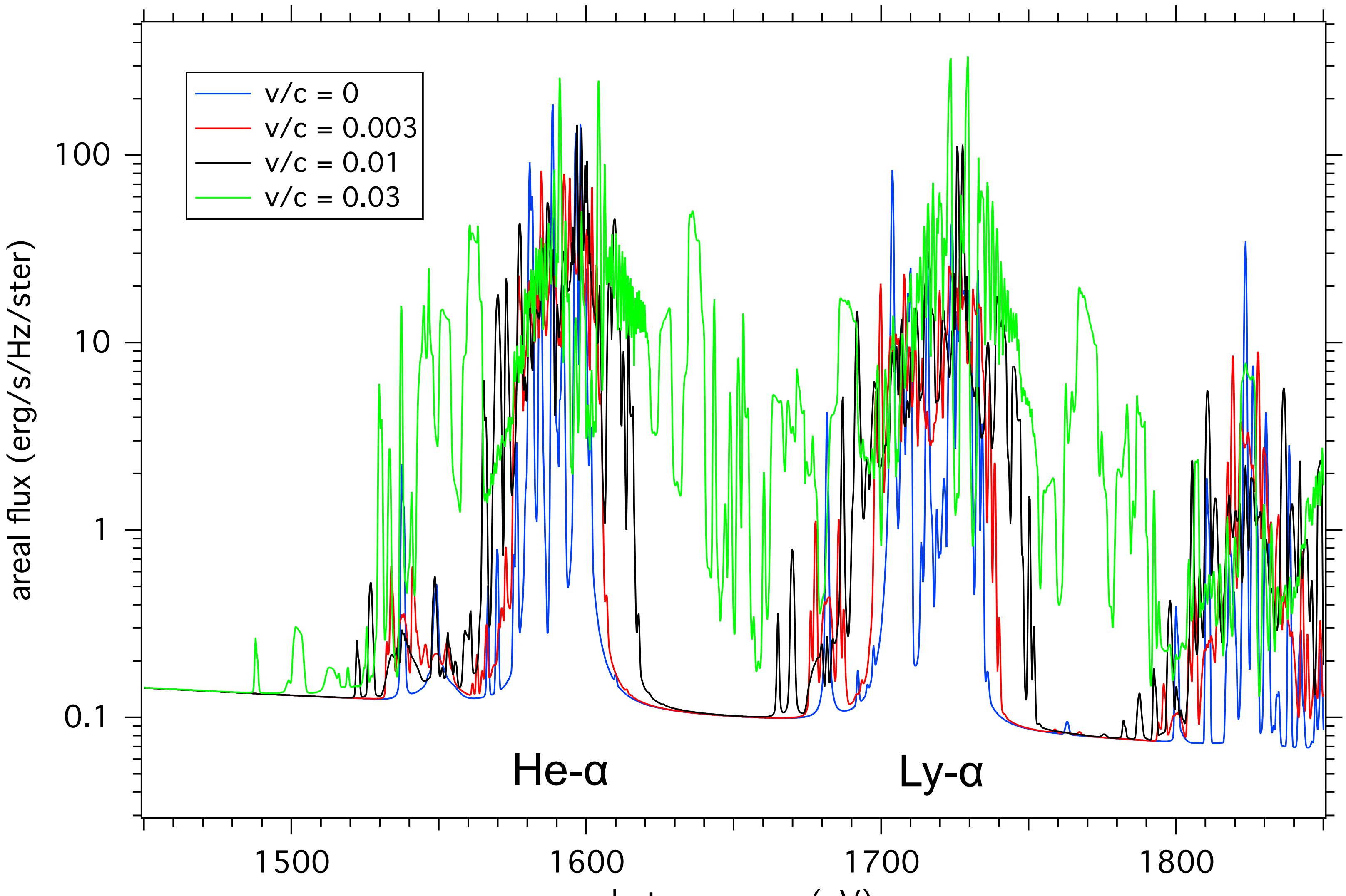
T_e = 500 eV
$\rho = 10^{-3}$ g/cm^3
R_{outer} = 1.0 cm
R_{inner} = 0.9 cm







Al sphere w/ uniform expansion velocity



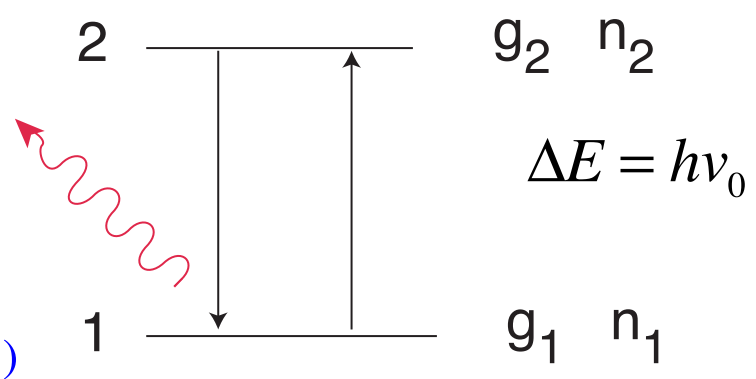
2-Level Atom

Rate equation for two levels in steady state:

