Master thesis

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October 30, 2019

Contents

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Goal of the thesis   Compute multiline transfer. With Monte Carlo techniques.

Part I
Radiative Transfer: theory

1   Very broad introduction & Summary

The material here originates from the master thesis of Nicolas Moens [Moe18] and from the course notes *Introduction to numerical methods for radiation in astrophsyics* from professor Sundqvist.

1.1   Definition of specific intensity

The definition of the specific intensity is

$$I_\nu = \frac{dE_\nu}{\cos(\theta)d\Omega dt d\nu} = \frac{dE_\nu}{\mu d\Omega dt d\nu} \tag{1}$$

On the other hand, for the total energy of a collection of N photons holds that

$$E_\nu = N E_{\nu,\text{photon}} \tag{2}$$

To the point   From this we deduce that

$$I_\nu \mu = \frac{N(\mu)dE_{\nu,\text{photon}}}{d\Omega dt d\nu} \tag{3}$$

and thus

$$\boxed{I_{nu}\mu d\mu \sim N(\mu)d\mu} \tag{4}$$

Considering the solid angle   In spherical geometry $d\Omega = \sin(\theta)d\theta d\phi = d\mu d\phi$.

1.2   Radiation equations

Material from [Iva14] Specific intensity $I(s,\lambda,x,y,t)$ satisfies the Radiative Transfer Equation:

$$\boxed{\frac{\delta I(q,t)}{\delta s} = \eta(q,t) - \chi(q,t)I(q,t)} \tag{5}$$

In cartesian coordinates (with propagation vector $\vec{n} = \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} = \begin{bmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ \cos(\theta) \end{bmatrix}$):

$$\frac{1}{c}\frac{\partial I}{\partial t} + \sin(\theta)\cos(\phi)\frac{\partial I}{\partial x} + \sin(\theta)\sin(\phi)\frac{\partial I}{\partial y} + \cos(\theta)\frac{\partial I}{\partial z} = \eta - \chi I \tag{6}$$

- 1D planar atmosphere: $\frac{\partial I}{\partial x} = \frac{\partial I}{\partial y} = 0$:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial z} = \eta - \chi I \tag{7}$$

- diffusion limit

- Definition of J in Equation (3.15)

Plane parallel geometry

- restrict oursevels to time-independent, one-dimensional (1D) case $I(s, \theta, \lambda)$ where s is the direction of the light ray

- it satisfies Radiation Transfer Equation (RTE) $\boxed{\dfrac{dI_\lambda}{d\tau_\lambda} = S_\lambda - I_\lambda}$

- with 'formal' solution $\boxed{I(\lambda, \tau_\lambda) = I_0(\lambda)e^{-\tau_\lambda} \int_0^{\tau_\lambda} S(t)e^{-t}dt}$

  - no emissivity $S = 0$ then $I(\lambda)I_0(\lambda)e^{-\tau_\lambda}$
  - no opacity then $I_0(\lambda) = \displaystyle\int_0^s \eta_\lambda(s)ds$
  - constant source function $I(\lambda, \tau) = I_0(\lambda)e^{-\tau_\lambda} + S(1 - e^{-\tau_\lambda})$
  - if $S = a + b\tau$ then $I(\lambda) = a + \dfrac{b}{k_\lambda}$ with k_λ the opacity. A jump in opacity leads to the jump in intensity of the opposite sign.

Specific intensity and its angular moments

specific intensity	$\Delta\epsilon = \boxed{I_\nu} A_1 A_2/r^2 \Delta\nu \Delta t$
energy density	$E = \dfrac{1}{c}\displaystyle\iint I_\nu d\nu d\Omega$
flux vector	$F = \displaystyle\iint I_\nu n d\nu d\Omega$
pressure tensor	$P = \displaystyle\iint I_\nu nn d\nu d\Omega$
mean intensity	$J_\nu = \dfrac{c}{4\pi}E_\nu$
Eddington flux	$H_\nu = \dfrac{1}{4\pi}F_\nu$
Eddington's K	$K_\nu = \dfrac{c}{4\pi}P_\nu$

Eddington factor   In general, the Eddington factor is a tensor, for 1D systems it is reduced to a scalar.

$$f_\nu = \frac{K_\nu}{J_\nu} = \frac{P_\nu}{E_\nu} \tag{8}$$

- isotropic radiation field

- radiation field stronly peaked in radial (i.e. vertical in cartesian) direction

1.3   Radiative Diffusion Approximation

The radiative diffusion approximation bridges two regimes: regimes with ...

- on one hand, large optical depth $\tau \gg 1$: diffusion equation: temperature structure in a static stellar atmosphere

- on the other hand, where radiative *transport* is important

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The diffusive approximation is the following: replace $\boxed{I = B}$ or $I_\nu = B_\nu$.

$$I_\nu = B_\nu - \mu \frac{dB_\nu}{k_\nu dz} \qquad (9)$$

This equation can be derived as a random walk of photons!

1.4   Radiation Hydrodynamical equations

The full RHD equations consist of

- five partial differential equations

- one HD closure equation, e.g. (i) variable Eddington tensor method or (ii) flux limited diffusion

Heat flux   The heat flow rate density $\vec{\phi}$ satisfies the Fourier law $\vec{\phi} = -k\nabla T$. More information can be found for instance on [Wik18].

1.5   Overview of symmetry assumptions

plane-parallel	1D atmosphere
	bounded by horizontal surfaces
spherical symmetry	

1.6   Overview of units and key variables

specific intensity I_ν	$\left[\frac{ergs}{cm^2.sr.Hz.s}\right] = \left[\frac{J}{cm^2.sr.Hz.s}\right]$
opacity $\alpha = k_\nu$	$\left[\frac{m^2}{kg}\right]$
optical depth $\tau = \int_0^l \alpha(s)ds$	[/]
	$\boxed{\tau = 0}$ leave atmosphere

- expanding flow: photons are redshifted (lower frequency - higher wavelength)

- compressing flow: photons are blueshifted (higher frequency - lower wavelength)

2 The mathematics of Radiative Transfer

The material in this section is based on the book [Bus60].

2.1 Auxiliary mathematics

- $\cos(\Theta) = cos(\theta)\cos(\theta') + \sin(\theta)\sin(\theta')\cos(\phi - \phi')$

- phase function $\boxed{p(\mu, \phi, \mu', \phi', \tau) = \sum_{n=0}^{N} \omega_n P_n(\cos(\Theta))}$

  - isotropic scattering $p(\tau) = \omega_0(\tau)$

- equation of transfer $\boxed{\mu\dfrac{\partial I(\tau, \mu, \phi)}{\partial \tau} = I(\tau, \mu, \phi) - \mathcal{S}(\tau, \mu, \phi)}$

  with $\mathcal{S}(\tau, \mu, \phi) = B_1(\tau) + \dfrac{1}{4\pi}\displaystyle\int_{-1}^{1} d\mu' \int_{0}^{2\pi} I(\tau, \mu', \phi')p(\mu, \phi, \mu', \phi')d\phi'$

  - axially symmetric with isotropic scattering
    $$\mathcal{S}(\tau) = \frac{\omega_0(\tau)}{2}\int_{-1}^{1} I(\tau, \mu')d\mu' = B_1(\tau) + \frac{\omega_0(\tau)}{2}\int_{0}^{\tau_1} \mathcal{S}(t)E_1(|t - \tau|)dt$$
  - the Milne equation of the problem $(1 - \omega_0\bar{\Lambda})\{ mahtcalS(t)\} = B(\tau)$
    * solve for $\mathcal{S}(t)$
    * then find $I(\tau, \mu)$

2.2 Background: integral equations

Based on the book [BHR02].

1. integral equation from differential equation

2. types of integral equations

3. operator notation and existence of solutions

4. closed-form solutions

   - separable kernels
   - integral transform method (Fourier transform)
   - differentiation

5. Neumann series

6. Fredholm theory

7. Schmidt-Hilbert theory

Fredholm equation first kind

$$0 = f + \lambda\mathcal{K}y \tag{10}$$

Fredholm equation second kind

$$y = f + \lambda\mathcal{K}y \tag{11}$$

3 Challenges in Radiative Transfer

The material here originates from an oral discussion with Ivan Milic.

3.1 Overview of the problem

$$I_\lambda^* \longrightarrow \boxed{T(\tau) \ , \ \rho(\tau) \ , \ \vec{B}(\tau) \ , \ \vec{v}(\tau)} \longrightarrow I_\lambda^+$$
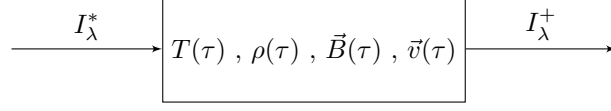
Forward problem

The forward problem is schematically represented

$$\vec{T}, \rho, \vec{B}, \vec{v} \longrightarrow \boxed{\begin{array}{c} \text{forward problem} \\ I_\lambda^+ = F(\vec{T}, \rho, \vec{B}, \vec{v}) \end{array}} \longrightarrow I_\lambda^+$$
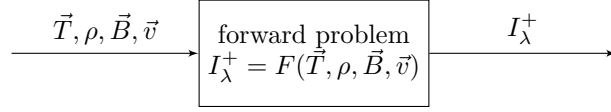
In fact solve for intensity vector $\vec{I} = \begin{pmatrix} I \\ Q \\ \alpha \\ V \end{pmatrix}$ obeying the equation

$$\frac{d\vec{I}}{d\tau} = -X(\vec{T}, \rho, \vec{B}, \vec{v})\vec{I} - \vec{j}(\vec{T}, \rho, \vec{B}, \vec{v}) \tag{12}$$

and the solution

$$I_\lambda^+ = I_0^+ e^{-\int} + \int \vec{j} e^{-\int} d\tau \tag{13}$$

Example Source function $S = a\tau + b$ then $\int_0^{\tau_{max}} (a\tau + b)e^{-\tau} d\tau = ...$

Inverse problem

The inverse problem is schematically represented

$$I_\lambda^+ \longrightarrow \boxed{\begin{array}{c} \text{inverse problem} \\ F^{-1}(I_\lambda^{obs}) \end{array}} \longrightarrow \vec{T}, \rho, \vec{B}, \vec{v}$$
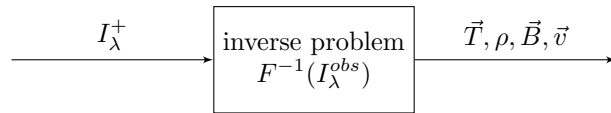
Via least-squares approximation

$$\min_{\vec{T}, \rho, \vec{B}, \vec{v}} \sum \left(I_\lambda^{obs} - I_\lambda(\vec{T}, \rho, \vec{B}, \vec{v}) \right)^2 \tag{14}$$

3.2 Challenging domains of application

- Lyman alpha in Galaxy Halos

- Dusty torii (AGD)

- protoplanetary disks

- circumstellar disks

- athmospheres

4 Stellar Winds

From [**introStellarWindsLamersCassinelli1999**]

4.1 Chronology of stellar wind studies

1. early history: similarties between spectra of nova and luminous stars

2. diagnostics of structure of oouter atmospheres of the sun and stars

3. the development of the solar wind theory, further evidence for outflows

4. rocket and early satellite observations of stellar winds

5. instabilities and non-speherical effects in winds

There are still many things of stellar winds that are uncertain.

4.2 Observations & Formation of spectral lines in stellar winds

- line scattering
  - resonance scattering: from ground state of atom

4.2.1 Pcygni profiles

5 Glossary

- LASER: Light Amplification by Stimulated Emission of Radiation
- (spectral) Line-force: force on material in stellar atmosphere
- MASER: Microwave Amplification by Stimulated Emission of Radiation
- SED: spectral energy distribution

Part II

Radiative Transfer: numerical techniques

forewarned is forearmed   General guidelines for good practices in scientific computing are found in [Wil+14].

6   Introduction to Monte Carlo Radiation Transfer

The material is taken from [**WWBW2001**] and from [**WWBW2013**].

6.1   Elementary principles

specific intensity	I_ν
radiant energy	dE_ν
surface area	dA
angle	θ
solid angle	$d\Omega$
frequency range	$d\nu$
time	dt
flux	F_ν
cross section	σ
scattering angle	χ
	$\mu = \cos(\chi)$
mean intensity	J
flux	H
radiation pressure	K

6.2   Example: plane parallel atmosphere

1. emission of photons: select two angles (3D space). In isotropic scattering
   - θ met $\mu = \cos(\theta)$
     - $\mu = 2\xi - 1$ (isotropic scattering)
     - $\mu = \sqrt{\xi}$ (A slab is heated from below. Then $P(\mu) = \mu$)
   - $\phi = 2\pi\xi$

2. propagation of photons
   - sample optical depth from $\tau = -\log(\xi)$
   - distance travelled $L = \dfrac{\tau z_{max}}{\tau_{max}}$

3. conclusion of emission and propagation

$$
\begin{aligned}
x &= x + L\sin(\theta)\cos(\phi) \\
y &= y + L\sin(\theta)\sin(\phi) \\
z &= z + L\cos(\theta)
\end{aligned}
\tag{15}
$$

4. Binning: once the photon exists the slab. Produce histograms of the distribution function. Finally, we wish to compute the output flux or the intensity.

7 Asymptotic Preserving Monte Carlo methods for transport equations in the diffusive limit

A very interesting article about Monte Carlo methods for radiative transfer problems, from a mathematical point of view, is [DPS18]. I am currently trying to reproduce the numerical experiments that are reported in the article.

8 Fluid and hybrid Fluid-Kinetic models (for neutral particles in plasma edge) (Horsten2019)

The material is mainly taken from [Hor19].

- Kinetic Boltzmann equation: neutral velocity distribution $f_n(r, v)$

- If you taken into account (e.g. microscopic processes for atomic deuterium) then the kinetic Boltzmann equation becomes

$$v \nabla f_n(r, v) = S_r(r, v) + S_{cx}(r, v) - f_n(r, v)(R_{cx}(r, v) + R_i(r)) \tag{16}$$

- Numerical solution strategies

    - finite differences/volumes/elements :computationally infeasible
    - spectral methods (series expansion of $f_n(r, v)$: not suitable for modelling discontinuties
    - stochatic approach: the whole velocity distribution is discretized by finite set of particles

- from Equation (16), the fluid model and the hybrid model is derived.

    - Fluid model: 3 state equations (continuity - momentum - energy) with boundary conditions
        * pure-pressure equation: maximum error of 10 - 28 %
        * with parallel momentum source: error 10 %
        * with ion energy source: error 30 %
    - hybrid model based on micro-macro decomposition

9 Overview of existing (Monte Carlo) radiative transfer codes

9.1 Synthesis codes

As is pointed out in [Chr15], there are basically two methods to solve the radiative transfer problem: ray-tracing and Monte Carlo methods.

