Lecture Notes on Radiation Transport for Spectroscopy

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Radiation Transport for Spectroscopy

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 \( I_v \), or the photon distribution function \( f \)
- Unpolarized radiation
- Neglect index of refraction effects (n=1, \( \omega >> \omega_p \))
- Photons travel in straight lines
- Neglect true scattering (mostly)
- Static material (for now)
- Single reference frame

Angular Moments

0th moment \( J_v = \frac{1}{4\pi} \int I_v d\Omega \) = energy density \( \times c/4\pi \)
1st moment \( H_v = \frac{1}{4\pi} \int n_v d\Omega \) = flux \( \times 1/4\pi \)
2nd moment \( K_v = \frac{1}{4\pi} \int n_v d\Omega \) = pressure tensor \( \times c/4\pi \)

For isotropic radiation, \( K_v \) is diagonal with equal elements:
\[ K_v = \frac{1}{3} f_v \mathbf{I} \] (\( P = \frac{1}{3} E \))
In this case, radiation looks like an ideal gas with \( Y = 4/3 \)

Radiation Transport Equation

\[ \frac{1}{c} \frac{dI_v}{dt} + \tilde{\Omega} \cdot \nabla I_v = -\alpha_v I_v + \eta_v \]
\( \alpha_v \) = absorption coefficient (fraction of energy absorbed per unit length)
\( \eta_v \) = emissivity (energy emitted per unit time, volume, frequency, solid angle)

Boltzmann equation for the photon distribution function:
\[ \frac{1}{c} \frac{d f_v}{dt} + \tilde{\Omega} \cdot \nabla f_v = \left( \frac{\partial f_v}{\partial \omega} \right)_{\text{coll}} - \eta_v \frac{2 \hbar^2}{c} \left( \frac{\omega}{c^2} \right)^3 f_v \]
- 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 \( \lambda_v = 1/\alpha_v \)

Radiation Description

Macroscopic - specific intensity \( I_v \)
- energy per (area x solid angle x time) within the frequency range \( (\nu, \nu + d\nu) \)
\[ dE = I_v(\nu, \Omega) d\nu d\Omega \]
- \( dE = \) energy crossing area \( dA \) within \( d\Omega d\nu dt \)

Microscopic - photon distribution function
\[ dE = \sum_{\nu} \left( h\nu f_v(\tilde{\nu}, \tilde{\Omega}) \right) d\nu d\Omega d\tilde{\nu} d\tilde{\Omega} \]
\[ f_v = \frac{1}{e^{\hbar\nu/kT} - 1} \]

Energy density
\[ E_{\text{int}}(T_v) = \frac{3}{4} \int_0^\infty B_v(T_v) d\nu = a T_v^4 \]
For \( T_v = T^4 \) and \( n_p = 10^3 \text{ cm}^3 \):
\[ E_{\text{int}} = E_{\text{eos}}, \Rightarrow T = 300 \text{ eV} \]

LTE (Local Thermodynamic Equilibrium) - particles have thermal distributions \( (T_v, T^4) \) photon distribution can be arbitrary

Thermal Equilibrium

Intensity: Planck function
\[ B_v = \frac{2 \hbar^3}{c^3} \frac{1}{e^{\hbar\nu/kT} - 1} \]
Distribution function: Bose-Einstein
\[ f_v = \frac{1}{e^{\hbar\nu/kT} - 1} \]

Characteristic Form

Define the source function \( S_v \) and optical depth \( \tau_v \):
\[ S_v = \eta_v/n_v = B_v \text{ in LTE} \]
\[ d\tau_v = -I_v + S_v \Rightarrow I_v(\tau_v) = I_v(0)e^{-\tau_v} + \int_0^{\tau_v} e^{-(\tau_v-\tau)} S_v(\tau) d\tau \]
This solution is useful when material properties are fixed, e.g. postprocessing for diagnostics