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

$$\bar{J}_{12} = \int_0^\infty J_\nu \phi_{12}(\nu)\,d\nu \;,\; C_{12} = \tfrac{g_2}{g_1} e^{-h\nu_0/kT} C_{21}$$

Two energy level system



Absorption / Emission:

$$\alpha_\nu = \frac{h\nu}{4\pi}(n_1 B_{12} - n_2 B_{21})\phi_{12}(\nu) \;,\; \eta_\nu = \frac{h\nu}{4\pi} n_2 A_{21}\phi_{12}(\nu)$$

Source Function:

$$S_\nu = {n_2 A_{21}}\big/{n_1 B_{12} - n_2 B_{21}} = (1-\varepsilon)\bar{J}_{12} + \varepsilon B_\nu \quad , \quad \frac{\varepsilon}{1-\varepsilon} = \frac{C_{21}}{A_{21}}\left(1 - e^{-h\nu_0/kT}\right)$$

S_ν is independent of frequency and linear in $\bar{J}$

- solution methods exploit this dependence

A Popular Solution Technique

For a single line, the system of equations can be expressed as

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \Rightarrow I_\nu = \overleftrightarrow{\lambda}_\nu S_\nu(\bar{J})$$

$$S_\nu = a_\nu + b_\nu \bar{J} \ , \ \bar{J} = \frac{1}{4\pi}\int d\Omega \int_0^\infty I_\nu \phi(\nu)\, d\nu$$

where the lambda operator $\overleftrightarrow{\lambda}_\nu$ and the source function depend on the populations through the absorption and emission coefficients.

A numerical solution for $\bar{J}$ uniquely specifies the entire system.

Since $\overleftrightarrow{\lambda}_\nu$ depends on $\bar{J}$ through the populations, the full system is non-linear and requires iterating solutions of the rate equations and radiation transport equation.

The dependence of $\overleftrightarrow{\lambda}_\nu$ on $\bar{J}$ is usually weak, so convergence is rapid.

Solution technique for the linear source function:

$$I_\nu = \overleftrightarrow{\lambda}_\nu \left[a_\nu + b_\nu \bar{J} \right]$$

$$\Rightarrow \qquad \bar{J} = \frac{1}{4\pi} \int d\Omega \int_0^\infty \overleftrightarrow{\lambda}_\nu \left[a_\nu + b_\nu \bar{J} \right] \phi(\nu) \, d\nu$$

$$\Rightarrow \qquad \bar{J} = \left[1 - \overleftrightarrow{\Lambda} \right]^{-1} \frac{1}{4\pi} \int d\Omega \int_0^\infty \overleftrightarrow{\lambda}_\nu a_\nu \phi(\nu) \, d\nu$$

$$\overleftrightarrow{\Lambda} = \frac{1}{4\pi} \int d\Omega \int_0^\infty \overleftrightarrow{\lambda}_\nu b_\nu \phi(\nu) \, d\nu$$

This linear system can (in principle) be solved directly for $\bar{J}$ and in 1D this is very efficient

The (angle,frequency)-integrated operator $\overleftrightarrow{\Lambda}$ includes $1 - e^{-\tau_\nu}$ factors, so $\left[1 - \overleftrightarrow{\Lambda} \right]^{-1}$ amplifies $\bar{J}$ (radiation trapping)

Efficient solution methods approximate key parts of $\overleftrightarrow{\Lambda}$

NLTE – local frequency scattering

LTE (linear in ΔT_e) – non-local coupling

Multi-Level Atom

For multiple lines, the source function for each line can be put in the two-level form – ETLA (Extended Two Level Atom) – or the full source function can be expressed in the following manner:

$$S_\nu = \frac{\eta_\nu^c + \sum_\ell \eta_\nu^\ell(\bar{J}_\ell)\phi_\nu^\ell}{\alpha_\nu^c + \sum_\ell \alpha_\nu^\ell(\bar{J}_\ell)\phi_\nu^\ell}$$

Solve for each $\bar{J}^\ell$ individually (if coupling between lines is not important) or simultaneously.