- RADICAL [**RADICAL**] (Ray-tracing, 2D, multi-purpose)

- MULTI [Car] [Car86] (computer program for solving multi-level non-LTE radiative transfer problems in moving or static atmospheres, very old: Uppsala 1986 - 1995)

- SKIRT [CB2] (continuum (Monte Carlo) radiation transfer in dusty astrophysical systems, such as spiral galaxies and accretion disks, from Ugent)

- TORUS [Har+19] (Monte Carlo radiation transfer and hydrodynamics code. Adopts 1D, 2D, 3D adaptive mesh refinement. Suitable for radiative equilibrium and creation of synthetic images and SED)

- RADMC-3D [Dul17] (Monte Carlo code that is especially applicable for dusty molecular clouds, protoplanetary disks, circumstellar envelopes, dusty tori around AGN and models of galaxies. Python interface with Fortran main code)

- TLUSTY and SYNSPEC [HL17a], [HL17b], [HL17c].

9.2 Inversion codes

- VFISV

- ASP/HAO

- HeLIx+

- SNAPI (not publicly available, created by Ivan Milic)

- multiple codes available from Instituto de Astrofyiica de Canarias (IAC)

- STiC: the Stockholm inve rsion code

Part III

Practical work and Exercises

10 Overview of exercises (PART I)

1. limb-darkening scattering exercise we did during the course. — You can look into your notes from that, and I attach here also a sample program which you can use a base. After you have familiarised yourself with this, you can start to think about how you would go about to extend this to a 3D setting (assuming isotropic scattering).

2. (As prep for Monte-Carlo school) here is a script computing a UV resonance P-Cygni line in spherically symmetric wind with v beta-law. At top of routine, a few exercises are given, where you can modify and play around with code. Monte-Carlo program which computes a UV resonance spectral line from a fast outflowing spherically symmetric stellar wind (if you were not cc'd on that email, let me know so that I can send you the files as well). At the top of that little script, there are a few suggestions for exercises (additions) you could do to that program, in order to learn a bit more about the general workings of Monte-Carlo radiative transfer in this context. — So that might be a good idea for you to do as well ! (And you can also ask the others in the group for some tips etc. then.)

3. Some background reading:

   - Attached mc manual by Puls.
   - Paper by Sundqvist+ 2010 (Appendix, I think).

11 Overview of exercises (PART II)

1. Calculate the probability distribution to sample from in the case of Eddington limb darkening for the initial distribution (see Section 20.3).

   - finished + Ok

2. Calculate analytical solution for simplified problem in the case that `mu = 1` (see Section 20.1).

   - finished + Ok + can be further studied

3. Perform convergence analysis (see Section 20.5).

12 Overview of exercises (PART III)

1. Revisit 3D limb darkening. ϕ should be sampled between 0 and 2π (see Section 19.6). (OK)

2. Revisit convergence analysis: adapt plot formatting and standard deviation is defined as square root of variance (see Section 20.5).

3. Test variance reduction technique (see Section 20.6).

4. Some general considerations about the definitiion of specific intensity (see Section 1.1). (OK)

5. For the Monte Carlo approximation of the diffusion equation, why do wo have $N \sim \tau$ for low optical depth $\tau \ll 1$ (see Section 28).

6. Revisit the radial streaming approximation in `pcyg.f90` for lower optical depth (e.g. `xk0=0.5`). (see Section 20.1).

7. What happens when you add a line (e.g. $x = 0.5 = a$)? How would you do that? (see Section **??**)

8. Towards a mathematical description of the problem.

13 Overview of exercises (PART IV)

1. Convergence analysis: also fit a line through the points. Formally, we write $V = CN^x$ and determine both C and X from experimental data. Correspondingly, $\log(V) = \log(C) + x\log(N)$. This is fitted using least-squares (see Section 20.5).

2. Variance reduction technique

   - averaging over different stochastic realizations?
   - take `xk0=0.5`
   - try to also discretize μ

3. Adding a second line: develop computer code in the radial streaming assumption (use analytic formulas) $\mu = 1$ (see Section **??**).

   - a following improvement is the use of a grid instead of using the bisection method.

4. Limb darkening. Have a look at section 19.3.1.

14 Multiline transfer (PART I)

1. What happens when you add a line (e.g. $x = 0.5 = a$)? How would you do that? (see section **??**)

15 Multiline transfer (PART II)

1. calculate force from one line (see section 25).

   - discretize in shells
   - assume $\epsilon_i = cte$

2. compare to analytic expressions

16 Preparation for Equation meeting on 15 October

See Section 24.

17 Preparation for meeting on 21 October

I have been working on Section 22 and on Section 24.

questions

- also take into account the photons where no scattering takes place?
- language of master thesis?
- analytical expression for $L(r)$?

18 Introductory exercises

18.1 Analytical exercises

From course material from (prof. Sundqvist - CMPAA course).

1. introduction

2. radiation quantities

   - exercise p.3:
     - on one hand, we know that $\Delta\epsilon \sim C/r^2$
     - on the other hand, from the definition we know that $\Delta\epsilon = I_\nu A_1 A_2/r^2 \Delta\nu\Delta t$
     - combining these equations shows that I_ν is independent from r

   - exercise p.4:
     -

   - exercise 1:
     - $F_x = \int_0^\pi \left[I_\nu(\theta)\sin^2(\theta) \int_0^{2\pi} \cos(\phi) \right] d\theta d\phi = 0$
     - the same reasoning for $F_y = 0$

   - exercise 2:
     - the equation follows from $d\mu = d\cos(\theta) = \sin(\theta)d\theta$

   - exercise 3:
     - isotropic radiation field (i.e. $I(\mu) = I$) then we have $F_\nu = 2\pi \int_{-1}^1 I\mu d\mu = 2\pi I \left.\frac{x^2}{2}\right|_{-1}^1 = 0$

   - exercise 4:
     - $F_\nu = 2\pi \int_{-1}^1 I(\mu)\mu d\mu = 2\pi \int_{-1}^0 I_\nu^- \mu d\mu + 2\pi \int_0^1 I_\nu^+ \mu d\mu = 2\pi I_\nu^+$

   - exercise p.7:
     - isotropic radiation field:
       * although the radiation pressure is a tensor, we will denote it as a scalar $P_\nu = \dfrac{4\pi I_\nu}{c}$
       * the radiation energy density $E_\nu = \dfrac{12\pi I_\nu}{c}$
       * thus $f_\nu = \dfrac{1}{3}$
     - very strongly peaked in radial direction (beam): $I_\nu = I_0\delta(\mu - \mu_0)$ with $\mu_0 = 1$
       * pressure tensor $P_{nu} = \dfrac{1}{c}\int I_0\delta(\mu - \mu_0)nnd\Omega$
       * energy density $E_\nu = \dfrac{1}{c}\int I_\nu d\Omega$
       * in this case $P_\nu = E_\nu$ thus $f_\nu = 1$

3. radiation transport vs. diffusion vs. equilibrium

   - exercise p. 12: 1D, Cartesian geometry, plane-parallel, frequency-independent and isotropic emission/extinction
     - radiation energy equation
       * The equation follows by integrating Equation (**??**)
       * By definition, $E = \dfrac{1}{c}\iint I_\nu d\nu d\Omega$
       * thus $\dfrac{dE}{dr} = \int (j - kI)d\nu d\Omega$ thus $\boxed{\dfrac{dE}{dr} = \dfrac{(j - kI)4\pi(\nu_1 - \nu_0)}{c}}$

 * work out the integral taking into account frequency-independent and isotropic coefficients:

– zeroth momentum equations

 * One must also take into account the specific form of the flux vector

$$F = \iint I_\nu n d\nu d\Omega = 2\pi \int_{-1}^{1} I_\nu(\mu)\mu d\mu$$

 * thus $\frac{dF}{dr} = \frac{1}{c}\int(j - kI)nd\nu d\Omega$ thus $\boxed{\dfrac{dF}{dr} = \dfrac{(j - kI)4\pi(\nu_1 - \nu_0)n}{c}}$

– first moment equation

 * similar reasoning

 * $\dfrac{dP}{dr} = \int(j - kI)n.nd\nu d\Omega$ thus $\boxed{\dfrac{dF}{dr} = \dfrac{(j - kI)4\pi(\nu_1 - \nu_0)n}{c}}$

• first exercise p. 15

– $P = \dfrac{1}{c}\iint I_\nu\mu^2 d\Omega d\nu = \dfrac{2\pi}{c}\int_\nu\int_{-1}^{1} I_\nu\mu^2 d\mu d\nu = \dfrac{4\pi}{3c}\int B_\nu d\nu = \dfrac{aT^4}{3} = \dfrac{E}{3}$

• second exercise p.15

– assuming the diffusion limit,

– flux-weighted mean opacity $\kappa_F = \dfrac{\int F_\nu \kappa_\nu d\nu}{\int F_\nu d\nu}$

– Rosseland mean opacity $\dfrac{1}{\kappa_R} = \dfrac{\int_0^\infty \frac{1}{\kappa_\nu}\frac{dB_\nu}{dT}}{\int_0^\infty \frac{dB_\nu}{dT}d\nu}$.

 * in the diffusion limit, $F_\nu = -\dfrac{4\pi}{3}\dfrac{dB_\nu}{k_\nu dz}$ thus $\dfrac{dB_{nu}}{dT} =$

 *

• third exercise p.15

4. the equations of radiation-hydrodynamics

5. numerical techniques for the radiative diffusion approximation

6. applications and approximations for a dynamically important radiative force in supersonic flows

• exercise p.27: $L_{SOB} = \Delta r = \dfrac{v_{th}}{dv/dr} = \dfrac{10[km/s]}{1000[km/s]/R_*} = 0.01R_*$

7. Appendix A: properties of equilibrium black-body radiation

• exercise p. 29

– this should be satisfied: $B_\nu d\nu = -B_\lambda d\lambda$ and also $\nu = \dfrac{c}{\lambda}$

– this is equivalent to saying that $0 = \nu d\lambda + \lambda d\nu$ or $d\lambda = -\dfrac{\lambda}{\nu}d\nu$ thus $B_\lambda = \dfrac{\nu}{\lambda}B_\nu$

– $B_\lambda(T) = \dfrac{\nu}{\lambda}\dfrac{2h\nu^3}{(\lambda\nu)^2}\dfrac{1}{e^{hc/\lambda kT} - 1} = \dfrac{2h\nu^2}{\lambda^3}\dfrac{1}{e^{hc/\lambda kT} - 1} = \dfrac{2hc^2}{\lambda^5}\dfrac{1}{e^{hc/\lambda kT} - 1}$

• first exercise p.31

– derive that $\lambda_{max}T = 2897.8[\mu mK]$

– ...

• second exercise p.31

– this is about the spectra of (unknown) stars

• first exercise p.32

– see exercise 7

• second exercise p.32

  – BB radiation: $I_\nu = \dfrac{2h\nu^3}{c^2} \dfrac{1}{e^{h\nu/kt} - 1}$

  – the radiative flux for isotropic BB radiation is zero. See also exercise 3. This dus also holds for BB radiation.

- exercise p. 33

  – <u>HR-diagram</u>

8. **Appendix B: Simple examples to the radiative transfer equation**

- first exercise p. 34

  – start from radiative transport equation $\mu\dfrac{dI}{ds} = \alpha - \eta I$ in which $\eta = 0$ thus $\boxed{\mu\dfrac{dI}{ds} = \alpha}$

  – solving the ODE in the general case that $\alpha(s)$ is not constant:

    * integrate the equation $\mu I = \displaystyle\int_0^D \alpha ds$

    * ...

  – second exercise p. 34

    * case $\tau(D) \gg 1$: then $I(D) \approx S$

    * case $\tau(D) \ll 1$: then $I(D) \approx I(0) + S(1 - 1) = I(0)$

  – first exercise p.35

    * is the plane-parallel approximation valid for the solar photosphere?

  – second exercise p.35

    * goal: find a solution to the equation $\mu\dfrac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu$ where $I(\tau, \mu)$

    * solution

- second exercise p.35

9. **Appendix C: connecting random walk of photons with radiative diffusion model**

- exercise p. 38. Computing the average photon mean-free path inside the Sun.
  $l = \dfrac{1}{\kappa\rho} = \dfrac{V_o}{\kappa M_o}[cm]$

- exercise p.39. Computing the random-walk time (diffusion time) for photons

18.2   Numerical exercises

18.2.1   Implicit 1D solver

Exercise from (20-11-2018).

Goal   Implement implicit solver for time-dependent diffusion equation

$$\partial_t u = \partial_{xx} u \tag{17}$$

Solution   The convergence behaviour of the method is shown in Figure 1.
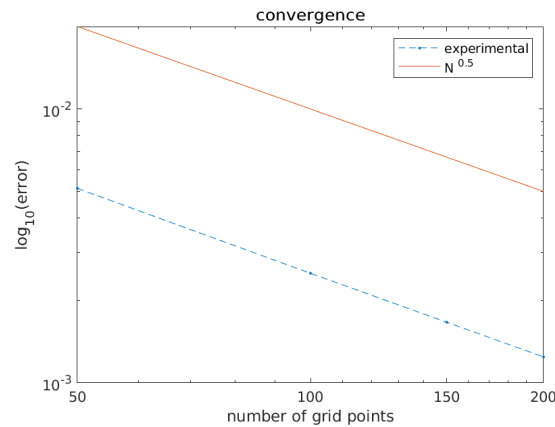

Figure 1: Convergence behaviour for 1D implicit solver (diffusion equation)

18.2.2   ADI 2D Solver

Goal   Implement implicit solver for time-dependent diffusion equation

$$\partial_t u(t, x, y) = \partial_{xx} u(t, x, y) + \partial_{yy} u(t, x, y) \tag{18}$$

Solution   There is still an error in the code.

18.2.3   Area of a circle

Goal   Develop Monte Carlo code

Solution

18.3   Other Exercises

From course material from Ivan Milic.

18.3.1   Lecture 7

1. Derive expressions for the emergent radiation when properties are the following:

   - optically thin slab at all wavelengths
   - wavelength-independent incident radiation

   Solution: see slide 14?