Important features:
- Explicit non-local relationship between \( I_v \) and \( S_v \)
- Escaping radiation comes from depth \( \tau_v = 1 \)
- Implicit \( S_v/\partial t \) dependence comes from radiation / material coupling

Self-consistently determining \( S_v \) and \( I_v \) is the hard part of radiation transport
Absorption / emission coefficients

**Macroscopic** description – energy changes
- Energy removed from radiation passing through material of area $dA$, depth $dx$, over time $dt$
  \[ dE = -\alpha_n dA dx \tau_{ij} \int d\nu \]
- Energy emitted by material
  \[ dE = \eta_n dA dx \tau_{ji} \int d\nu \]

**Microscopic** description – radiative transitions
- Absorption and emission coefficients are constructed from atomic populations $y_j$ and cross sections $\sigma_{ij}$:
  \[ \alpha_{ij} = \sum_j \sigma_{ij} (y_j - \gamma_j), \quad \eta_{ij} = \frac{2h\nu_j}{c} \sum_j \sigma_{ij} \gamma_j \]

Cross section for absorption
\[ \sigma_{ij} = \frac{h\nu_j}{4\pi} B_{ji} \phi_j = \frac{2\pi e^2}{mc} f_{ij} \phi_j \]  
Oscillator strength $f_{ij}$ relates the quantum mechanical result to the classical treatment of a harmonic oscillator
- Strong transitions have $j \approx 1$
- Sum rule $\sum_j f_{ij} = Z$ (for $Z$ bound electrons)

Absorption and emission coefficients:
\[ \alpha_{ij} = n_i \pi e^2 \frac{2h\nu_j}{mc} f_{ij} \phi_j \]  
\[ \eta_{ij} = \frac{2h\nu_j}{c} \frac{\pi e^2}{mc} f_{ij} \phi_j \]  

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

**Bound-bound Transitions**

Probability (per unit time) of:
- Spontaneous emission: $A_{ji}$
- Absorption: $B_{ji}$
- Stimulated emission: $J_{ji}$

$A_{ji}$, $B_{ji}$, $J_{ji}$ are Einstein coefficients

\[ g_i B_{ji} = g_j A_{ji}, \quad J_{ji} = 2h\nu_j^3 g_i B_{ji} \]

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

\[ \int \phi(\nu) d\nu = 1 \]

Transition rate from level 1 to level 2

\[ R_{ji} = B_{ji} J_{ji}, \quad J_{ji} = \int \phi(\nu) d\nu \]

(assuming that the linewidth $<< \Delta E$)

**Bound-free absorption**
Absorption cross section from state of principal quantum number $n$ and charge $Z$

\[ \sigma_n = 7.91 \times 10^{-19} n^3 \left( \frac{v_e}{c} \right)^2 \left( 1 - e^{-h\nu_{thv}} \right) \text{ cm}^2 \]

Gauß factor
$\nu_{thv} = \text{threshold energy}$

**Free-free absorption**
Absorption cross section per ion of charge $Z$

\[ \sigma_z = 3.69 \times 10^{-3} \left( \frac{Z^2}{n} \right)^{3/2} g_\nu a_{\nu} \left( 1 - e^{-h\nu_{thv}} \right) \text{ cm}^2 \]

Gauß factor

The term $1 - e^{-h\nu_{thv}}$ 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

\[ \text{Note: frequency shift from scattering is } \sim \frac{h\nu}{m_e c^2} \]

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 \( (T_e, T_i, n_e) \)

Effective scattering

Photons also “scatter” by e.g. resonant absorption / emission

Upper level 2 can decay
- a) radiatively \( A_{21} \)
- b) collisionally \( \eta_i C_{2i} \)

Two energy level system

<table>
<thead>
<tr>
<th>Energy level</th>
<th>( g_2 )</th>
<th>( n_2 )</th>
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<tbody>
<tr>
<td>1</td>
<td>( g_1 )</td>
<td>( n_1 )</td>
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The fraction \( \times \) of photons are destroyed / thermalized