(Complete) linearization – expand S_ν in terms of $\Delta\bar{J}_\ell$

$$S_\nu = S_\nu(\bar{J}_\ell{}^0) + \sum_\ell \frac{\partial S_\nu}{\partial \bar{J}_\ell}\left(\bar{J}_\ell - \bar{J}_\ell{}^0\right)$$

and solve as before.

Partial redistribution usually converges at a slightly slower rate.

Numerical methods need to fulfill <u>2</u> requirements

1. Accurate <u>formal</u> transport solution which is
   - conservative,
   - non-negative
   - 2nd order (spatial) accuracy (diffusion limit as $\tau >> 1$)
   - causal (+ efficient)

   Many options are available – each has advantages and disadvantages

2. Method to converge solution of <u>coupled</u> implicit equations
   - Multiple methods fall into a few classes
     - Full nonlinear system solution
     - Accelerated transport solution
     - Incorporate transport information into other physics
   - Optimized methods are available for specific regimes, but no single method works well across all regimes

Method #1 – Source (or lambda) iteration

1. Evaluate source function
2. Formal solution of radiation transport equation
3. Use intensities to evaluate temperature / populations

iterate to convergence

Advantages –

Simple to implement

Independent of formal transport method

Disadvantages –

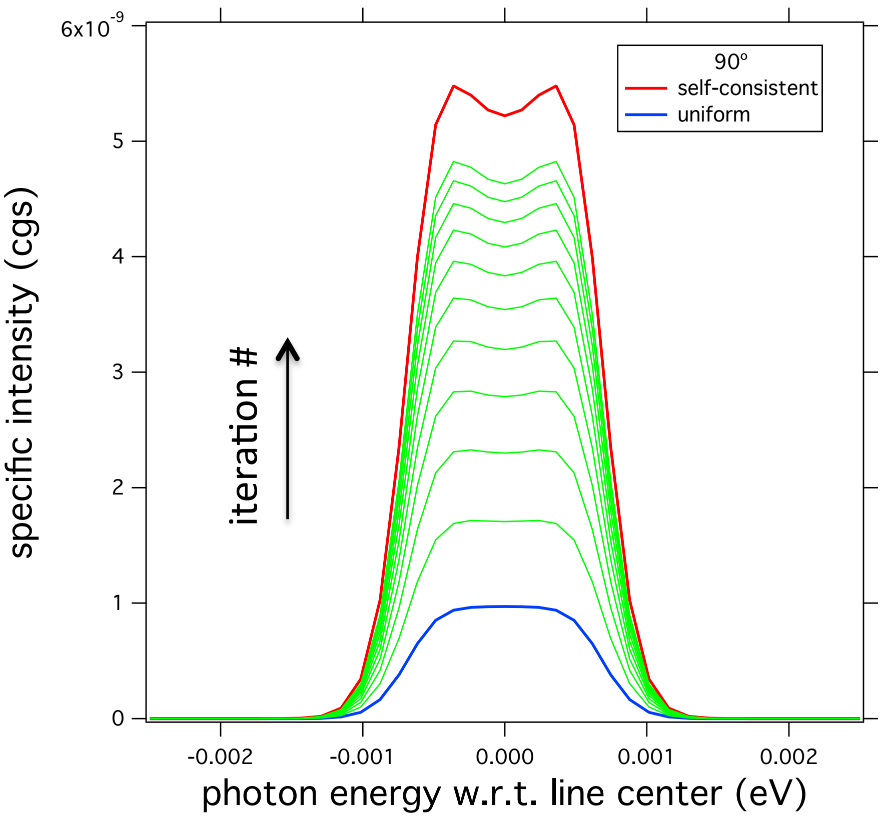
Can require many iterations: # iterations ~ τ^2