2. Derive ralations between Einstein coefficients.

3. Calculate electron density in atmosphere from FALC model

19   Limb darkening

19.1   Formulation of the problem

- The radiative transfer equation 5 in this situtation becomes an integro-differential equation with
$S(\tau) = \frac{1}{4\pi} \int I(\tau, \mu) d\Omega$

$$
\begin{aligned}
\mu \frac{dI(\tau, \mu)}{d\tau} &= -I(\tau, \mu) + S(\tau) \\
&= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) d\Omega
\end{aligned}
\tag{19}
$$

- The difficulty resides in the (evaluation of) the source function. Monte Carlo simulation avoids explicit calculation source function: source function implicit in Monte Carlo simulation. There the physics are simulated IN BETWEEN TWO CONSECUTIVE SCATTERING EVENTS as follows

$$
\frac{dI}{dz} = -\alpha I
\tag{20}
$$

thus $I = I_0 e^{-\delta\tau}$ and then τ is sampled according to $\tau = -\log(X_{\text{random}})$

19.2   Solving the (integro-differential) radiative transfer equation

Analytical Solution of Equation (19)   Ik heb de mosterd gehaald op [Esp].

$$
I(0, \mu) = \int_0^\infty S(\tau) exp\left(\frac{-\tau}{\mu}\right) d\left(\frac{\tau}{\mu}\right)
\tag{21}
$$

Numerical Solution of Equation (19)   First rewrite the equation

$$
\begin{aligned}
\mu \frac{dI(\tau, \mu)}{d\tau} &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) \sin(\theta) d\theta d\phi \\
&= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) d\mu d\phi \\
&= -I(\tau, \mu) + \frac{1}{2} \int I(\tau, \mu) d\mu
\end{aligned}
\tag{22}
$$

Discretization scheme:

$$
???
\tag{23}
$$

19.3   Eddington-Barbier approximation

$$
J(\tau) = S(\tau) = \left(\tau + \frac{2}{3}\right) 3H
\tag{24}
$$

Together with the time-independent radiative transfer equation (5) in a gray (frequency-independent) planar medium gives

$$
\mu \frac{\partial I(\tau, \mu)}{\partial \tau} = I(\tau, \mu) - \left(\frac{2}{3} + \tau\right) 3H
\tag{25}
$$

The emergent intensity $I(0, \mu)$ is a solution of Equation (25). Its solution for $\tau = 0$ equals

$$
\boxed{I(\tau = 0, \mu) = I_1\left(\frac{2}{5} + \frac{3\mu}{5}\right) = a + b\mu}
\tag{26}
$$

with $a = \frac{\sigma}{2\pi} T_{eff}^4$ and $b = \frac{3\sigma}{4\pi} T_{eff}^4$

19.3.1 Validity of the Eddington-Barbier approximation

If we assume Equuation (24) then $I = I_1(a + b\mu)$ thus

$$J = \frac{1}{2} \int I(\tau, \mu) d\mu = \frac{1}{2} \int_0^1 (a + b\mu) d\mu \tag{27}$$

But we can not really compute this since we only know $I(0, \mu)$.

The thing is that Eddington specifies $S(\tau)$ but not $S(\mu)$ directly. If that expression is used into the expression of a semi-infinite atmosphere (namely that the specific intensity is the Laplace transform of the source function), then we get the desired result AT THE OUTER EDGE OF THE ATMOSPHERE. See also [Mihalas] p. 571.

> dat ziet er hier niet goed uit

19.4 2D Case

We again have $\mu = \cos(\theta)$. The solution of the radiative transfer equation in plane-parallel syummetry with frequency-independent absorption and emission, is

$$I(\mu) = I_1(0.4 + 0.6\mu) \tag{28}$$

In the Monte Carlo code, the photons are sorted according to the direction that they leave the atmosphere.

Goal Calculates the angular dependence of photon's emitted from a plane-parallel, grey atmosphere of radial optical depth `taumax`. The value of `tau` determines the position of the photon

Variables and Algorithm

- `muarray` contains emergent photons

- `na` number of channels

- `dmu` $= 1/$`na` width of channels

- `nphot` number of photons

- `taumax` maximum optical depth

Figure 2 is according to what is expected $I = I_0(0.4 + 0.6\mu)$. The input parameters are as follows
`Limb_Darkening(number_of_channels = 20, number_of_photons = ` 10^5`,`
`maximum_optical_depth = 10)`.


Algorithm 1 Limb darkening: compute quantitiy of photons

---

initialization
    radial optical depth τ
    direction μ
for all photons **do**
    $\boxed{\tau = \tau_{max}}$
    while tau ≥ 0 **do**
        compute scattering angle mu
        if tau $\geq$ taumax **then** $\boxed{mu = sqrt(x)}$ (initial distribution)
        else $\boxed{mu = 2 * x = 1}$ (isotropic scattering)
        tau_i = -log(x2)
        tau = tau - tau_i*mu
    end while
    now we know that the photon has left the photosphere
    compute the distribution of all angles mu at which the photon left the photosphere
end for
visualisation:

- plot photon numbers from $\mu d\mu$ against mu

- plot specific intensity from $d\mu$ against mu against

---
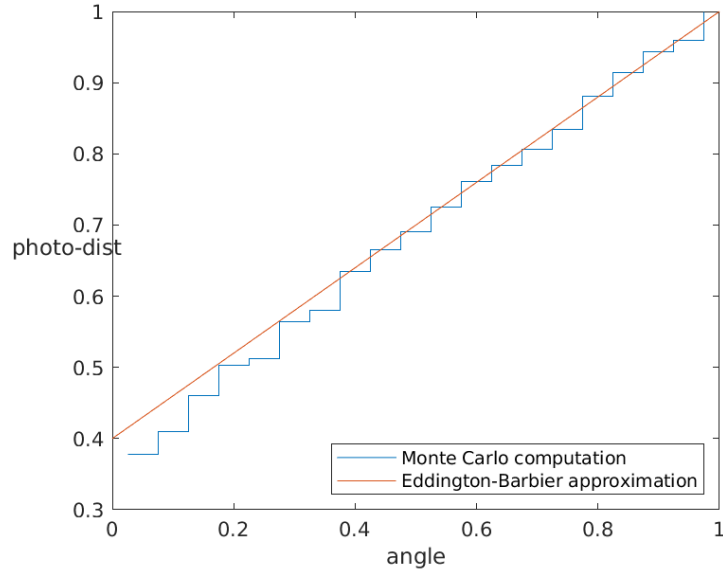
Figure 2: histogram for mu

19.5 Calculating the moments of intensity: study

Limb darkening. Expected results in Equation (28). The first angular moment $J(r)$ of the intensity should approximately equal Equation (24), if the Eddington-Barbier approximation is valid. I am now also interested in computing $J(r)$, numerically. Photons are counted using formula in Table 1.
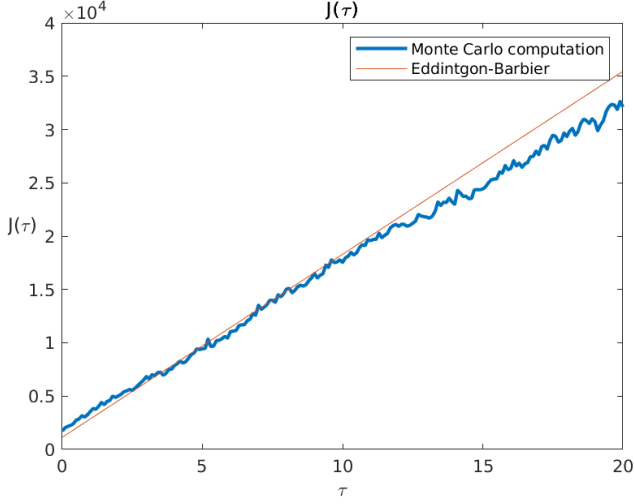
(a) $J(\tau)$ as numerically computed with MC method
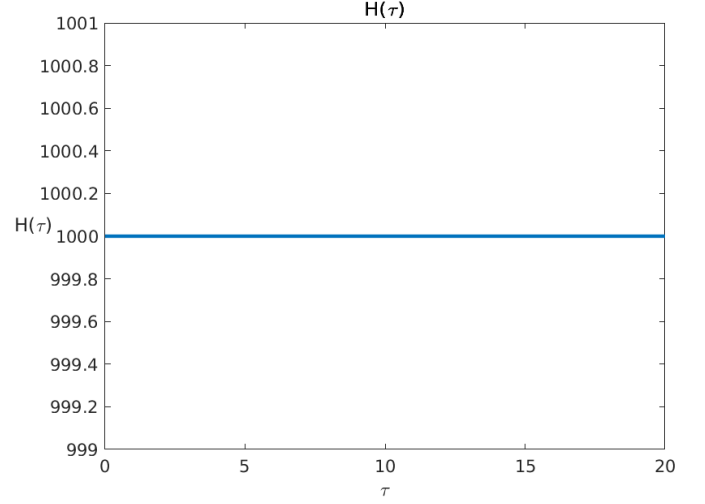
(b) $H(\tau)$ as numerically computed with MC method

One (numerical) problem here is that photons with $\mu_i \to 0$ would give a very high contribution to $J(r)$. To overcome this, only photons with an angle $\mu > 0.1$ are counted.

Problem   From Figure 4 (output of Monte Carlo simulation), $J(\tau) \equiv J$ seems to be constant. This is not as predicted in Equation (24).

Explanation   One can understand this result as follows: photons are counted according to the sign of their angle. But of course all photons eventually reach the zone where $\tau = 0$ and zones where a photon *goes for a little walk* does not contribute to the moment J.
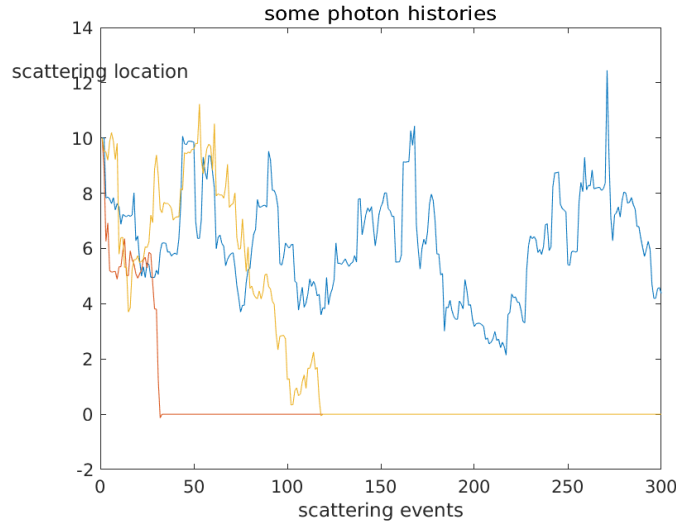

Figure 4: $J(\tau)$

19.6   3D Case

What changes is this:

- introduction of a new angle ϕ

- the optical depth is not updated with respect to ϕ
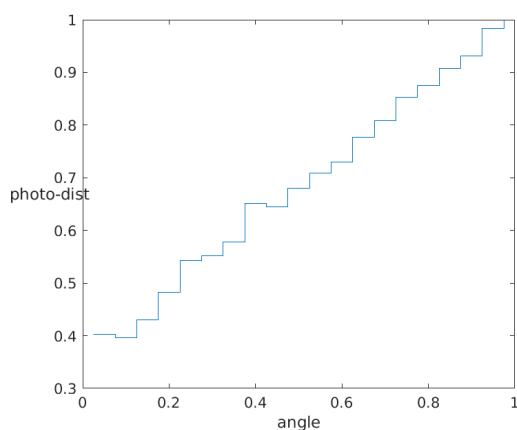

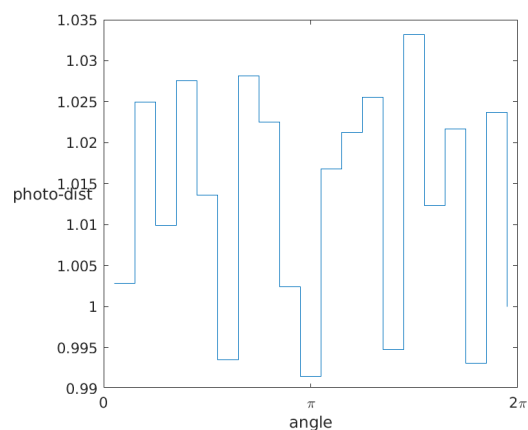Figure 5: histogram for `mu`

Figure 6: histogram for `phi`

Figure 5 and Figure 6 are the result of the function `Limb_Darkening_3D` with the following input parameters: `Limb_Darkening_3D(number_of_channels = 20, number_of_photons = ` 10^5 `, maximum_optical_depth = 10)`. The results according to what is expected, namely $I = I_0(0.4 + 0.6\mu)$ and ϕ follows a uniform distribution.
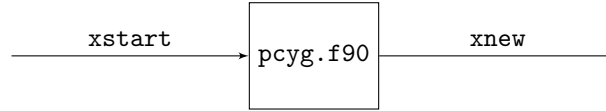
Extension: make version where the optical depth is updated with respect to ϕ

Via this link, you can go back to the exercises overview: Section <u>12</u>.

Part IV
Spectral line formation: pcyg.f90

20 Basics

This section is about the study of line formation in an expanding wind.

```
           xstart              xnew
  ─────────────────→ ┌──────────┐ ─────────────────→
                     │ pcyg.f90 │
                     └──────────┘
```

- spherical geometry

20.1 First adaptation: what if all photons are released radially from photosphere?

20.1.1 Release photons radially: numerical MC experiments

What would happen with line-profile, if you assumed all photons were released radially from photopshere?

- In other words `xmuestart = 1`.

- This is implemented under the test case `test_number=1`.

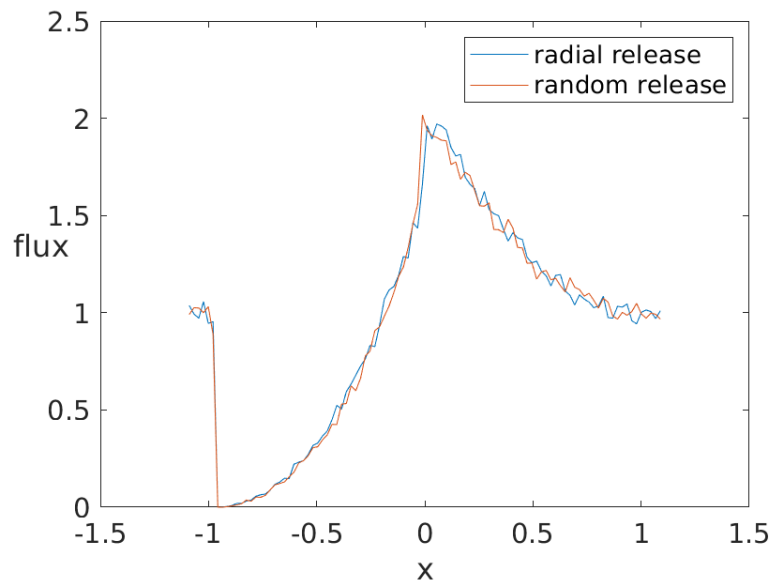- Results in Figure 30 for opacity `xk0 = 100`.