The fraction \( \times \) of photons are “scattered”
- energy changes only slightly (mostly Doppler shifts)
- undergo many “scattering” before being thermalized

Note: \( \times \ll 1 \) is the condition for a strongly non-LTE transition and is easily satisfied for low density or high \( \Delta E \)

Summary of absorption / emission coefficients

- Summed over populations and radiative transitions:

\[ \alpha_e = \sum_i \left( \frac{n_i}{m_e} \right) \left( \frac{2\nu}{mc^2} \right) \left( 1 + \frac{\text{photon energy}}{\text{atomic energy}} \right) \]

\[ \eta_e = \frac{2\nu}{mc^2} \sum_i \left( \frac{n_i}{m_e} \right) \left( 1 + \frac{\text{photon energy}}{\text{atomic energy}} \right) \]

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

\[ S_e = S_e (n_i, T_e, y_i (J_e)) \]

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

\[ S_e = B_e (T_e) \]

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

Radiation transport equation with scattering (and frequency changes):

\[ \frac{1}{c} \frac{dI}{dt} + \Omega \cdot \nabla I = -\alpha_e I + \eta_i + \sigma \int \frac{d\nu}{c} \left[ -R(\nu' \Omega, \nu, \Omega) \frac{\nu}{V} B_e (\nu + \nu') + R(\nu' \Omega, \nu, \Omega) \frac{\nu}{V} B_e (\nu + \nu') \right] \]

The redistribution function \( R \) describes the scattering of photons \( (\nu, \Omega) \to (\nu', \Omega') \)

Neglecting frequency changes, this simplifies to:

\[ \frac{1}{c} \frac{dI}{dt} + \Omega \cdot \nabla I = - (\alpha_e + \sigma) I + \eta_i + \sigma I \left( \frac{\nu}{V} B_e (\nu + \nu') \right) \]

for isotropic scattering

Scattering contributes to both absorption and emission terms (and may be denoted separately or included in \( \sigma \) and \( \eta_i \))

Population distribution

LTE: Saha-Boltzmann equation

- Excited states follow a Boltzmann distribution

\[ \frac{N_i}{N_{eq}} = \frac{2}{\pi} \frac{U_i}{U_{eq}} \left( \frac{kT}{\pi m_i} \right)^{3/2} \]

- Ionization stages obey the Saha equation

\[ \frac{N_i}{N_{eq}} = \frac{2}{\pi} \frac{U_i}{U_{eq}} \left( \frac{kT}{\pi m_e e^2} \right) \]

NLTE: Collisional-radiative model

- Calculate populations by integrating rate equations

\[ \frac{dN_i}{dt} = \dot{N}_i - \partial_i = -\sigma_{ji} I + \eta_{ji} \]

Opacity & mean opacities

\[ \text{opacity} = \alpha_e / \rho \]

Rosseland mean opacity:
- emphasizes transmission
- includes scattering appropriate for average flux

Planck mean opacity:
- emphasizes absorption
- no scattering appropriate for energy exchange

\[ \kappa_e = \frac{2}{c^2} \left( \frac{1}{c} \frac{dI}{dt} + \Omega \cdot \nabla I \right) \]

Hydrogen, again \( (T_e = 2 \, \text{eV}, n_e=10^{14} \, \text{cm}^{-3}) \)
Flux from a uniform sphere revisited

Example – Hydrogen Ly-α
Ly-α emission from a uniform plasma
- $T_e = 1 \text{ eV}, n_e = 10^{14} \text{ cm}^{-3}$
- Moderate optical depth: $\tau \sim 5$
- Viewing angles 90° and 10° show optical depth broadening