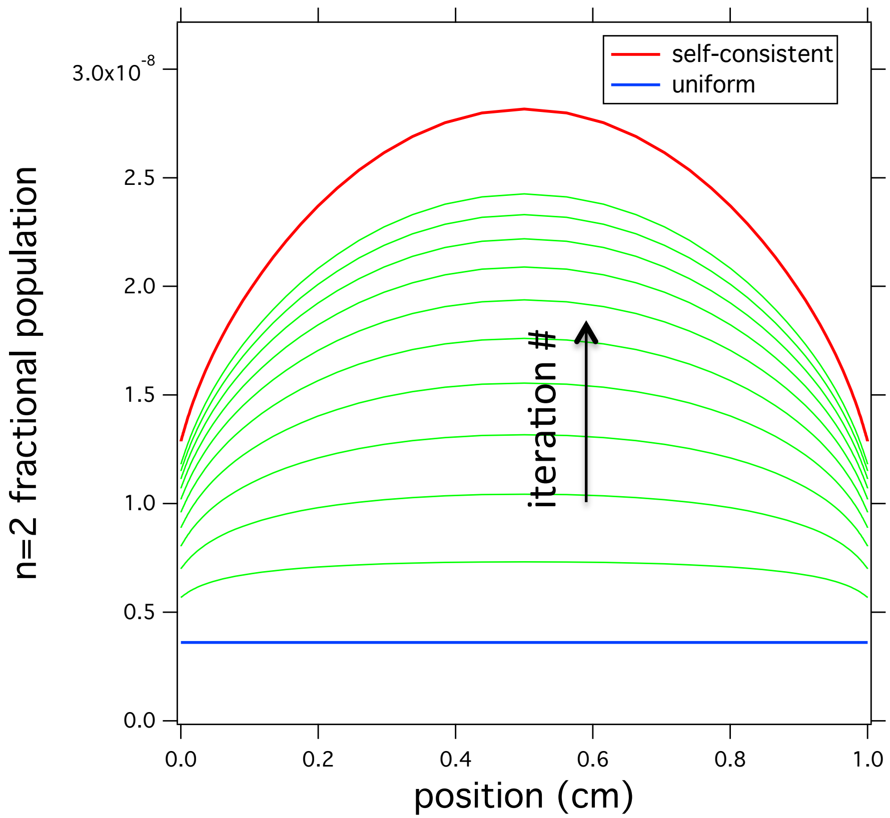
False convergence is a problem for $\tau >> 1$

Hydrogen Lyman-α revisited

- Source iteration (green curves) approaches self-consistent solution slowly
- Linearization achieves convergence in 1 iteration

$$S_{ij} = a + b\bar{J}_{ij}, \bar{J}_{ij} = \int J_\nu \phi_\nu \, d\nu$$ ← linear function of $\bar{J}$





Method #2 – Monte Carlo

Formal solution method –

1) Sample emission distribution in (space, frequency, direction) to create "photons"
2) Track "photons" until they escape or are destroyed

Advantages –

Works well for complicated geometries

Not overly constrained by discretizations ➔ does details very well

Disadvantages –

Statistical noise improves slowly with # of particles

Expense increases with optical depth

Iterative evaluation of coupled system is not possible / advisable

Semi-implicit nature requires careful timestep control

Convergence –

A procedure that transforms absorption/emission events into effective scatterings (Implicit Monte Carlo) provides a semi-implicit solution

Symbolic IMC provides a fully-implicit solution at the cost of a solving a single mesh-wide nonlinear equation

Method #3 – Discrete Ordinates (S_N)

Formal solution method –

Discretization in angle converts integro-differential equations into a set of coupled differential equations (provides lambda operator)

Advantages –

Handles regions with τ<<1 and τ>>1 equally well
Modern spatial discretizations achieve the diffusion limit
Deterministic method can be iterated to convergence

Disadvantages –

Ray effects due to preferred directions
angular profiles become inaccurate well before angular integrals
Required # of angles in 2D/3D can become enormous
Discretization in 7 dimensions requires large computational resources

Convergence –

Effective solution algorithms exist for both LTE and NLTE versions [6] –
e.g. LTE – synthetic grey transport (or diffusion)
NLTE – complete linearization (provides linear source function)
+ accelerated lambda iteration in 2D/3D

(Note: this applies to all deterministic methods)

Method #4 – Escape factors

Escape factor p_e is used to eliminate radiation field from net radiative rate

$$y_j B_{ji} \bar{J} - y_i B_{ij} \bar{J} = y_j A_{ji} p_e$$

Equivalent to incorporating a (partial) lambda operator into the rate equations
➔ combines the formal solution + convergence method

Advantages –

- Very fast – no transport equation solution required
- Can be combined with other physics with no (or minimal) changes

Disadvantages –

- Details of transport solution are absent
- Escape factors depend on line profiles, system geometry
- Iterative improvement is possible, but usually not worthwhile

Escape factor is built off the single flight escape probability $e^{-\tau_\nu}$

$$p_e = \frac{1}{4\pi}\int d\Omega \int_0^\infty e^{-\tau_\nu}\,\phi(\nu)\,d\nu$$

Iron's theorem – this gives the correct rate on average
(spatial average weighted by emission)

$$\left\langle 1 - \bar{J}/S \right\rangle = \left\langle p_e \right\rangle$$

Note that the optical depth depends on the line profile, plus continuum

Asymptotic expressions for large optical depth:

Gaussian profile

$$p_e \approx 1\Big/4\tau\sqrt{\ln\left(\tau/\sqrt{\pi}\right)}$$

Voigt profile

$$p_e \approx \tfrac{1}{3}\sqrt{a/\tau}$$

Evaluating p_e can be complicated by overlapping lines, Doppler shifts, etc.

Many variations and extensions exist in a large literature

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