Figure 7: The number of photons equals 10^5, `xk0=100`

20.1.2 Derive analytic expression

See also slide 26/49 [Sundqvist course material].

- since `xmuein = 1` we have for the velocity profile

$$v = v_\infty (1 - b/r)^\beta \tag{29}$$

A scaled version of Equation (29) yields

$$u = \frac{v(r)}{v_\infty} = \left(1 - \frac{b}{r}\right)^\beta \tag{30}$$

with $u \in [0..1]$

- Doppler shift for the frequency of the photons: $x_{CMF} = x_{REF} - \mu u$.

- Condition for resonance from Sobolov approximation (to be studied later): $\boxed{x_{CMF} = 0}$ thus

$$x_{REF} = \mu u \tag{31}$$

or thus $x_{REF} = \boxed{u_{\text{interaction}}}$ and than solve Equation 30 for $r_{\text{interaction}}$

- If $\mu = 1$ then

$$x = \left(1 - \frac{b}{r}\right)^\beta \tag{32}$$

$$x^{1/\beta} = 1 - \frac{b}{r}$$

$$r(1 - x^{1/\beta}) = b$$

$$\boxed{r(x) = \frac{b}{1 - x^{1/\beta}}} \tag{33}$$

- From the location of interaction r, the incident angle can be calculated

$$\texttt{xmuein} = \sqrt{1 - \left[\frac{\texttt{pstart}}{r}\right]^2} = \sqrt{1 - \left[\frac{\sqrt{1 - \texttt{xmuestart}^2}}{r}\right]^2} \tag{34}$$

Now also taking into account that `xmuestart = 1`

$$\texttt{xmuein = 1} \tag{35}$$

- The calculation of the optical depth goes as follows:

$$\tau = \frac{\texttt{xk0}}{rv^{2-\alpha}(1 + \texttt{xmuein}^2\sigma)} \tag{36}$$

Now also taking into account that `xmuestart = 1` gives

$$\tau = \frac{\texttt{xk0}}{rv^2(1 + \sigma)} \tag{37}$$

where $\boxed{v(x) = \left(1 - \frac{b}{r}\right)^\beta}$ and $\frac{dv}{dr} = \frac{\beta b}{r^2}\left(1 - \frac{b}{r}\right)^{\beta-1}$

and $\sigma(x) = \frac{dv}{dr}\frac{r}{v} - 1$ thus $\boxed{\sigma(x) = \frac{\beta b}{r}\left(1 - \frac{b}{r}\right)^{-1}}$

- Assuming that $\beta = 1$ then $\boxed{v(x) = 1 - \frac{b}{r}}$ and $\frac{dv}{dr} = \frac{\beta b}{r^2}$ and $\boxed{\sigma(x) = \frac{\beta b}{r}}$.

- `xmueou` follows the distribution as given by the function `xmueout`, namely

$$p(x) = \frac{1 - e^{-\tau}}{\tau} \tag{38}$$

with $\tau = \dfrac{\texttt{tau0}}{1 + \texttt{X}^2 \sigma}$ where `X` is a random number, so actually this comes down to

$$p(x) = \frac{1 - e^{-\frac{\tau_0}{1+x^2\sigma(x)}}}{\frac{\tau_0}{1+x^2\sigma(x)}} \tag{39}$$

- Finally one can combine these results to get the distribution of the photons according to the frequency x via the relation

$$\texttt{xnew = xstart + v(xmueou-xmuein) = xstart + v(xmueou -1)} \tag{40}$$

In words, we initially have an isotropic distribution for `xstart`. The number of photons that are leaving the atmosphere at different frequencies is however not isotropic through complex interactions that are incorporated into $p(x)$. One must also take into account that not all of the photons that are released actually escape from the atmosphere and also that sometimes no resonance is possible, and then Equation (40) is not applicable.

TO DO: proceed from this to the analytical expression for the flux. Here I am stuck for the moment.

20.1.3 Experiments with other opacities
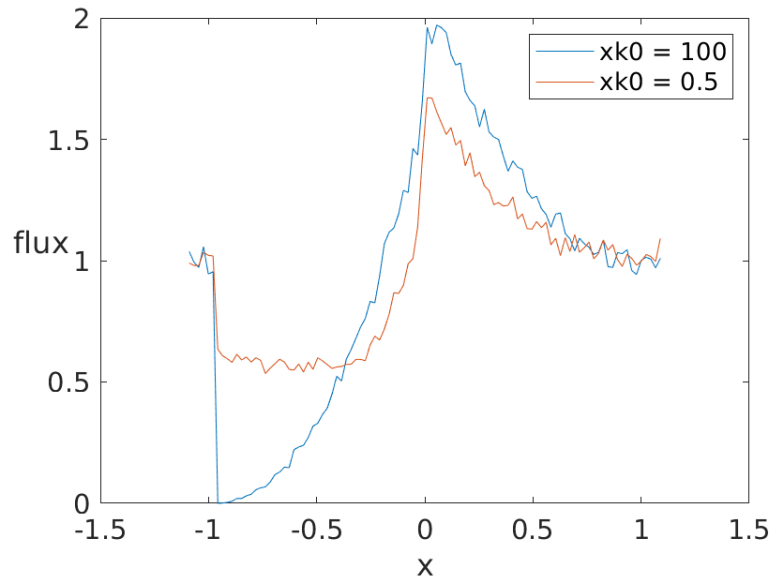
The results for `xk0=0.5` are shown in Figure 8.

Figure 8: The number of photons equals 10^5, `xk0=0.5`

Via this link, you can go back to the exercises overview: Section <u>12</u>.

20.2 Second adaptation: isotropic scattering

What would happen to line-profile, is you assumed scattering was isotropic
(i.e., NOT following Sobolev-distrobution)

- in the implementation, `test_number = 2`
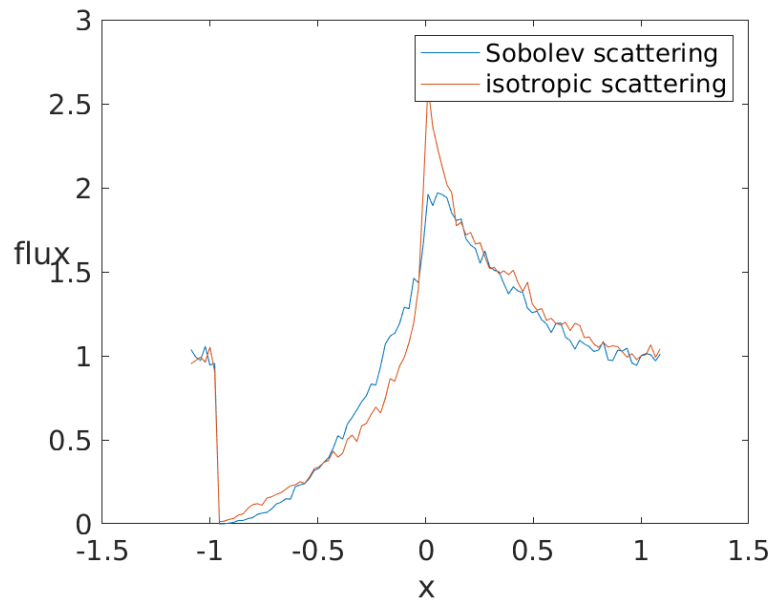
- the results are shown in Figure 9.

Figure 9: The number of photons equals 10^5

It is clear from Figure 9 that the peak around $x = 0$ is higher and sharper.

Analyse this behaviour more closely

20.3 Third adaptation: introduction of Eddington limb-darkening

Goal Put Eddington limb-darkening in. What happens?

20.3.1 Construction of probability distribution corresponding to Eddington limb darkening

For a general (introductory) discussion about Eddington limb darkening, please refer to Section **??**

1. Let us thus first review the emmission case where <u>the flux in each direction is isotropic</u> i.e. $I(\theta) = I$ (as experimented in paragraph 20.2)

   - the specific intensity is defined as $I_\nu(\mu) = \dfrac{dE_\nu}{\cos(\theta)dAdtd\nu d\Omega} = \dfrac{dE_\nu}{\mu dAdtd\nu d\Omega}$

   - the flux $F_\nu = \displaystyle\int_\Omega I_\nu \cos(\theta)d\Omega$ is in this case isotropic thus

$$\xi = \int_0^\mu F_\nu d\mu = \int_0^\mu \int_\Omega I_\nu \cos(\theta)d\Omega d\mu = A\int_0^\mu \mu d\mu \tag{41}$$

   together with the condition that μ satisfies a probability distribution:

$$1 = \int_{-1}^1 F_\nu d\mu = \int_{-1}^1 \int_\Omega I_\nu \cos(\theta)d\Omega d\mu = \frac{A}{2} \tag{42}$$

   thus $A = 2$. Photons need to be sampled according to $\mu d\mu$.

2. Now we look at a new case where the photons need to be emitted following a distrubution that corresponds to $I(\theta) = I(0)(0.4 + 0.6\cos(\theta))$.

   - in this case the flux $F_\nu = \displaystyle\int_\Omega I_\nu \cos(\theta)d\Omega$ is isotropic but also satisfies

$$F_\nu = \int_\Omega I_\nu(0)[0.4 + 0.6\cos(\theta)]\cos(\theta)d\Omega \tag{43}$$

   > I am not sure about the correctness of the assumption of isotropy of the flux

$$\xi = \int_0^\mu F_\nu d\mu = A\int_0^\mu (0.4 + 0.6\mu)\mu d\mu \tag{44}$$

   subject to the normalisation condition -very similar to Equation (42) - that

$$1 = \int_0^1 F_\nu d\mu = \frac{2A}{5} \tag{45}$$

   thus $A = \dfrac{5}{2}$. Photons need to be sampled according to

$$\frac{5}{2}(0.4 + 0.6\mu)\mu d\mu \tag{46}$$

   In the code `pcyg.f90` this corresponds to `test_number = 3` (not yet implemented).

   The results of an accept-reject method that samples the probability distribution in Equation (46).

Via this link, you can go back to the exercises overview: Section <u>11</u>.
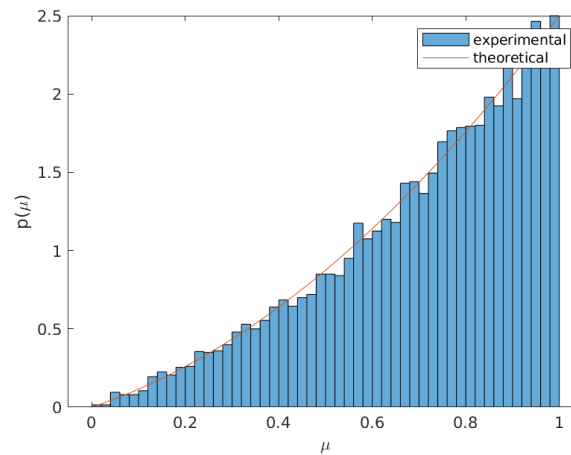
Figure 10: Accept-reject method for Eddington limb darkening

20.4 Fourth adaptaion: photospheric line-profile

Challening: Put photospheric line-profile (simple Gaussian) in. What happens? Test on `xk0=0` (opacity = 0) case.

- test case number 4
- This is still to be implemented.

20.5 Convergence analysis

Zero opacity The convergence of the Monte Carlo method is tested with the following input parameters

kx0	alpha	beta	test_number
0	0	1	0

for a varying amount of photons, as shown in Figure 11. We expect the method to have $\frac{1}{\sqrt{N}}$ convergence, where N is the number of photons. However, the methods strangely seems to have a faster convergence rate.
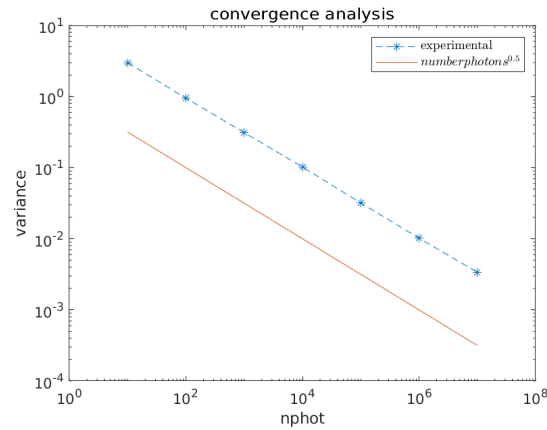

Figure 11: Original version of the code: convergence analysis (xk0=0)

Nonzero opacity The convergence test is set up as follows: different Monte Carlo simulations (with increasing number of photons) are compared to an *expensive* simulation with 10^7 photons. As can be seen in Figure 12, the spectrum profile behaves according to a $N^{0.5}$ law.
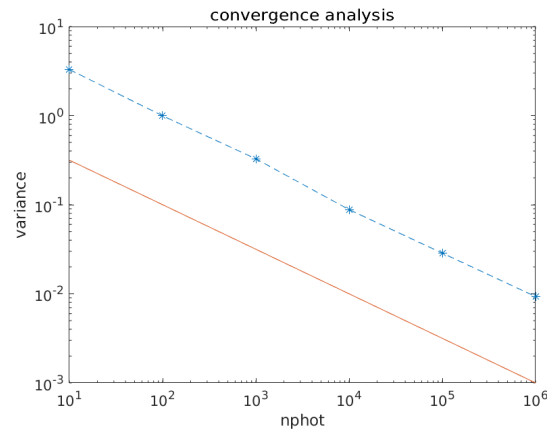

Figure 12: Original version of the code: convergence analysis (xk0=100)

Via this link, you can go back to the exercises overview: Section 11.

20.6   Variance reduction experiment

We will set up the test as follows

- run the code with `xk0=100` and number of photons $N = 10^7$

- run the code again for lower number of photons (e.g. $N = 10^3$), both with random sampling and pseudo-random sampling

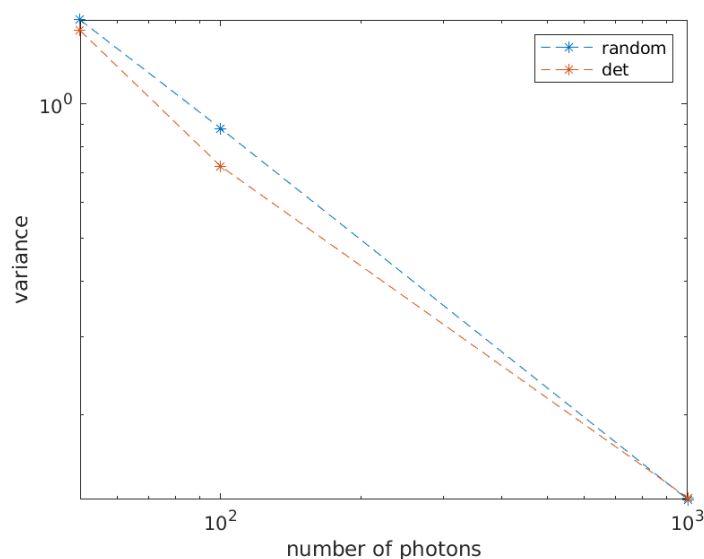- compute variance w.r.t. *expensive* simulation and compare

- `test_number = 5`

Figure 13: Original version of the code: convergence analysis (xk0=0)

`xk0=100`   Possible improvement: average over different stochastic realizations.