Example – Hydrogen Ly-α
Ly-α emission from a plasma with uniform temperature and density
- $T_e = 1 \text{ eV}, n_e = 10^{14} \text{ cm}^{-3}$
- Self-consistent solution displays effects of:
  - Radiation trapping / pumping
  - Non-uniformity due to boundaries

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
  \[
  \frac{dE}{dt} = 4\pi \int_0^{\infty} \alpha_i (J_i - S_i) d\nu
  \]
- Indirect radiation-material coupling through energy/temperature
- Collisions couple all frequencies locally independent of $J_i$
- Solution methods concentrate on non-local aspects

NLTE / spectroscopy:
- Coupled to rate equations
  \[
  \frac{dY_i}{dt} = A_i Y_i (T_e, J_i) = A_i \tau_i J_i
  \]
- 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 ($\Delta \nu_0$)
- Collisional broadening ($\nu_c, T_e$)
- Doppler broadening ($\Gamma$)
- Stark effect (plasma microfields)

\[
\phi(\nu) = \frac{1}{\Delta \nu_0 \sqrt{\pi}} H(\alpha, x) = \frac{1}{\Delta \nu_0} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{\alpha^2}} dy
\]

Gaussian, Voigt and Lorentzian Profiles

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

The emission profile $\Psi_e$ is determined by multiple effects:
- collisional excitation $\rightarrow$ natural line profile (Lorentzian)
- photo excitation $+$ coherent scattering $\rightarrow$ absorption profile
- Doppler broadening

This is described by the redistribution function $R(v', v'')$:

$$\int R(v', v'') \, dv'' = \phi(v'') \quad \Psi_e(v) = \int R(v', v'') \, dv'' \int \phi(v'') \, dv''$$

Complete redistribution (CRD): $\Psi_e = \phi$

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

A good approximation for partial redistribution (PRD) is often

$$R(v', v'') = (1 - f) \phi(v') \delta(v' - v') + f \frac{1}{\tau}$$

where $f < 1$ for X-rays is the ratio of elastic scattering and de-excitation rates, $\tau$ includes coherent scattering and Doppler broadening

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

2-Level Atom

Rate equation for two levels in steady state:

$$\frac{d}{dt} n = \lambda_{1} (n_{1} - n_{2}) + \eta_{1} (n_{1} - n_{2})$$

Two energy level system:

$$\frac{d}{dt} n_{1} = \frac{1}{\tau} \int \lambda_{1} \phi(v) \, dv$$

Absorption / Emission:

$$\frac{d}{dt} n_{1} = - \frac{1}{\tau} \int \lambda_{1} \phi(v) \, dv$$

Solution Function:

$$n_{1} = \frac{n_{2} \lambda_{2}}{\lambda_{1} \lambda_{2} - n_{1} \lambda_{2}} (1 - e^{-\tau_{1}/\tau})$$

Scales independent of frequency and line shape in $\tau$
- solution methods exploit this dependence

Solution technique for the linear source function:

$$\int \lambda_{1} [n_{1} + \lambda_{1} \tau] \phi(v) \, dv$$

$$\int \lambda_{1} [1 - \lambda_{1} \lambda_{2} / n] \phi(v) \, dv$$

$$\frac{1}{\tau} \int \lambda_{1} \phi(v) \, dv$$

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

The (angle, frequency)-integrated operator $\lambda$ includes $1 - e^{-\tau}$ factors, so $\lambda$ amplifies $\tau$ (radiation trapping)

Efficient solution methods approximate key parts of $\lambda$

- NLTE – local frequency scattering
- LTE (linear in $\Delta \lambda$) – 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:

\[ S_y = \sum_i n_i J_i \left( \frac{\alpha_i}{\alpha_e} \right) \]

Solve for each \( J \) individually (if coupling between lines is not important) or simultaneously.

(Complete) linearization – expand \( S_y \) in terms of \( \Delta J \)

\[ S_y = S_y \Delta J + \sum_i \frac{\partial S_y}{\partial J_i} \Delta J_i \]

and solve as before.