Via this link, you can go back to the exercises overview: Section 12.

20.7   Mathematical description of the problem & Looking at literature

Have a look at [NS19] (see Appendix).

21 Transferring the code to Matlab

21.1 Limit variables

	xmin	xmax	vmin	vmax
Fortran	-1.1	1.1	0.01	0.98
Fortran (reverse order for scattering distribution)	-1.1	1.1	-0.98	-0.01
Matlab (with `resonance_x = 0`	-1	1	-0.8	0

21.2 Comparison

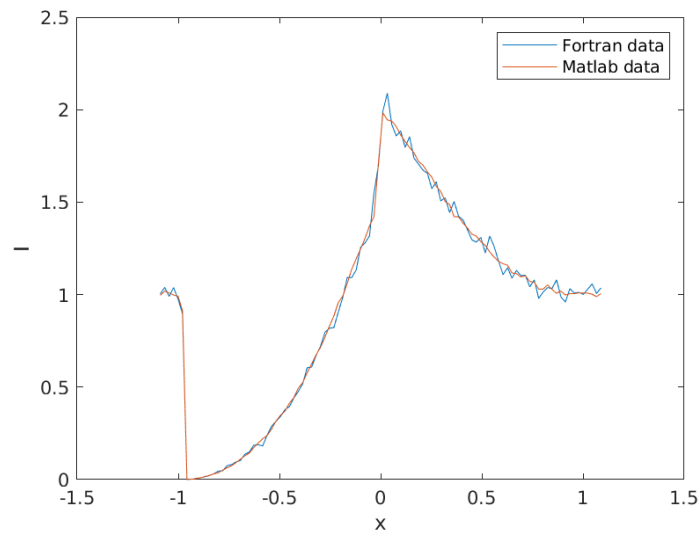### 21.2.1 Literal Matlab version

Figure 14: Comparison of Fortran code and Matlab code (unchanged version - `xk0 = 100`)
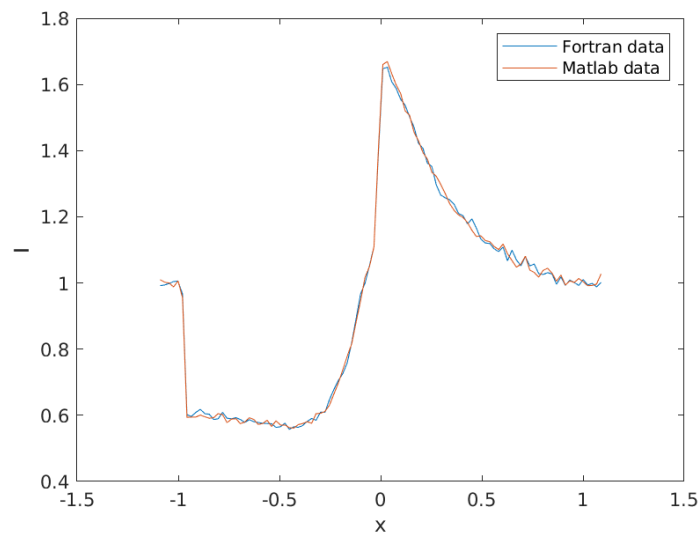

Figure 15: Comparison of Fortran code and Matlab code (unchanged version - `xk0 = 0.5`)
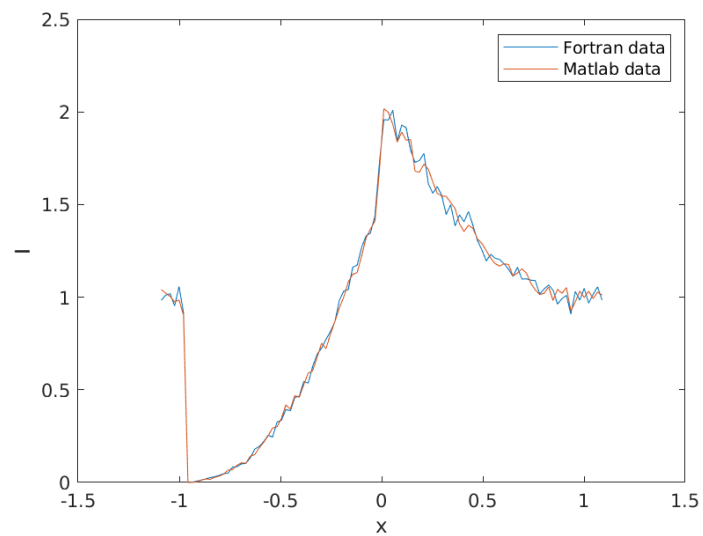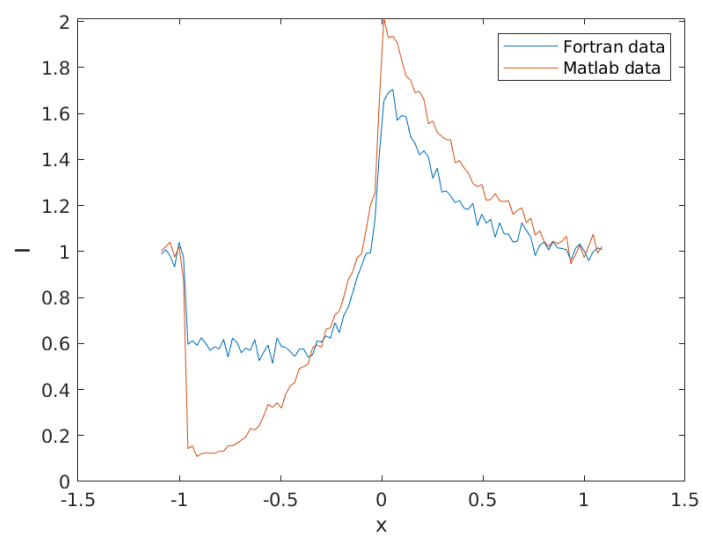
21.2.2 More freely translated version

Figure 16: Comparison of Fortran code and Matlab code (freely adapted version)

Figure 17: Comparison of Fortran code and Matlab code (unchanged version - `xk0 = 0.5`)

21.3 Optimizations

21.3.1 Already implemented

21.3.2 To be implemented

- generation of random numbers that undergo no scattering: replace with continuum profile

22 Theoretical background

Algorithm 2 `pcyg.f90:   one resonance line`

---

for all photons **do**

1. Release photon with frequency x

2. Check if interaction is uberhaupt possible.

3. Solve for distance (radius r) of interaction using Sobolev approximation $x_{CMF} = x_{REL} - \mu v(r)$ with $\boxed{x_{CMF} = 0}$ and compute Sobolev optical depth

4. Check whether the photon is scattered:

   if $\tau_S > -log(\xi)$ **then**
   Interaction: the photon is scattered. Update the frequency
   else
   No interaction

4. update the frequency according to the scattering event

end for
collect photons and perform visualisation

22.1 General things

- $\lambda\nu = c$. Mostly stellar spectra are recorded for increasing λ, thus decreasing ν

- the β-velocity law

$$v = \left(1 - \frac{b}{r}\right)^\beta \tag{47}$$

where we want $v = \in [v_{\min}, v_{\max}]$. Thus on one hand $b = 1 - x_{v_{\min}}^{1/\beta} > 0$ and then we can compute the radius where $v = v_{\max}$, namely $r_{\max} = b/(1 - v_{\max}^{1/\beta})$

  - Minimal velocity. Without angle correction (see Section 22.2), the minimal velocity is given by $(1 - b)^\beta$. With angle correction,

$$v = \cos(\alpha)\left(1 - \frac{b}{r}\right)^\beta \tag{48}$$

  then the minimal velocity is slightly higher.
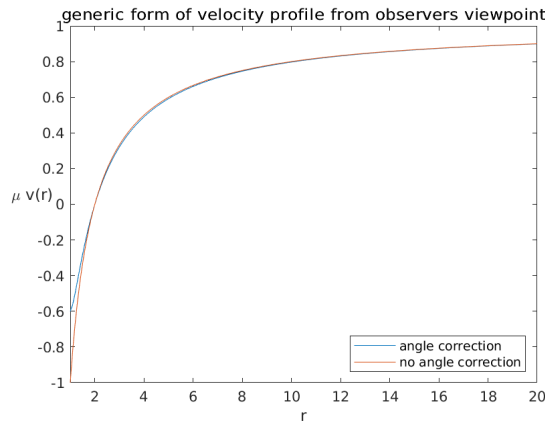 - Maximal velocity equals v_{max}

Figure 18: Example of velocity profile (give paramters)

22.2 Geometry

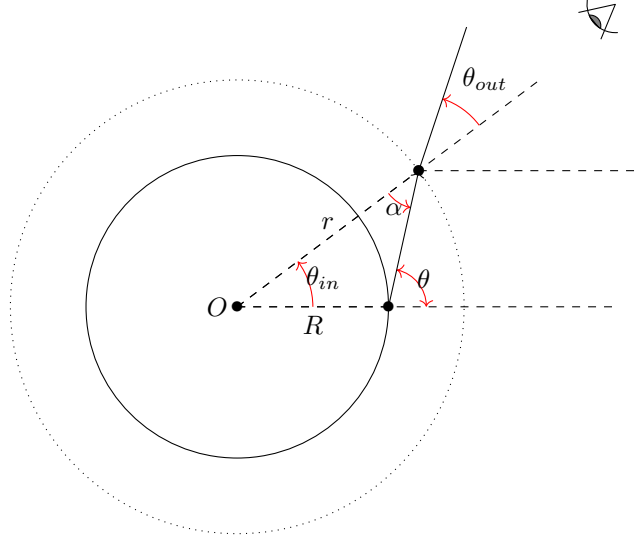Spherical symmetry. Scattering at point P

Figure 19: 2D Geometry for scattering

We can derive an expression, but first the sum of the angles in a triangle equals π which leads to $\alpha = \theta_{in} - \theta$. We then have the sine rule, namely that, with

$$\frac{\sin(\alpha)}{R} = \frac{\sin(\pi - \theta)}{r} = \frac{\sin(\theta)}{r} \tag{49}$$

and thus, with $R = R_* = 1$,

$$\cos(\alpha) = \sqrt{1 - \left(\frac{\sin(\theta)}{r}\right)^2} \tag{50}$$

Per definition

- $\texttt{xmuestart} = \cos(\theta)$

- $\texttt{pstart} = R_* \sin(\theta)$

- $\texttt{xmuein} = \cos(\alpha)$

- $\texttt{xmueou} = \cos(\theta_{\text{out}})$

22.2.1 Condition for hitting the core

Check this only for inwards streaming photons!

$$\begin{aligned}
\texttt{pcheck} &= \sqrt{r^2 \left(1 - \cos(\theta_{\text{out}})^2\right)} \\
&= r \sin(\theta_{\text{out}})
\end{aligned} \tag{51}$$

22.2.2 Slightly more general version

When $R_* \neq 1$, Equation (50) is replaced by

$$\cos(\alpha) = \sqrt{1 - \left(\frac{R_* \sin(\theta)}{r}\right)^2} \tag{52}$$

22.3 Sobolev approximation

- In fact, the absolute frequency of the photons does not change. However, in an observer's frame, we observe that the photon frequency changes at a scattering event. After a scattering event, the oberserver's frame frequency is updated as follows:

$$\texttt{xnew = xstart + u(xmueou - xmuein)} \tag{53}$$

- Sobolev condition for resonance:

$$x_{REF} - \mu u = 0 \tag{54}$$

with $u = \dfrac{v}{v_\infty} \in [0, 1]$ and $\mu = \cos(\theta) \in [-1, 1]$ then

$$x_{REF} \in [0, 1] \tag{55}$$

- The radius of interaction, we solve for $v_{photon} = x > 0$, for a specific ν_0

$$\sqrt{1 - \left(\frac{p}{r}\right)^2} \left(1 - \frac{b}{r}\right)^{\beta} = \frac{\nu - \nu_0}{\nu_0} \frac{c}{v_\infty} \tag{56}$$

Now we are going to invest the effect of

- – increasing $\nu_0 \uparrow$. What then happens is that the RHS decreases, thus $r \downarrow$.
- – Inversely, $\nu_0 \downarrow$, then $r \uparrow$

22.4 Can resonance in the same resonance line happen twice?

After a first scattering event, the frequency is updated according to Equation (53). In my opinion, it is possible to have multiple scatterings.

22.5 Meaning of the parameters

- $\texttt{xk0}$ is a characteristic scale of opacity $\chi = \dfrac{\texttt{xk0}}{rv^{2+\alpha}}$

- opacity $\chi = \dfrac{\texttt{xk0}}{rv^{2+\alpha}} \propto \kappa\rho \propto \dfrac{\kappa}{rv^2}$

- from this we deduce that $\kappa \propto \dfrac{1}{v^\alpha}$

22.6 Special case: $\texttt{xmuestart = 1}$

- FIRST SCATTTERING: from Equation (53) we have that $\texttt{xstart = u}$ and then

$$\begin{aligned}
\texttt{xnew} &= \texttt{xstart + u(xmueou- 1)} \\
&= \texttt{xstart.xmueou}
\end{aligned} \tag{57}$$

Thus, since $\texttt{xmueou} \in [-1, 1]$ and $\texttt{xmin} \le \texttt{xstart} \le \texttt{xmax}$

$$\texttt{xmin} \le \texttt{xnew} \le \texttt{xmax} \tag{58}$$

23 Development of computer code (in `Matlab`)

23.1 Implementation in Matlab: user's manual

Run the function `test_function(test_number)`.

| test_number	parameter settings
0	original version
1	first adaptation: radial release
2	isotropic scattering – higher peak
3	Eddington limb darkening
4	photospheric line-profile
5	simple well
6	other resonance frequency (thus introducing shift)
7	formation of two lines, only radially streaming photons (thus also radial release
8	formation of two lines, with radial release
9	formation of two lines, full scattering possibilities

Via this link, you can go back to the exercises overview: Section 13.

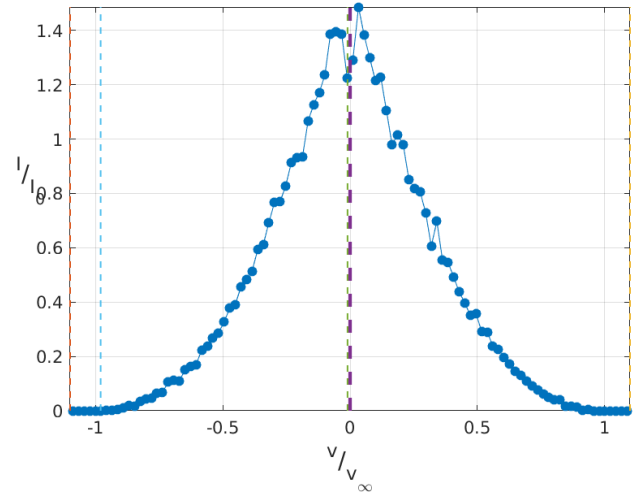## 23.2 Keeping track of the photon path

$$
\begin{bmatrix}
\texttt{xstart} \\
\texttt{xmuestart} \\
\texttt{goto\_end\_of\_loop} \\
\hline
\texttt{r\_new} \\
\texttt{xmueou} \\
\texttt{xnew} \\
\texttt{x\_selected} \\
\hline
\vdots
\end{bmatrix}
\tag{59}
$$

24 Experiments and results

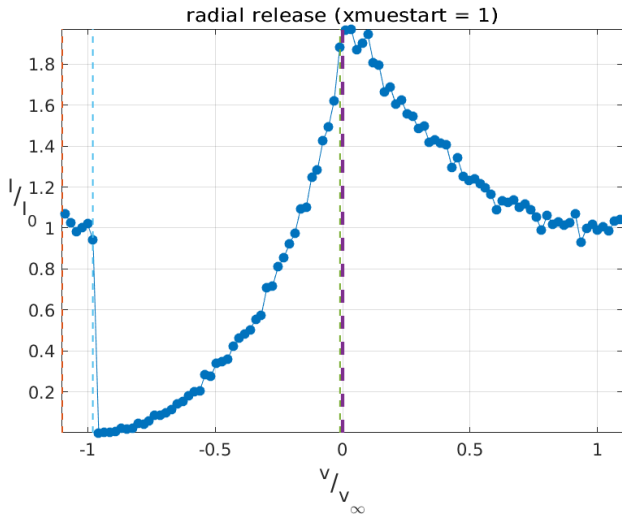## 24.1 About the scattering probability distribution
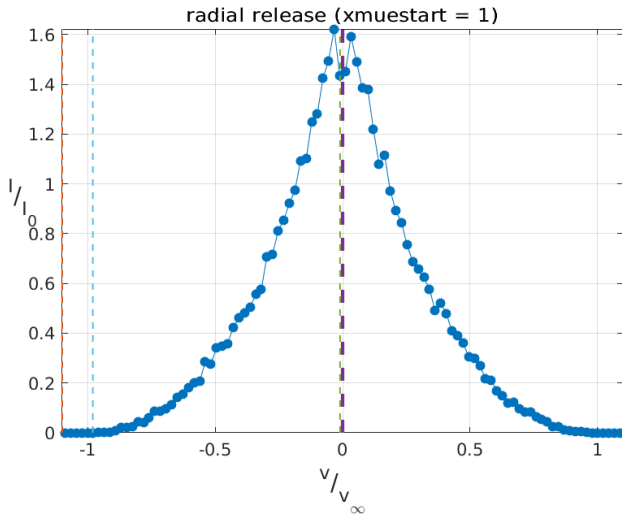
(a) Radial release

(b) Random release

Figure 20: Scattering distribution

24.2 Single resonance line

(a) Radial release
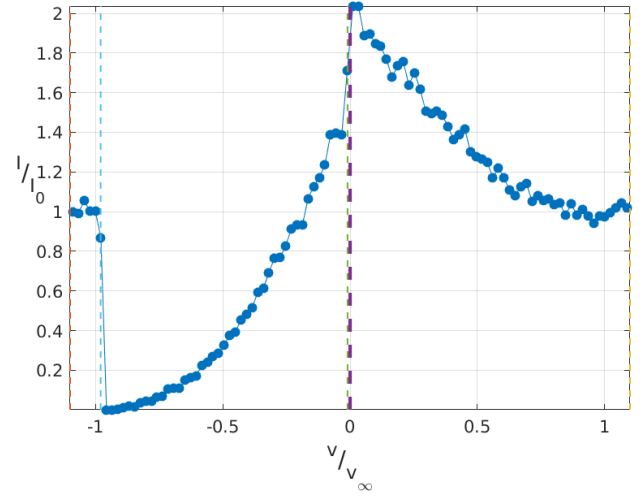
(b) Random release

Figure 21: Single line formation with Sobolev approximation

24.3 Multiple line formation

- NON-INTERACTING LINES
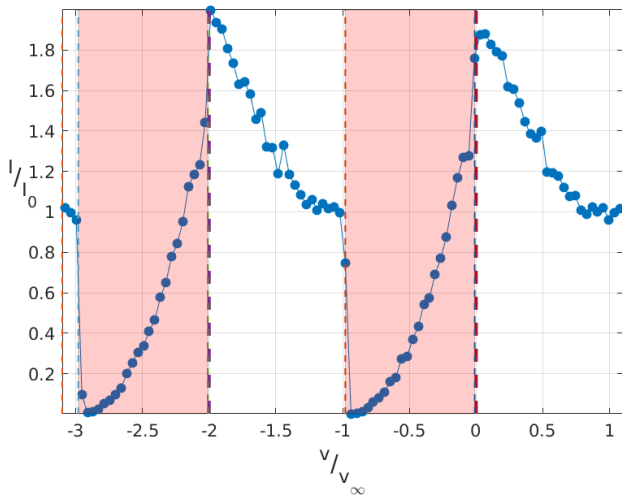
Figure 22: Multiple lines (distant lines, non-interacting)

- OVERLAPPING LINES

Figure 23: Multiple lines (distant lines, non-interacting)

24.4 Effect of the opacity
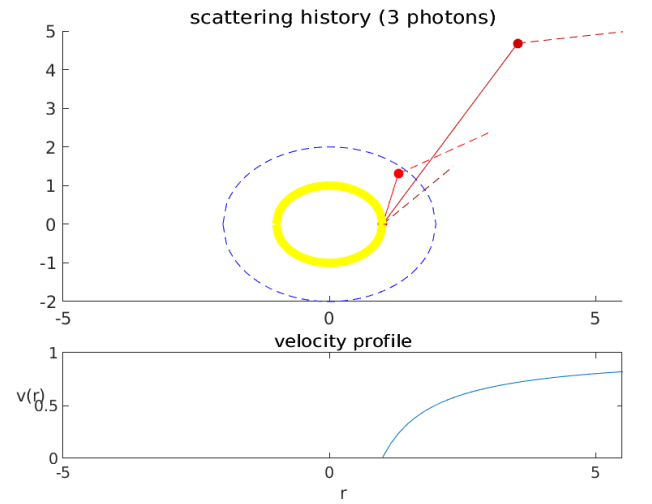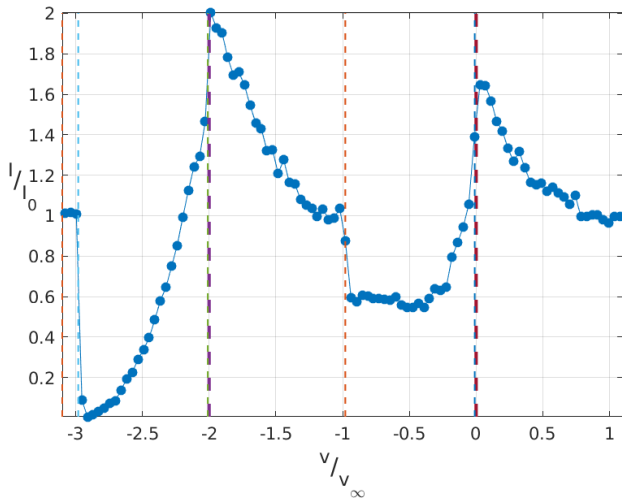
Figure 24: Multiple lines (left `xk0 = 100` and right `xk0 = 0.5`)

24.5 Observations

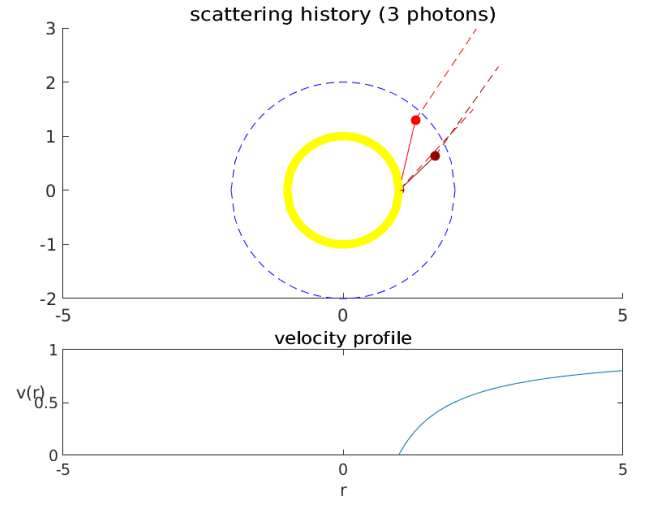Figure 25 shows the profile when the scattering angle is allowed to lie in the interval $\mu_{\text{out}} \in [-1, 1]$. Figure 26 shows the same computations, but with $\mu_{\text{out}} \in [0, 1]$
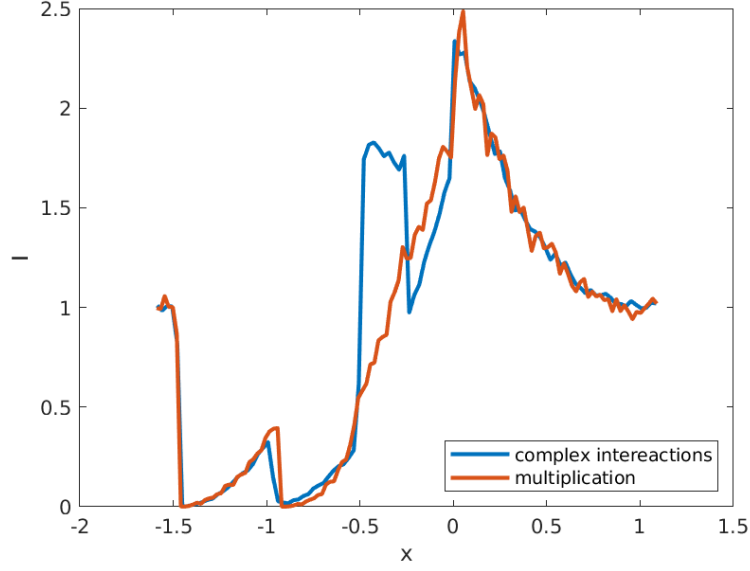
Figure 25: Comparison with multiplied profile ($\mu_{\text{out}} \in [-1, 1]$)
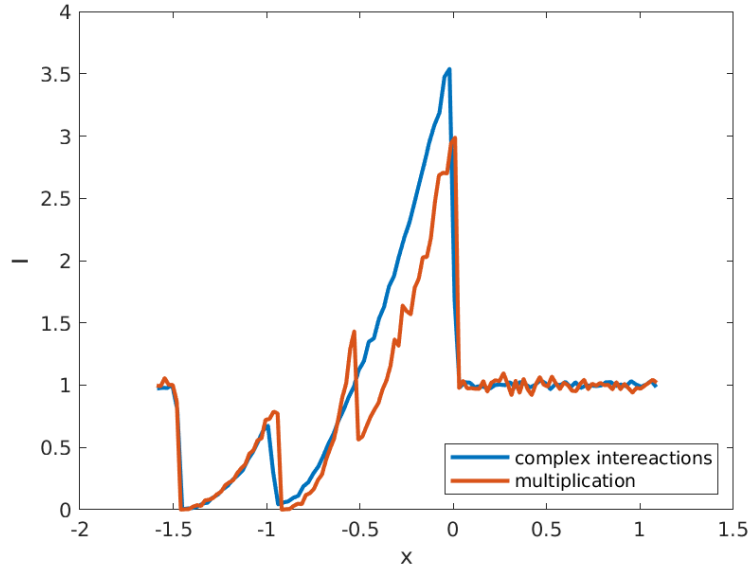
Figure 26: Comparison with multiplied profile ($\mu_{\text{out}} \in [0, 1]$)

Loosely speaking, one can understand this result because in Figure 26, photons are not allowed to be backscattered to the first resonance line.

24.6 Convergence behaviour
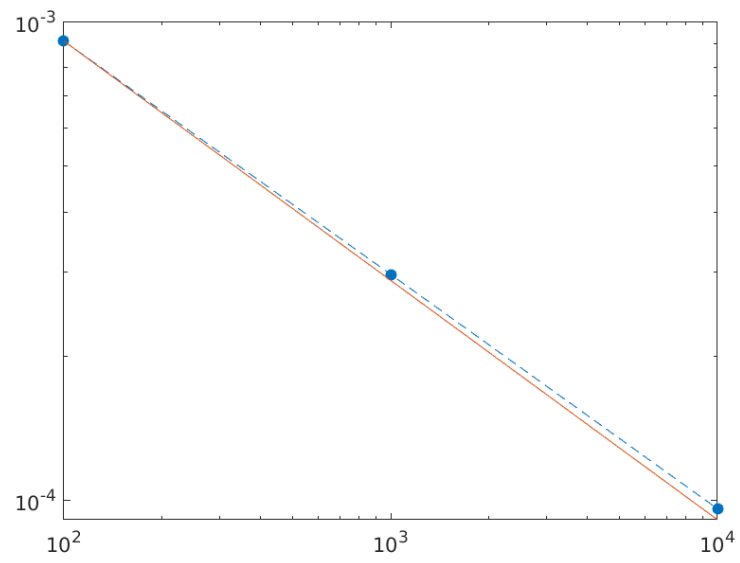
Figure 27: Convergence behaviour

24.7   Some theoretical observations

- The resonance frequencies need to lie close enough to each other, otherwise no resonance is possible.

  - if the lines are close enough to each other, resonance ends always at the rightmost frequency because you can indeed have a pumping up, but the leftmost peak is then in the absorption zone of the rightmost, thus it is scattered again! You can indeed see that the joint zone is depleted - and actaully makes the rightmost line stronger.