Partial redistribution usually converges at a slightly slower rate.

Method #1 – Source (or lambda) iteration

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

Advantages –
- Simple to implement
- Independent of formal transport method

Disadvantages –
- Can require many iterations: \# iterations \( \sim \) \( \tau^2 \)
- False convergence is a problem for \( \tau >> 1 \)

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 \( \tau << 1 \) and \( \tau >> 1 \) 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 [8] – 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 \( p \) is used to eliminate radiation field from net radiative rate

\[ y_B J - y_B \overline{J} = y_A p \]

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

Numerical methods need to fulfill 2 requirements

1. Accurate formal 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 coupled 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

Hydrogen Lyman-α revisited

\[ S_y = a + b J_y J = \int J_y \phi \, dv \]

\( \phi \) is used to eliminate radiation field from net radiative rate

\[ 1 - \overline{J_y} = (p) \]

\( \overline{J} \) is the average of the source function over the volume

\( \overline{J_y} = \left( \frac{1}{\Omega} \right) \int J_y \phi \, dv \)

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

Asymptotic expressions for large optical depth:

- Gaussian profile
- Voigt profile

\[ p = \sqrt[3]{\frac{1}{2 \pi} \log(\sqrt{2 \pi})} \]

Evaluating \( p \) can be complicated by overlapping lines, Doppler shifts, etc.

Many variations and extensions exist in a large literature
References


Laser Absorption

For narrow band optical laser, can neglect emission but must consider index of refraction $n$

\[ n^2 < 0 \text{ for } n^e \text{ above a critical density:} \]

\[ n_{\text{crit}}^e = \frac{m_e}{4\pi e^2} \omega^2 \]

$10^{17}$ cm$^{-3}$ for 1.06 micron laser

Refractive effects - curved photon paths
modified absorption / emission
invariant phase space quantity is $I/n^2$ instead of $I$

\[
\frac{1}{c} \frac{\partial}{\partial t} \left( \frac{I}{n^2} \right) + \mathbf{n} \cdot \nabla \left( \frac{I}{n^2} \right) + \frac{d}{ds} \left( \frac{I}{n^2} \right) + n \eta \nabla \frac{I}{n^2} = -n\alpha \left( \frac{I}{n^2} \right) + n\eta
\]

$\alpha$=unit vector

Radiation transport effects with plasma transport

- Plasma transport model explicitly treats ion and (ground state) neutral atoms
- Excited states are assumed to be in equilibrium on transport timescales:

\[ n_i = n_{i0} + n_i^e \quad f_i^e = n_i^e / n_i \]

- Transport model uses effective ionization / recombination and energy loss coefficients which account for excited state distributions, e.g.

\[
\frac{dn}{dt} + \nabla \cdot (n \nabla) = -n\alpha \left( \frac{I}{n^2} \right) + n\eta
\]

- Tabulated coefficients are evaluated with a collisional-radiative code in the optically thin limit

Detached divertor simulations exhibit large radiation effects

Specifications: $L=2$ m, $n=10^{20}$ m$^{-3}$, $q_{in}=10$ MW/m$^2$, $\beta=0.1$

<table>
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<tr>
<th>Flux</th>
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<th>$q_{out}$</th>
</tr>
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<tr>
<td>CR</td>
<td>-0.805</td>
<td>+0.195</td>
</tr>
<tr>
<td>NLTE</td>
<td>-0.555</td>
<td>+0.445</td>
</tr>
<tr>
<td>ESC</td>
<td>-0.537</td>
<td>+0.463</td>
</tr>
</tbody>
</table>

$Q_n$: radiative flux
$q_{out}$: particle flux

CR: collisional-radiative tables (optically-thin)
NLTE: collisional-radiative model w/ radiation transport
ESC: parameterized tables

Qualitative description of the detached divertor region remains unchanged, Quantitative details of the particle and power balance change dramatically.