- Calculation of scattering probability for overlapping regions. Define ...

  - the 'one-time scattering probability' p_1.

  - probabiltiy of the overlapping region $p_2 = \dfrac{\text{length of overlapping region}}{\text{union of the length of the 'one-scattering' regions}}$.

  - HOWEVER take also into account that not all scattered photons are scattered.

  Then we have
  $$p_{\text{total}} = p_1(1 + 2p_2(1 + 2p_2(1 + ...))) \tag{60}$$

25 Computing the radiation force & luminosity $L(r)$

This is based upon material from the text provided by professor Sundqvist, and the Phd thesis from Uwe Springmann [**UweSpringmannPHD**] where sperically symmetric Wolf-Rayet stars are discussed.

25.1 Theoretical formulas

1. Formal definition

$$g_{\text{radiation}} = \frac{\Delta p}{\Delta t \Delta m} = \frac{\Delta E}{v} \frac{1}{\Delta t} \frac{v}{M \Delta r} = -\frac{1}{\dot{M}} \frac{dL}{dr} \tag{61}$$

2. Numerical approximation, we count photons according to formulas in Table 1.

25.2 Solution strategy

Loop over all photons. In that loop, loop over all r values and assign the corresponding angle. Update the array at each scattering event.

- create a grid for r

- for each r on the grid, look at the

- calculate $L(r)$

- then calculate $\dfrac{dL}{dr}$ numerically on that grid

In the case $\mu_{\text{out}} < 0$ then
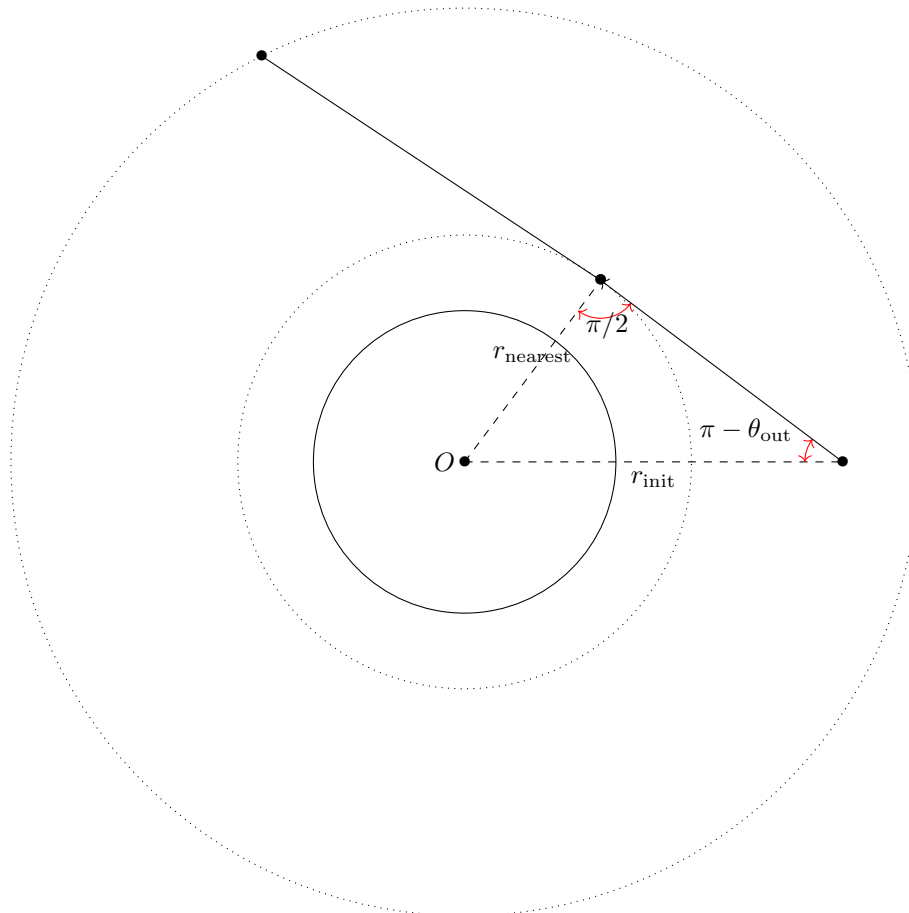
Figure 28: Trick when computin $L(r)$

25.3 Checking the correctness of the program

Enforce algorithmically that all photons stream in one direction (no scattering with `xmueout < 0`). Comment out the line `xmueou = -xmueou` in the function `scatter.m`.
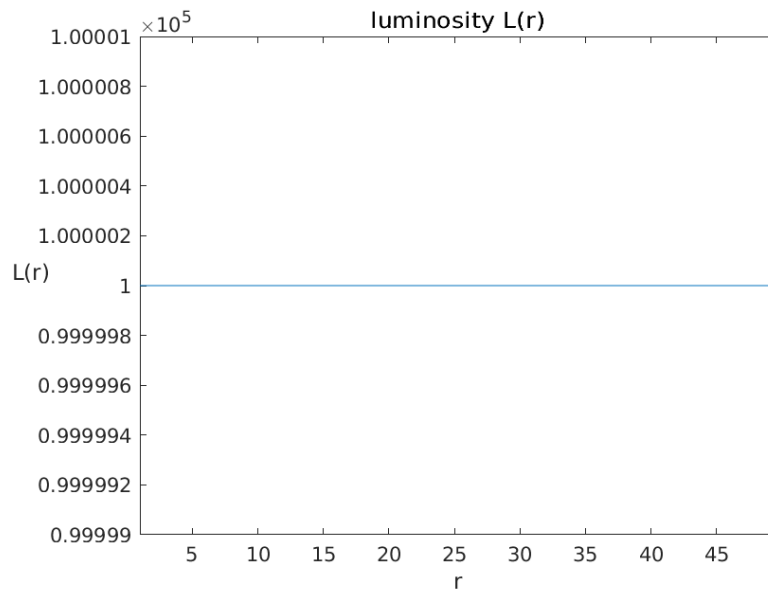
Figure 29: Luminosity $L(r)$ (for one resonance line) - test situation

25.4 Computing the radiation force for one line

Basic, well-known test situation.

(a) Luminosity $L(r)$ (for one resonance line)

(b) dL/dr
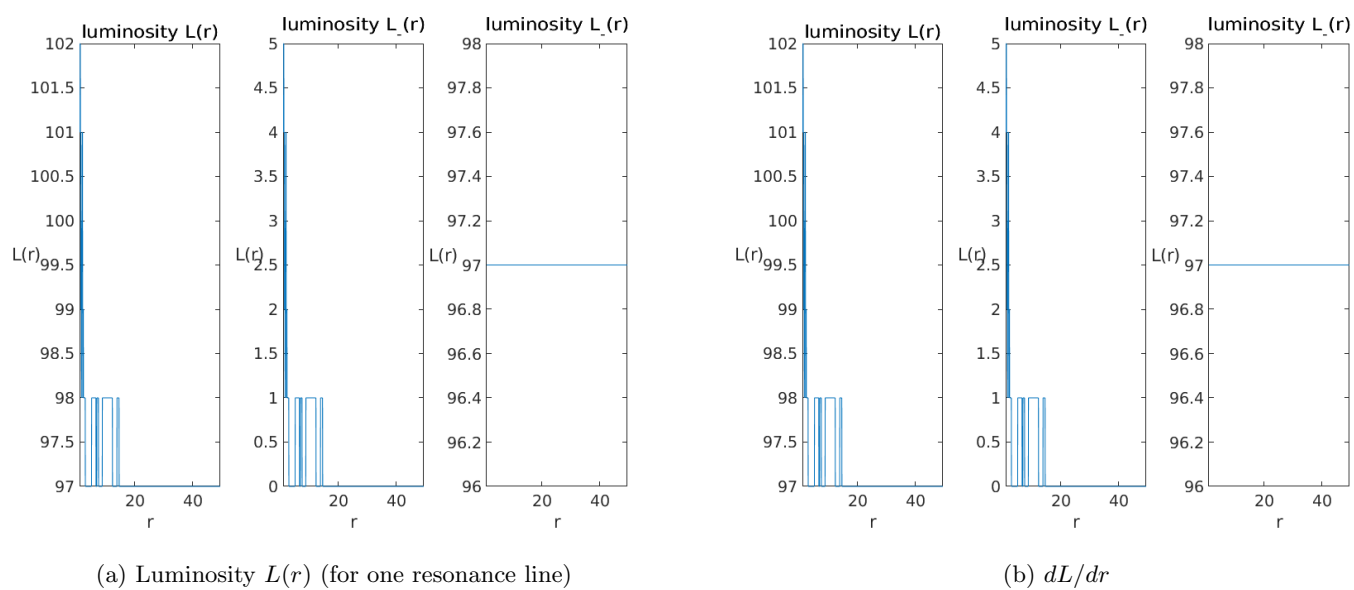
Figure 30: Scattering distribution

25.5 Multiple lines
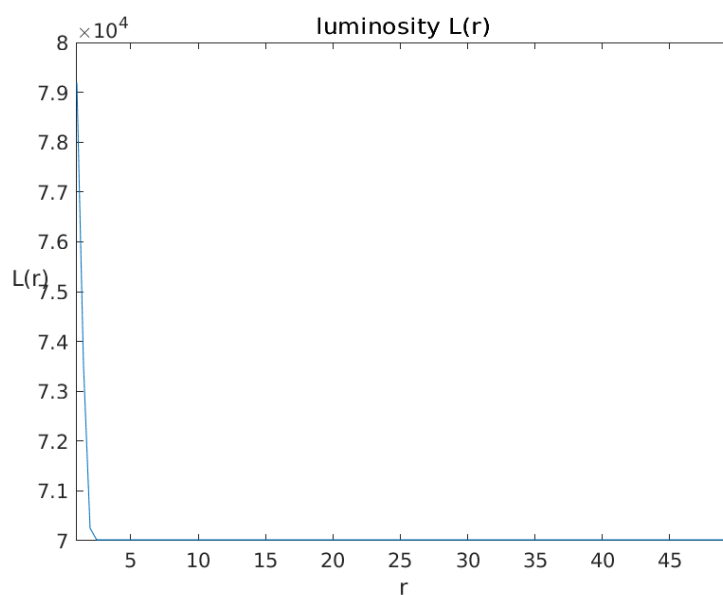
Figure 31: Luminosity $L(r)$ (for multiple resonance line)

25.6 Theoretical considerations

25.6.1 Analytical quantities

Theoretical From the course notes on radiative processes

$$g_{\text{radiation}} = g_{\text{line}} = g_{\text{line}}^{\text{thin}} \frac{1 - e^{-\tau_S}}{\tau_S} \qquad (62)$$

- expression for g_{thin}

$$g_{\text{thin}} = g_e q = \frac{F_\nu^0 k_L}{\rho c} \qquad (63)$$

- the Sobolev optical depth

$$\tau_S = \frac{\kappa_0}{r^2 v \left| \frac{dv_l}{dl} \right|} = \frac{\kappa_0}{r v^2 (\mu^2 \sigma + 1)} \qquad (64)$$

$$\frac{dv_l}{dl} = \mu^2 \frac{dv_r}{dr} + (1 - \mu^2) \frac{v_r}{r} \qquad (65)$$

- the density - mass loss relation

$$\dot{M} = \rho 4\pi r^2 v \qquad (66)$$

$$\rho = \frac{\dot{M}}{4\pi r^2 v} \qquad (67)$$

- expression for the extinction coefficient k_L

> @ Luka, do you know where this expression comes from?

$$k_L = \frac{\kappa_0 \rho 4\pi R_* v_\infty^2}{\dot{M} \lambda_0} = \frac{\kappa_0 R_* v_\infty^2}{r^2 v \lambda_0} \qquad (68)$$

Conclusion Combining these quantities gives

$$g_{\text{radiation}} = \frac{F_{\nu_0}}{c} k_L \frac{1}{\rho} \frac{1 - e^{-\tau_S}}{\tau_S} \qquad (69)$$

$$g_{\text{radiation}} = \frac{F_{\nu_0}}{c} \frac{\kappa_0 R_* v_\infty^2}{\lambda_0 r^2 v} \frac{4\pi r^2 v}{\dot{M}} \frac{r^2 v \left| \frac{dv_l}{dl} \right|}{\kappa_0} \left(1 - e^{-\tau_S} \right) \qquad (70)$$

$$g_{\text{radiation}} = \frac{F_{\nu_0}}{c\lambda_0} \frac{4\pi R_* v_\infty^2}{\dot{M}} r^2 v \left| \frac{dv_l}{dl} \right| \left(1 - e^{-\tau_S} \right) \qquad (71)$$

Now since we are assuming spherical symmetry then $F_{\nu_0} = \dfrac{L_0}{4\pi r^2}$

$$g_{\text{radiation}} = \frac{L_{\nu_0}}{c\lambda_0} \frac{4\pi R_* v_\infty^2}{\dot{M}} v \left| \frac{dv_l}{dl} \right| \left(1 - e^{-\tau_S} \right) \qquad (72)$$

Special case $\beta = 1$ Averaging over all μ angles, we have

$$\frac{dv_l}{dl} = \mu^2 \left(\beta(1 - b/r)^{\beta-1} \frac{b}{r^2} \right) + (1 - \mu^2)(1 - b/r)^\beta \frac{1}{r} = \mathcal{O}(r^{-2}) \qquad (73)$$

$$\frac{g_{\text{rad}}}{\dot{M}} = \mathcal{O}(r^{-3}) \qquad (74)$$

From numerical computations On the other hand we have

$$g_{\text{radiation}} = -\frac{1}{\dot{M}} \frac{dL}{dr} \qquad (75)$$

These quantities should equal and also accounting for spherical symmetry. Also taking the limit $\tau_S \gg 1$ and assuming the β-velocity law, wet get

$$\frac{dL}{dr} = -\frac{C^{te}}{4\pi r^2} r^2 v \left| \frac{dv_l}{dl} \right| \tag{76}$$

$$\frac{dL}{dr} = \mathcal{O}(r^{-2}) \tag{77}$$

25.6.2 The same quantities in dimensionless units

Theoretical The dimensionless units (those used in the computer code) for the wind velocity and for the radius are $v' = \dfrac{v}{v_\infty}$ and $r' = \dfrac{r}{R_*}$. Thus $v = v' v_\infty$ and $r = r' R_*$.

- for Sobolev optical depth

$$\tau_S' = \frac{\kappa_0}{r'^2 v' \left| \frac{dv_l'}{dl'} \right|} = R_*^2 v_\infty \tau_S \tag{78}$$

$$\frac{dv_l'}{dl'} = \frac{v_\infty}{R_*} \frac{dv_l}{dl} \tag{79}$$

- extinction coefficient

$$k_L' = \frac{\kappa_0 v_\infty}{\lambda_0 R_* r'^2 v'} = R_*^2 v_\infty k_L \tag{80}$$

- density versus mass-loss rate

$$\rho' = \frac{\dot{M}}{R_*^2 v_\infty 4\pi r'^2 v'} \tag{81}$$

Putting these together

$$g_{\text{radiation}} = \frac{F_{\nu_0}}{c} k_L' \frac{1}{\rho'} \frac{1 - e^{-\tau_S'}}{\tau_S'} \tag{82}$$

$$g_{\text{radiation}}' = \frac{F_{\nu_0}}{c} \frac{\kappa_0 v_\infty}{\lambda_0 R_* r'^2 v'} \frac{R_*^2 v_\infty 4\pi r'^2 v'}{\dot{M}} \frac{r'^2 v' \left| \frac{dv_l'}{dl'} \right|}{R_*^2 v_\infty \kappa_0} \left(1 - e^{-\tau_S} \right) \tag{83}$$

$$\boxed{g_{\text{radiation}}' = \frac{1}{R_*} \frac{F_{\nu_0}}{c} \frac{\kappa_0}{\lambda_0 r'^2 v'} \frac{4\pi r'^2 v'}{\dot{M}} \frac{r'^2 v' \left| \frac{dv_l'}{dl'} \right|}{\kappa_0} \left(1 - e^{-\tau_S} \right)} \tag{84}$$

From numerical computations

$$g_{\text{radiation}}' = -\frac{R_*}{\dot{M}} \frac{dL}{dr'} \tag{85}$$

These quantities should equal

25.6.3   These quantities should equal (dimensionless units?)

For optically thick lines ($\tau_S \gg 1$)

$$g_{\text{radiation}}^{\text{numerical}} = -\frac{1}{\dot{M}}\frac{dL}{dr} = g_{\text{radiation}}^{\text{analytical}} = \frac{F_{\nu_0}\nu_0}{\dot{M}c^2}\frac{dv_l}{dl} \tag{86}$$

$$\frac{dL}{dr} = \frac{1}{4\pi r^2 c^2}\frac{F_{\nu_0}}{F}\frac{dv}{dr} \tag{87}$$

Combining that with a β-velocity profile

$$v = \left(1 - \frac{b}{r}\right)^\beta \tag{88}$$

Then we have

$$\boxed{\frac{dL}{dr} = \frac{F_{\nu_0}}{4\pi c^2}\frac{b}{r^3}\left(1 - \frac{b}{r}\right)^{\beta-1}} \tag{89}$$

and for $\beta = 1$

$$\frac{dL}{dr} = \frac{F_{\nu_0}}{4\pi c^2}\frac{b}{r^4} \tag{90}$$

$$\left|\frac{dL}{dr}\right| = C^{te}\frac{1}{r^4} \tag{91}$$

54

25.6.4 From random notes, global mass-loss rates

- definition of luminosity

$$g_{\rm rad} = -\frac{1}{\dot{M}}\frac{dL}{dr} \tag{92}$$

- steady-state equation of motion

$$v\frac{dv}{dr} = -\frac{GM}{r^2} + g_{\rm rad}(r) \tag{93}$$

using Equation (92)

– assuming that $\dot{M}(r) \equiv \dot{M}$

$$\int_{R_*}^{\infty} v\frac{dv}{dr}dr = -\int_{R_*}^{\infty}\frac{GM}{r^2}dr - \frac{1}{\dot{M}}\int_{R_*}^{\infty}\frac{dL}{dr}dr \tag{94}$$

we then get

$$\frac{v^2}{2}\Big|_{R_*}^{\infty} = -\frac{GM}{r}\Big|_{R_*}^{\infty} - \frac{1}{\dot{M}}L\Big|_{R_*}^{\infty} \tag{95}$$

with $v(R_*) = 0$

$$\frac{v(\infty)^2}{2} - \frac{GM}{R_*} = \frac{L(R_*) - L(\infty)}{\dot{M}} \tag{96}$$

– in general

$$\int_{R_*}^{\infty} v\frac{dv}{dr}dr = -\int_{R_*}^{\infty}\frac{GM}{r^2}dr - \frac{1}{4\pi\rho}\int_{R_*}^{\infty}\frac{1}{r^2 v}\frac{dL}{dr}dr \tag{97}$$

25.7 With high `xk0`

TO BE UPDATED

26 Backup from theory

Transport step and collision step. There is no absorption.

26.1 Moments of the intensity

definition	numerical estimation (spherical symmetry)	(plane-parallel)
I_ν	tally the number of photons	"
$J_\nu = \frac{1}{4\pi} \int I_\nu d\Omega$	$J(r) = \frac{1}{16\pi^2 r^2} \frac{\epsilon_0}{\Delta t} \sum_i \frac{\epsilon_i}{\epsilon_0} \frac{1}{\|\mu_i(r)\|}$	$J(\tau) = \frac{\epsilon_0}{\Delta t} \sum_i \frac{\epsilon_i}{\epsilon_0} \frac{1}{\|\mu_i(\tau)\|}$
$H_\nu = \frac{1}{4\pi} \int \mu I_\nu d\Omega$	$H(r) = \frac{1}{16\pi^2 r^2} \frac{\epsilon_0}{\Delta t} \sum_i \frac{\epsilon_i}{\epsilon_0} \mathrm{sign}(\mu_i(r))$	$J(\tau) = \frac{\epsilon_0}{\Delta t} \sum_i \frac{\epsilon_i}{\epsilon_0} \mathrm{sign}(\|\mu_i(\tau)\|)$
$K_\nu = \frac{1}{4\pi} \int \mu^2 I_\nu d\Omega$	$K(r) = \frac{1}{16\pi^2 r^2} \frac{\epsilon_0}{\Delta t} \sum_i \frac{\epsilon_i}{\epsilon_0} \|\mu_i(r)\|$	$J(\tau) = \frac{\epsilon_0}{\Delta t} \sum_i \frac{\epsilon_i}{\epsilon_0} \|\mu_i(\tau)\|$

Table 1: Moments of intensity

We are interested

- in $F \propto H$ which is an average of I over $d\Omega$ (but only at 'shell of release')

- in L, which is then both an average of I over $d\Omega$ and over $d\nu$

26.2 Computing total photon distance and time that it has travelled

See figure 19.

27 Extension to higher dimensions

add angle ϕ

28 Closer look at Monte Carlo simulations

28.1 Random walk (diffusion equation)

A more simple experiment that simulates the diffusion equation (1D random walk) is also set up. The results are shown in Figure 32. We observe that $N \sim \tau^2$, as can also be derived from theory.
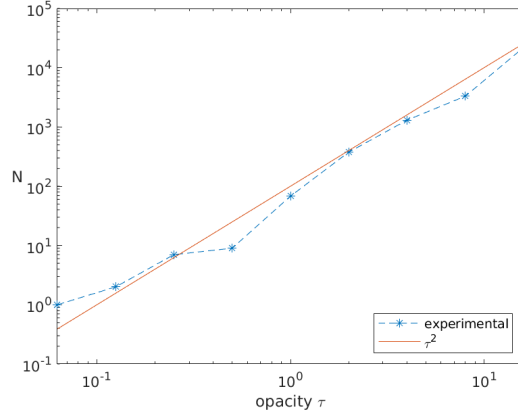
Figure 32: Number of interactions (scattering events) versus opacity, random walk

- When starting from an initial condition $x_0 = 0$ and

$$x_N = x_{N-1} \pm l \tag{98}$$

  we have for the variance that $\langle x_N \rangle^2 = N l^2$

- If we require a photon to cover a distance R then $N = \dfrac{R^2}{l^2}$ and

  - the relation between mean-free path l and opacity α is $l = \dfrac{1}{\alpha}$

  - with $\tau = \displaystyle\int_0^R \alpha ds = \dfrac{R}{l}$

  then we have that $N = \tau^2$. This corresponds with the observations in Figure 32.

28.2 Limb darkening

We first look at results from the limb darkening program, as studied in Section 19. In Figure 33, the number of scattering events is plotted versus the opacity of the medium.

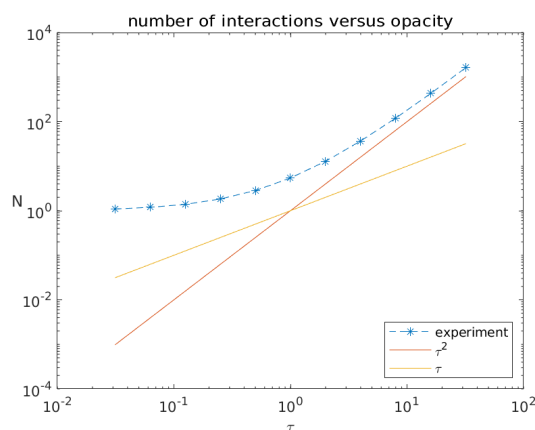
Figure 33: Number of interactions (scattering events) versus opacity, kimb darkening

- For high opacity $\tau \gg 1$ we observe that $N \sim \tau$.

- Bridging regime.

- For opacity $\tau \ll 1$ we observe that $N \sim 1$: namely the photons travels very far during the first emission event.

If you assume constant opacity then $\tau = \alpha z$

Part V
Questions

29 Questions for professor Sundqvist

- What are the equations governing the processes in `pcyg.f90`

- What does this mean? `xnew=xstart+(v-sign(0.06,xmueou))*xmueou-v*xmuein`

- Pcygni profiles: Why don't we just take the absorption and the emission and add them together.

30 Questions for professor Samaey

Important

- In [DPS18], Equation (31) why does it correspond to diffusion (more specifically the second term on the right hand side).

- MC voor radiative transfer problem in [DPS18]

- taal van masterproef

- geen vergelijlijking van het probleem (zie e-mail)

Not important

- what is the difference between Monte Carlo and equation-free computing?

31 Questions for Dylan

- what happens @ limb darkening: why is $J(\tau)$ apparently constant from the numerical results? Section 19.5.

Thank you very much ! :)

32   Questions for Luka

- question about derivation concerning $\frac{dL}{dr}$ in Section 25.6.1. Could you please quickly check out the derivation in 25.6.1. The scaling factors are not such important for me at this moment, what bothers me primarily is the scaling relation between $\frac{dL}{dr}$ and r in Equation 77.

Thank you very much ! :)

33 Solved questions

- Sundqvist+ 2009: what is thermal velocity (see Wikipedia)

- Sundqvist+ 2009: what is line force (see explanation Dylan)

- unclassified: what is a flux limiter? (see course notes)

- unclassified: what is cross section of scattering (see Wikipedia)

- Puls manual: p.26: how does the Milne equation appear? (see library book)

- pcyg.f90: what are p-rays? (see anwser professor Sundqvist)

    - parallel rays leaving the atmosphere (of, e.g. a star)
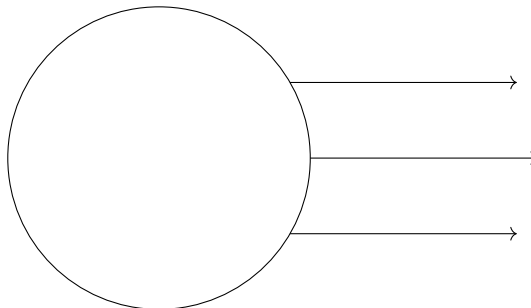
- pcyg.f90: what is meant by Eddington limb-darkening? (see answer professor Sundqvist)

    - standard limb darkening

- Sundqvist+ 2009: what is the geometry of a *slice*?

- CMFAA course notes p.13 (the example) what is understood by plane-parallel geometry and is it 1D or 2D? (see answer professor Sundqvist)

    -

- CMFAA course notes p.15: why is this called diffusion $F = T^3 \frac{dT}{dx}$ (flux proportional to local gradient in temperature)?

- unclassified: what is the terminal velocity v_∞?

- unclassified: what is Sobo-distribution? (Sobolev distribution)

- pcyg.f90: for `test_number = 2`, why do we call it isotropic since isotropy of `mu` does not imply isotropy of `theta`? (myself, see definition of intensity)

- (for which star are the exerpimental data and what assumptions are used in the theory?) (see ... and derive some formulas)

- book *Stellar Atmospheres* [Mihalas] (bought)

- ordening of array `freq` (adapted the code, experimented with it)

    - why `freq(1) = xmax-5*deltax`?

    - frequency binning: how are you sure that no lower/higher frequencies can occur?
      derive this analytically

- `Pcyg.f90` does it take into account that photons are scattered away from the observer? (via assumption of radial symmetry)

- what is the meaning of I_ν versus I? ($I = \int I_\nu d\nu$)

34 Interesting problems

- inverse radiative transfer problem

might be interesting for looking at

- splitting methods
- Eddington factors

35 Do not forget

- convergence plots

Part VI
Thesis meetings

36 Meeting on 6 September 2019

- overview of Petnica summer institute on Astrophysics

- question: manual by Puls: why is isotropic distribution sampled from $\mu\mu$?

- `pcyg.f90` program

- practical arangements

- SKIRT code

- discussion of paper (Dimarco+2018)

37 Meeting on 23 September 2019

- convergence plots

- relation $N \sim \tau + \tau^2/2$

- limb darkening

38 Meeting on 30 September 2019

- discussion about $x_{\min}$ and $x_{\max}$

- discussion about introduction of second line.

  - take into account the Doppler shift because you have two different frames
  - make them radially streaming (release)
  - do step for step:
    * begin with creating a correct well

- normalized frequency: $x = \dfrac{\nu - \nu_0}{\nu_0} \dfrac{c}{v_{infty}}$

- adding other resonance frequencies, involves enlarging the frequency frame.

- about the goal of the master thesis. Making a master thesis is not doing a course where all is well-defined and *a priori* known.

39 Meeting on 30 October

with Dylan and Luka.

- question about MC limb darkening

- the quantity $\dot{M}$ is a constant. From continuity of mass

$$\frac{d\rho}{dt} + \nabla.(\rho v) = 0 \tag{99}$$

In steady-state and in sperical symmetry

$$\frac{1}{r^2}\frac{\partial(r^2 \rho v)}{\partial r} = 0 \tag{100}$$

- discussion about computing luminosity for pcyg profile. Take into account changing frequency for energy balance.

- change $\dfrac{dL}{dr}$ into $\dfrac{dL_\nu}{dr}$

Part VII
Equation meetings

- Meeting of 10 April 2019

- Meeting of 17 April 2019

- Meeting of 14 August 2019

- Meeting of 18 September 2019

- Meeting of 25 September 2019

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